

# Structural Bioinformatics Training Workshop & Hackathon 2017

MMTF JavaScript API &  
NGL Viewer/Library

Alexander Rose  
RCSB PDB

*Structural Bioinformatics Laboratory  
San Diego Supercomputer Center  
UC San Diego*

- *Simplicity*: Complex code fits neither into processor caches nor into programmer minds. It is thus prone to be slow, faulty and not widely implemented.

J. Huwald, et al., J. Comp. Chem. (2016) 37, 1897-1906




# MMTF JS Decoder ~6kb (~2kb gzipped)

```
var decodeStructure=function(t){"use strict";function t(t){function r(t){for(var r={},e=0;e<t;e++){var n=o();r[n]=o();return r}function e(r){var e=t.subarray(i,i+r);return i+=r,e}function n(r){var e=t.subarray(i,i+r),n=String.fromCharCode.apply(null,e);return i+=r,n}function a(t){for(var r=new Array(t),e=0;e<t;e++){r[e]=o();return r}function o(){var o,s,c,f,t[i];if(0==(128&f))return i++,f;if(128==(240&f))return s=15&f,i++,r(s);if(144==(240&f))return s=15&f,i++,a(s);if(160==(224&f))return s=31&f,i++,n(s);if(224==(224&f))return o=u.getInt8(i),i++,o;switch(f){case 192: return i++,null;case 194: return i++,1;case 195: return i++,0;case 196: return s=u.getUint8(i+1),i+=2,e(s);case 197: return s=u.getUint16(i+1),i+=3,e(s);case 198: return s=u.getUint32(i+1),i+=5,e(s);case 199: return s=u.getUint8(i+1),c=u.getUint8(i+2),i+=3,[c,e(s)];case 200: return s=u.getUint16(i+1),c=u.getUint8(i+3),i+=4,[c,e(s)];case 201: return s=u.getUint32(i+1),c=u.getUint8(i+5),i+=6,[c,e(s)];case 202: return o=u.getFloat32(i+1),i+=5,o;case 203: return o=u.getFloat64(i+1),i+=9,o;case 204: return o=t[i+1],i+=2,o;case 205: return o=u.getUint16(i+1),i+=3,o;case 206: return o=u.getUint32(i+1),i+=5,o;case 207: return i+=9,0;case 208: return o=u.getUint8(i+1),i+=2,o;case 209: return o=u.getInt16(i+1),i+=3,o;case 210: return o=u.getInt32(i+1),i+=5,o;case 211: return i+=9,0;case 212: return c=u.getUint8(i+1),i+=2,[c,e(1)];case 213: return c=u.getUint8(i+1),i+=2,[c,e(2)];case 214: return c=u.getUint8(i+1),i+=2,[c,e(4)];case 215: return c=u.getUint8(i+1),i+=2,[c,e(8)];case 216: return c=u.getUint8(i+1),i+=2,[c,e(16)];case 217: return s=u.getUint8(i+1),i+=2,n(s);case 218: return s=u.getUint16(i+1),i+=3,n(s);case 219: return s=u.getUint32(i+1),i+=5,n(s);case 220: return s=u.getUint16(i+1),i+=3,a(s);case 221: return s=u.getUint32(i+1),i+=5,a(s);case 222: return s=u.getUint16(i+1),i+=3,r(s);case 223: return s=u.getUint32(i+1),i+=5,r(s)}throw new Error("Unknown type 0x"+f.toString(16))}var i=0,u=new DataView(t.buffer);return o()}function r(t,r){var e=new DataView(t.buffer),n=t.byteOffset,a=t.byteLength;r||(r=new Int8Array(a));for(var o=0;o<a;o++)r[o]=e.getInt8(n+o);return r}function e(t,r,e){var n=new DataView(t.buffer),a=t.byteOffset,o=t.byteLength;r||(r=new Int16Array(o/2));for(var i=0,u=0/2;u<i;u++)r[i]=n.getInt16(a+2*i,e);return r}function n(t,r,e){var n=new DataView(t.buffer),a=t.byteOffset,o=t.byteLength;r||(r=new Int32Array(o/4));for(var i=0,u=0/4;u<i;u++)r[i]=n.getInt32(a+4*i,e);return r}function a(t,r){var e,n;if(!r){var a=0;for(e=0,n=t.length;n>e;e+=2)a+=t[e+1];r=new t.constructor(a)}var o=0;for(e=0,n=t.length;n>e;e+=2)for(var i=t[e],u=t[e+1],s=0;u>s;u++)r[o]=i,o+=1;return r}function i(t){for(var r=1,e=t.length;e>r;r++)t[r]=t[r-1];return t}function u(t,r,e){var n=t.length/2+r.length/2;e||(e=new Int32Array(n));for(var a=0,o=0,i=0,u=t.length;u>i;i+=2){var s=t[i],c=t[i+1];e[a]=s,0===i&&e[a]=e[a-1],a+=1;for(var f=0;f<u;f++)e[a]=e[a-1]+r[o],a+=1,o+=1}return e}function s(t,r,o,i,s){var c,i&&(c=new Int32Array(i.buffer,i.byteOffset,i.byteLength/4));var f=u(n(t,void 0,s),e(r,void 0,s),c);return a(f,o,i)}function c(t,r){for(var e,n,t.resOrder,a=n.byteOffset,o=n.byteLength,i=new DataView(n.buffer),u=0,s=0,c=0/4;c<s;s++)e=i.getInt32(a+4*s,r),u+=t.groupMap[e].bondOrders.length;return u}function f(e){e instanceof ArrayBuffer&&(e=new Uint8Array(e));var a=t(e);console.log(a);var u,f,_g,y=c(a),b=a.numAtoms,d=a.resOrder.length/4,w=a.chainList.length/4,U=a.chainsPerModel.length,v=a.groupMap,h=new Uint32Array(y.d),A=new Uint32Array(y.d),m=new Uint8Array(y.d),p=new Uint32Array(b),I=new Float32Array(b),C=new Float32Array(b),O=new Float32Array(b),x=new Float32Array(b),S=new Int32Array(b),F=new Uint8Array(b),L=new Uint32Array(d),D=new Uint32Array(d),M=new Uint16Array(d),V=new Uint16Array(d),Z=new Int32Array(d),P=new Uint8Array(d),G=new Uint16Array(w),K=new Uint32Array(w),q=new Uint32Array(w),B=new Uint8Array(4*w),E=new Uint32Array(U),T=new Uint32Array(U);if(s(a.cartn_x_small,1e3,I),s(a.cartn_y_big,a.cartn_y_small,1e3,C),s(a.cartn_z_big,a.cartn_z_small,1e3,O),a.b_factor_big&&s(a.b_factor_big,a.b_factor_small,100,x),a.atom_site_id&&i(o(n(a.atom_site_id),S)),a.atom_site_label_alt_id){for(u=0,f=a.atom_site_label_alt_id.length;f>u;u+=2){var j=a.atom_site_label_alt_id[u];?"===j?a.atom_site_label_alt_id[u]:a.atom_site_label_alt_id[u]=a.atom_site_label_alt_id[u].charCodeAt(0),a.atom_site_label_alt_id[u+1]=parseInt(a.atom_site_label_alt_id[u+1])}o(a.atom_site_label_alt_id,F)}r(a.chainList,B);var H,J,a.chainsPerModel,K=0;for(u=0;u<u;u++){for(H=J[u],E[u]=K,T[u]=H,_0=H;_0>H;_0++)J[_0]=K;var N,Q=a.groupsPerChain,R=0;for(u=0;u<u;u++){for(N=Q[u],k[u]=R,q[u]=N,_0=N;_0>N;_0++)L[_0]=u;R=N}i(o(n(a.atom_site_auth_seq_id),Z));var W(n(a.resOrder,V),X=r(a.secStruct),Y=_0,Z=0;for(u=0;u<u;u++){var $=v[W[u]],tt=$.atomInfo,rt=tt.length/2,et=$.bondIndices,nt=$.bondOrders;for(f=0,g=nt.length;g>f;f++)h[Z]=Y+et[2*f],A[Z]=Y+et[2*f+1],m[Z]=nt[f],Z+=1;for(P[u]=L[X[u]]||"L").charCodeAtAt(1),D[u]=Y,M[u]=rt,_0=rt;_0>_0;_0++)p[Y]=u,Y+=1}return{bondStore:{atomIndex:l,h,atomIndex2:A,bondOrder:m},atomStore:{groupIndex:p,x:I,y:C,z:O,bfactor:x,serial:S,altLoc:F},groupStore:{chainIndex:L,atomOffset:D,atomCount:M,groupTypeId:V,resno:Z,sstruc:P},chainStore:{modelIndex:G,groupOffset:k,groupCount:q,chainName:B},modelStore:{chainOffset:E,chainCount:T},groupMap:v,unitCell:a.unitCell,spaceGroup:a.spaceGroup,bioAssembly:a.bioAssembly,pdbCode:a.pdbCode,title:a.title,bondCount:y,atomCount:b,groupCount:d,chainCount:w,modelCount:U};var l={0:"i",1:"s",2:"h",3:"e",4:"g",5:"b",6:"t",7:"l","-1":"","-2":"","-3":"","-4":"","-5":"","-6":"","-7":"","-8":"","-9":"","-10":"","-11":"","-12":"","-13":"","-14":"","-15":"","-16":"","-17":"","-18":"","-19":"","-20":"","-21":"","-22":"","-23":"","-24":"","-25":"","-26":"","-27":"","-28":"","-29":"","-30":"","-31":"","-32":"","-33":"","-34":"","-35":"","-36":"","-37":"","-38":"","-39":"","-40":"","-41":"","-42":"","-43":"","-44":"","-45":"","-46":"","-47":"","-48":"","-49":"","-50":"","-51":"","-52":"","-53":"","-54":"","-55":"","-56":"","-57":"","-58":"","-59":"","-60":"","-61":"","-62":"","-63":"","-64":"","-65":"","-66":"","-67":"","-68":"","-69":"","-70":"","-71":"","-72":"","-73":"","-74":"","-75":"","-76":"","-77":"","-78":"","-79":"","-80":"","-81":"","-82":"","-83":"","-84":"","-85":"","-86":"","-87":"","-88":"","-89":"","-90":"","-91":"","-92":"","-93":"","-94":"","-95":"","-96":"","-97":"","-98":"","-99":"","-100":"","-101":"","-102":"","-103":"","-104":"","-105":"","-106":"","-107":"","-108":"","-109":"","-110":"","-111":"","-112":"","-113":"","-114":"","-115":"","-116":"","-117":"","-118":"","-119":"","-120":"","-121":"","-122":"","-123":"","-124":"","-125":"","-126":"","-127":"","-128":"","-129":"","-130":"","-131":"","-132":"","-133":"","-134":"","-135":"","-136":"","-137":"","-138":"","-139":"","-140":"","-141":"","-142":"","-143":"","-144":"","-145":"","-146":"","-147":"","-148":"","-149":"","-150":"","-151":"","-152":"","-153":"","-154":"","-155":"","-156":"","-157":"","-158":"","-159":"","-160":"","-161":"","-162":"","-163":"","-164":"","-165":"","-166":"","-167":"","-168":"","-169":"","-170":"","-171":"","-172":"","-173":"","-174":"","-175":"","-176":"","-177":"","-178":"","-179":"","-180":"","-181":"","-182":"","-183":"","-184":"","-185":"","-186":"","-187":"","-188":"","-189":"","-190":"","-191":"","-192":"","-193":"","-194":"","-195":"","-196":"","-197":"","-198":"","-199":"","-200":"","-201":"","-202":"","-203":"","-204":"","-205":"","-206":"","-207":"","-208":"","-209":"","-210":"","-211":"","-212":"","-213":"","-214":"","-215":"","-216":"","-217":"","-218":"","-219":"","-220":"","-221":"","-222":"","-223":"","-224":"","-225":"","-226":"","-227":"","-228":"","-229":"","-230":"","-231":"","-232":"","-233":"","-234":"","-235":"","-236":"","-237":"","-238":"","-239":"","-240":"","-241":"","-242":"","-243":"","-244":"","-245":"","-246":"","-247":"","-248":"","-249":"","-250":"","-251":"","-252":"","-253":"","-254":"","-255":"","-256":"","-257":"","-258":"","-259":"","-260":"","-261":"","-262":"","-263":"","-264":"","-265":"","-266":"","-267":"","-268":"","-269":"","-270":"","-271":"","-272":"","-273":"","-274":"","-275":"","-276":"","-277":"","-278":"","-279":"","-280":"","-281":"","-282":"","-283":"","-284":"","-285":"","-286":"","-287":"","-288":"","-289":"","-290":"","-291":"","-292":"","-293":"","-294":"","-295":"","-296":"","-297":"","-298":"","-299":"","-300":"","-301":"","-302":"","-303":"","-304":"","-305":"","-306":"","-307":"","-308":"","-309":"","-310":"","-311":"","-312":"","-313":"","-314":"","-315":"","-316":"","-317":"","-318":"","-319":"","-320":"","-321":"","-322":"","-323":"","-324":"","-325":"","-326":"","-327":"","-328":"","-329":"","-330":"","-331":"","-332":"","-333":"","-334":"","-335":"","-336":"","-337":"","-338":"","-339":"","-340":"","-341":"","-342":"","-343":"","-344":"","-345":"","-346":"","-347":"","-348":"","-349":"","-350":"","-351":"","-352":"","-353":"","-354":"","-355":"","-356":"","-357":"","-358":"","-359":"","-360":"","-361":"","-362":"","-363":"","-364":"","-365":"","-366":"","-367":"","-368":"","-369":"","-370":"","-371":"","-372":"","-373":"","-374":"","-375":"","-376":"","-377":"","-378":"","-379":"","-380":"","-381":"","-382":"","-383":"","-384":"","-385":"","-386":"","-387":"","-388":"","-389":"","-390":"","-391":"","-392":"","-393":"","-394":"","-395":"","-396":"","-397":"","-398":"","-399":"","-400":"","-401":"","-402":"","-403":"","-404":"","-405":"","-406":"","-407":"","-408":"","-409":"","-410":"","-411":"","-412":"","-413":"","-414":"","-415":"","-416":"","-417":"","-418":"","-419":"","-420":"","-421":"","-422":"","-423":"","-424":"","-425":"","-426":"","-427":"","-428":"","-429":"","-430":"","-431":"","-432":"","-433":"","-434":"","-435":"","-436":"","-437":"","-438":"","-439":"","-440":"","-441":"","-442":"","-443":"","-444":"","-445":"","-446":"","-447":"","-448":"","-449":"","-450":"","-451":"","-452":"","-453":"","-454":"","-455":"","-456":"","-457":"","-458":"","-459":"","-460":"","-461":"","-462":"","-463":"","-464":"","-465":"","-466":"","-467":"","-468":"","-469":"","-470":"","-471":"","-472":"","-473":"","-474":"","-475":"","-476":"","-477":"","-478":"","-479":"","-480":"","-481":"","-482":"","-483":"","-484":"","-485":"","-486":"","-487":"","-488":"","-489":"","-490":"","-491":"","-492":"","-493":"","-494":"","-495":"","-496":"","-497":"","-498":"","-499":"","-500":"","-501":"","-502":"","-503":"","-504":"","-505":"","-506":"","-507":"","-508":"","-509":"","-510":"","-511":"","-512":"","-513":"","-514":"","-515":"","-516":"","-517":"","-518":"","-519":"","-520":"","-521":"","-522":"","-523":"","-524":"","-525":"","-526":"","-527":"","-528":"","-529":"","-530":"","-531":"","-532":"","-533":"","-534":"","-535":"","-536":"","-537":"","-538":"","-539":"","-540":"","-541":"","-542":"","-543":"","-544":"","-545":"","-546":"","-547":"","-548":"","-549":"","-550":"","-551":"","-552":"","-553":"","-554":"","-555":"","-556":"","-557":"","-558":"","-559":"","-560":"","-561":"","-562":"","-563":"","-564":"","-565":"","-566":"","-567":"","-568":"","-569":"","-570":"","-571":"","-572":"","-573":"","-574":"","-575":"","-576":"","-577":"","-578":"","-579":"","-580":"","-581":"","-582":"","-583":"","-584":"","-585":"","-586":"","-587":"","-588":"","-589":"","-590":"","-591":"","-592":"","-593":"","-594":"","-595":"","-596":"","-597":"","-598":"","-599":"","-600":"","-601":"","-602":"","-603":"","-604":"","-605":"","-606":"","-607":"","-608":"","-609":"","-610":"","-611":"","-612":"","-613":"","-614":"","-615":"","-616":"","-617":"","-618":"","-619":"","-620":"","-621":"","-622":"","-623":"","-624":"","-625":"","-626":"","-627":"","-628":"","-629":"","-630":"","-631":"","-632":"","-633":"","-634":"","-635":"","-636":"","-637":"","-638":"","-639":"","-640":"","-641":"","-642":"","-643":"","-644":"","-645":"","-646":"","-647":"","-648":"","-649":"","-650":"","-651":"","-652":"","-653":"","-654":"","-655":"","-656":"","-657":"","-658":"","-659":"","-660":"","-661":"","-662":"","-663":"","-664":"","-665":"","-666":"","-667":"","-668":"","-669":"","-670":"","-671":"","-672":"","-673":"","-674":"","-675":"","-676":"","-677":"","-678":"","-679":"","-680":"","-681":"","-682":"","-683":"","-684":"","-685":"","-686":"","-687":"","-688":"","-689":"","-690":"","-691":"","-692":"","-693":"","-694":"","-695":"","-696":"","-697":"","-698":"","-699":"","-700":"","-701":"","-702":"","-703":"","-704":"","-705":"","-706":"","-707":"","-708":"","-709":"","-710":"","-711":"","-712":"","-713":"","-714":"","-715":"","-716":"","-717":"","-718":"","-719":"","-720":"","-721":"","-722":"","-723":"","-724":"","-725":"","-726":"","-727":"","-728":"","-729":"","-730":"","-731":"","-732":"","-733":"","-734":"","-735":"","-736":"","-737":"","-738":"","-739":"","-740":"","-741":"","-742":"","-743":"","-744":"","-745":"","-746":"","-747":"","-748":"","-749":"","-750":"","-751":"","-752":"","-753":"","-754":"","-755":"","-756":"","-757":"","-758":"","-759":"","-760":"","-761":"","-762":"","-763":"","-764":"","-765":"","-766":"","-767":"","-768":"","-769":"","-770":"","-771":"","-772":"","-773":"","-774":"","-775":"","-776":"","-777":"","-778":"","-779":"","-780":"","-781":"","-782":"","-783":"","-784":"","-785":"","-786":"","-787":"","-788":"","-789":"","-790":"","-791":"","-792":"","-793":"","-794":"","-795":"","-796":"","-797":"","-798":"","-799":"","-800":"","-801":"","-802":"","-803":"","-804":"","-805":"","-806":"","-807":"","-808":"","-809":"","-810":"","-811":"","-812":"","-813":"","-814":"","-815":"","-816":"","-817":"","-818":"","-819":"","-820":"","-821":"","-822":"","-823":"","-824":"","-825":"","-826":"","-827":"","-828":"","-829":"","-830":"","-831":"","-832":"","-833":"","-834":"","-835":"","-836":"","-837":"","-838":"","-839":"","-840":"","-841":"","-842":"","-843":"","-844":"","-845":"","-846":"","-847":"","-848":"","-849":"","-850":"","-851":"","-852":"","-853":"","-854":"","-855":"","-856":"","-857":"","-858":"","-859":"","-860":"","-861":"","-862":"","-863":"","-864":"","-865":"","-866":"","-867":"","-868":"","-869":"","-870":"","-871":"","-872":"","-873":"","-874":"","-875":"","-876":"","-877":"","-878":"","-879":"","-880":"","-881":"","-882":"","-883":"","-884":"","-885":"","-886":"","-887":"","-888":"","-889":"","-890":"","-891":"","-892":"","-893":"","-894":"","-895":"","-896":"","-897":"","-898":"","-899":"","-900":"","-901":"","-902":"","-903":"","-904":"","-905":"","-906":"","-907":"","-908":"","-909":"","-910":"","-911":"","-912":"","-913":"","-914":"","-915":"","-916":"","-917":"","-918":"","-919":"","-920":"","-921":"","-922":"","-923":"","-924":"","-925":"","-926":"","-927":"","-928":"","-929":"","-930":"","-931":"","-932":"","-933":"","-934":"","-935":"","-936":"","-937":"","-938":"","-939":"","-940":"","-941":"","-942":"","-943":"","-944":"","-945":"","-946":"","-947":"","-948":"","-949":"","-950":"","-951":"","-952":"","-953":"","-954":"","-955":"","-956":"","-957":"","-958":"","-959":"","-960":"","-961":"","-962":"","-963":"","-964":"","-965":"","-966":"","-967":"","-968":"","-969":"","-970":"","-971":"","-972":"","-973":"","-974":"","-975":"","-976":"","-977":"","-978":"","-979":"","-980":"","-981":"","-982":"","-983":"","-984":"","-985":"","-986":"","-987":"","-988":"","-989":"","-990":"","-991":"","-992":"","-993":"","-994":"","-995":"","-996":"","-997":"","-998":"","-999":"","-1000":"","-1001":"","-1002":"","-1003":"","-1004":"","-1005":"","-1006":"","-1007":"","-1008":"","-1009":"","-1010":"","-1011":"","-1012":"","-1013":"","-1014":"","-1015":"","-1016":"","-1017":"","-1018":"","-1019":"","-1020":"","-1021":"","-1022":"","-1023":"","-1024":"","-1025":"","-1026":"","-1027":"","-1028":"","-1029":"","-1030":"","-1031":"","-1032":"","-1033":"","-1034":"","-1035":"","-1036":"","-1037":"","-1038":"","-1039":"","-1040":"","-1041":"","-1042":"","-1043":"","-1044":"","-1045":"","-1046":"","-1047":"","-1048":"","-1049":"","-1050":"","-1051":"","-1052":"","-1053":"","-1054":"","-1055":"","-1056":"","-1057":"","-1058":"","-1059":"","-1060":"","-1061":"","-1062":"","-1063":"","-1064":"","-1065":"","-1066":"","-1067":"","-1068":"","-1069":"","-1070":"","-1071":"","-1072":"","-1073":"","-1074":"","-1075":"","-1076":"","-1077":"","-1078":"","-1079":"","-1080":"","-1081":"","-1082":"","-1083":"","-1084":"","-1085":"","-1086":"","-1087":"","-1088":"","-1089":"","-1090":"","-1091":"","-1092":"","-1093":"","-1094":"","-1095":"","-1096":"","-1097":"","-1098":"","-1099":"","-1100":"","-1101":"","-1102":"","-1103":"","-1104":"","-1105":"","-1106":"","-1107":"","-1108":"","-1109":"","-1110":"","-1111":"","-1112":"","-1113":"","-1114":"","-1115":"","-1116":"","-1117":"","-1118":"","-1119":"","-1120":"","-1121":"","-1122":"","-1123":"","-1124":"","-1125":"","-1126":"","-1127":"","-1128":"","-1129":"","-1130":"","-1131":"","-1132":"","-1133":"","-1134":"","-1135":"","-1136":"","-1137":"","-1138":"","-1139":"","-1140":"","-1141":"","-1142":"","-1143":"","-1144":"","-1145":"","-1146":"","-1147":"","-1148":"","-1149":"","-1150":"","-1151":"","-1152":"","-1153":"","-1154":"","-1155":"","-1156":"","-1157":"","-1158":"","-1159":"","-1160":"","-1161":"","-1162":"","-1163":"","-1164":"","-1165":"","-1166":"","-1167":"","-1168":"","-1169":"","-1170":"","-1171":"","-1172":"","-1173":"","-1174":"","-1175":"","-1176":"","-1177":"","-1178":"","-1179":"","-1180":"","-1181":"","-1182":"","-1183":"","-1184":"","-1185":"","-1186":"","-1187":"","-1188":"","-1189":"","-1190":"","-1191":"","-1192":"","-1193":"","-1194":"","-1195":"","-1196":"","-1197":"","-1198":"","-1199":"","-1200":"","-1201":"","-1202":"","-1203":"","-1204":"","-1205":"","-1206":"","-1207":"","-1208":"","-1209":"","-1210":"","-1211":"","-1212":"","-1213":"","-1214":"","-1215":"","-1216":"","-1217":"","-1218":"","-1219":"","-1220":"","-1221":"","-1222":"","-1223":"","-1224":"","-1225":"","-1226":"","-1227":"","-1228":"","-1229":"","-1230":"","-1231":"","-1232":"","-1233":"","-1234":"","-1235":"","-1236":"","-1237":"","-1238":"","-1239":"","-1240":"","-1241":"","-1242":"","-1243":"","-1244":"","-1245":"","-1246":"","-1247":"","-1248":"","-1249":"","-1250":"","-1251":"","-1252":"","-1253":"","-1254":"","-1255":"","-1256":"","-1257":"","-1258":"","-1259":"","-1260":"","-1261":"","-1262":"","-1263":"","-1264":"","-1265":"","-1266":"","-1267":"","-1268":"","-1269":"","-1270":"","-1271":"","-1272":"","-1273":"","-1274":"","-1275":"","-1276":"","-1277":"","-1278":"","-1279":"","-1280":"","-1281":"","-1282":"","-1283":"","-1284":"","-1285":"","-1286":"","-1287":"","-1288":"","-1289":"","-1290":"","-1291":"","-1292":"","-1293":"","-1294":"","-1295":"","-1296":"","-1297":"","-1298":"","-1299":"","-1300":"","-1301":"","-1302":"","-1303":"","-1304":"","-1305":"","-1306":"","-1307":"","-1308":"","-1309":"","-1310":"","-1311":"","-1312":"","-1313":"","-1314":"","-1315":"","-1316":"","-1317":"","-1318":"","-1319":"","-1320":"","-1321":"","-1322":"","-1323":"","-1324":"","-1325":"","-1326":"","-1327":"","-1328":"","-1329":"","-1330":"","-1331":"","-1332":"","-1333":"","-1334":"","-1335":"","-1336":"","-1337":"","-1338":"","-1339":"","-1340":"","-1341":"","-1342":"","-1343":"","-1344":"","-1345":"","-1346":"","-1347":"","-1348":"","-1349":"","-1350":"","-1351":"","-1352":"","-1353":"","-1354":"","-1355":"","-1356":"","-1357":"","-1358":"","-1359":"","-1360":"","-1361":"","-1362":"","-1363":"","-1364":"","-1365":"","-1366":"","-1367":"","-1368":"","-1369":"","-1370":"","-1371":"","-1372":"","-1373":"","-1374":"","-1375":"","-1376":"","-1377":"","-1378":"","-1379":"","-1380":"","-1381":"","-1382":"","-1383":"","-1384":"","-1385":"","-1386":"","-1387":"","-1388":"","-1389":"","-1390":"","-1391":"","-1392":"","-1393":"","-1394":"","-1395":"","-1396":"","-1397":"","-1398":"","-1399":"","-1400":"","-1401":"","-1402":"","-1403":"","-1404":"","-1405":"","-1406":"","-1407":"","-1408":"","-1409":"","-1410":"","-1411":"","-1412":"","-1413":"","-1414":"","-1415":"","-1416":"","-1417":"","-1418":"","-1419":"","-1420":"","-1421":"","-1422":"","-1423":"","-1424":"","-1425":"","-1426":"","-1427":"","-1428":"","-1429":"","-1430":"","-1431":"","-1432":"","-1433":"","-1434":"","-1435":"","-1436":"","-1437":"","-1438":"","-1439":"","-1440":"","-1441":"","-1442":"","-1443":"","-1444":"","-1445":"","-1446":"","-1447":"","-1448":"","-1449":"","-1450":"","-1451":"","-1452":"","-1453":"","-1454":"","-1455":"","-1456":"","-1457":"","-1458":"","-1459":"","-1460":"","-1461":"","-1462":"","-1463":"","-1464":"","-1465":"","-1466":"","-1467":"","-1468":"","-1469":"","-1470":"","-1471":"","-1472":"","-1473":"","-1474":"","-1475":"","-1476":"","-1477":"","-1478":"","-1479":"","-1480":"","-1481":"","-1482":"","-1483":"","-1484":"","-1485":"","-1486":"","-1487":"","-1488":"","-1489":"","-1490":"","-1491":"","-1492":"","-1493":"","-1494":"","-1495":"","-1496":"","-1497":"","-1498":"","-1499":"","-1500":"","-1501":"","-1502":"","-1503":"","-1504":"","-1505":"","-1506":"","-1507":"","-1508":"","-1509":"","-1510":"","-1511":"","-1512":"","-1513":"","-1514":"","-1515":"","-1516":"","-1517":"","-1518":"","-1519":"","-1520":"","-1521":"","-1522":"","-1523":"","-1524":"","-1525":"","-1526":"","-1527":"","-1528":"","-1529":"","-1530":"","-1531":"","-1532":"","-1533":"","-1534":"","-1535":"","-1536":"","-1537":"","-1538":"","-1539":"","-1540":"","-1541":"","-1542":"","-1543":"","-1544":"","-1545":"","-1546":"","-1547":"","-1548":"","-1549":"","-1550":"","-1551":"","-1552":"","-1553":"","-1554":"","-1555":"","-1556":"","-1557":"","-1558":"","-1559":"","-1560":"","-1561":"","-1562":"","-1563":"","-1564":"","-1565":"","-1566":"","-1567":"","-1568":"","-1569":"","-1570":"","-1571":"","-1572":"","-1573":"","-1574":"","-1575":"","-1576":"","-1577":"","-1578":"","-1579":"","-1580":"","-1581":"","-1582":"","-1583":"","-1584":"","-1585":"","-1586":"","-1587":"","-1588":"","-1589":"","-1590":"","-1591":"","-1592":"","-1593":"","-1594":"","-1595":"","-1596":"","-1597":"","-1598":"","-1599":"","-1600":"","-1601":"","-1602":"","-1603":"","-1604":"","-1605":"","-1606":"","-1607":"","-1608":"","-1609":"","-1610":"","-1611":"","-1612":"","-1613":"","-1614":"","-1615":"","-1616":"","-1617":"","-1618":"","-1619":"","-1620":"","-1621":"","-1622":"","-1623":"","-1624":"","-1625":"","-1626":"","-1627":"","-1628":"","-1629":"","-1630":"","-1631":"","-1632":"","-1633":"","-1634":"","-1635":"","-1636":"","-1637":"","-1638":"","-1639":"","-1640":"","-1641":"","-1642":"","-1643":"","-1644":"","-1645":"","-1646":"","-1647":"","-1648":"","-1649":"","-1650":"","-1651":"","-1652":"","-1653":"","-1654":"","-1655":"","-1656":"","-1657":"","-1658":"","-1659":"","-1660":"","-1661":"","-1662":"","-1663":"","-1664":"","-1665":"","-1666":"","-1667":"","-1668":"","-1669":"","-1670":"","-1671":"","-1672":"","-1673":"","-1674":"","-1675":"","-1676":"","-1677":"","-1678":"","-1679":"","-1680":"","-1681":"","-1682":"","-1683":"","-1684":"","-1685":"","-1686":"","-1687":"","-1688":"","-1689":"","-1690":"","-1691":"","-1692":"","-1693":"","-1694":"","-1695":"","-1696":"","-1697":"","-1698":"","-1699":"","-1700":"","-1701":"","-1702":"","-1703":"","-1704":"","-1705":"","-1706":"","-1707":"","-1708":"","-1709":"","-1710":"","-1711":"","-1712":"","-1713":"","-1714":"","-1715":"","-1716":"","-1717":"","-1718":"","-1719":"","-1720":"","-1721":"","-1722":"","-1723":"","-1724":"","-1725":"","-1726":"","-1727":"","-1728":"","-1729":"","-1730":"","-1731":"","-1732":"","-1733":"","-1734":"","-1735":"","-1736":"","-1737":"","-1738":"","-1739":"","-1740":"","-1741":"","-1742":"","-1743":"","-1744":"","-1745":"","-1746":"","-1747":"","-1748":"","-1749":"","-1750":"","-1751":"","-1752":"","-1753":"","-1754":"","-1755":"","-1756":"","-1757":"","-1758":"","-1759":"","-1760":"","-1761":"","-1762":"","-1763":"","-1764":"","-1765":"","-1766":"","-1767":"","-1768":"","-1769":"","-1770":"","-1771":"","-1772":"","-1773":"","-1774":"","-1775":"","-1776":"","-1777":"","-1778":"","-1779":"","-1780":"","-1781":"","-1782":"","-1783":"","-1784":"","-1785":"","-1786":"","-1787":"","-1788":"","-1789":"","-1790":"","-1791":"","-1792":"","-1793":"","-1794":"","-1795":"","-1796":"","-1797":"","-1798":"","-1799":"","-1800":"","-1801":"","-1802":"","-1803":"","-1804":"","-1805":"","-1806":"","-1807":"","-1808":"","-1809":"","-1810":"","-1811":"","-1812":"","-1813":"","-1814":"","-1815":"","-1816":"","-1817":"","-1818":"","-1819":"","-1820":"","-1821":"","-1822":"","-1823":"","-1824":"","-1825":"","-1826":"","-1827":"","-1828":"","-1829":"","-1830":"","-18
```

# Fetching


[MMTF.fetch](#) and [MMTF.fetchReduced](#) are helper functions to quickly load and decode PDB IDs in MMTF format.

– raw 

```
1 // Fetch PDB ID 3PQR in MMTF format and print the decoded MMTF data (or an loading/decoding error)
2 MMTF.fetch(
3     "3PQR",
4     // onLoad callback
5     function( mmtfData ){ console.log( mmtfData ) },
6     // onError callback
7     function( error ){ console.error( error ) }
8 );
```

# Traversal


`MMTF.traverse` is a helper function to loop over the structural data in the decoded MMTF data object.

— raw 

```
1 // `bin` is an Uint8Array containing the MMTF MessagePack
2 var mmtfData = MMTF.decode( bin );
3
4 // create event callback functions
5 var eventCallbacks = {
6     onModel: function( modelData ){ console.log( modelData ) },
7     onChain: function( chainData ){ console.log( chainData ) },
8     onGroup: function( groupData ){ console.log( groupData ) },
9     onAtom: function( atomData ){ console.log( atomData ) },
10    onBond: function( bondData ){ console.log( bondData ) }
11 };
12
13 // traverse the structure and listen to the events
14 MMTF.traverse( mmtfData, eventCallbacks );
```

# Decoding

The decoder is exposed as [MMTF.decode](#) which accepts an `Uint8Array` containing the MMTF MessagePack and returns the decoded MMTF data as an object. Note, when using [MMTF.fetch](#) or [MMTF.fetchReduced](#), decoding is not necessary.

— raw 

```
1 // bin is Uint8Array containing the mmtf msgpack
2 var mmtfData = MMTF.decode( bin );
3 console.log( mmtfData.numAtoms );
```

# MMTF JavaScript API - Resources

- **Github repository**
  - <https://github.com/rcsb/mmtf-javascript>
- **API docs**
  - <https://rcsb.github.io/mmtf-javascript/docs/api/v1.0.0/>
- **Examples**
  - JSON <https://codepen.io/arose/pen/LLzVXg>
  - Traversal <https://codepen.io/arose/pen/QgqbRG>
  - Loader <https://codepen.io/arose/pen/qjPdzQ>
- **CDN**
  - <https://cdn.rawgit.com/rcsb/mmtf-javascript/v1.0.0/dist/mmtf.js>



# Example

The following code creates a viewer and loads the structure of PDB entry *1CRN* from the [RCSB PDB](#). The result is seen on the right. For more information on how to control the viewer see the API reference, starting with the [Stage](#) class.

```
<!DOCTYPE html>
<html lang="en">
<head>
  <meta charset="utf-8">
</head>
<body>
  <script src="path/to/ngl.js"></script>
  <script>
    document.addEventListener( "DOMContentLoaded", function() {
      var stage = new NGL.Stage( "viewport" );
      stage.loadFile( "rcsb://1crn", { defaultRepresentation: true } );
    } );
  </script>
  <div id="viewport" style="width:400px; height:300px;"></div>
</body>
</html>
```



# NGL - Objects and Concepts

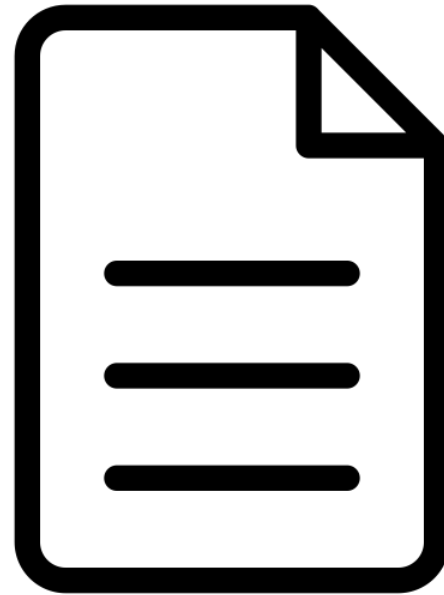
- Stage -> Component -> Representation

```
// create a `stage` object
var stage = new NGL.Stage("viewport");
// load a PDB structure and consume the returned `Promise`
stage.loadFile("rcsb://1CRN").then(function (component) {
  // add a "cartoon" representation to the structure component
  component.addRepresentation("cartoon");
  // provide a "good" view of the structure
  component.autoView();
});
```

<http://arose.github.io/ngl/api/manual/usage/embedding.html>  
<http://arose.github.io/ngl/api/class/src/stage/stage.js~Stage.html>

# NGL - File Formats

- **Structure**
  - mmCIF, PDB/PQR, GRO, SDF, MOL2, MMTF, PSF, DCD
- **Volume**
  - MRC/MAP/CCP4, DSN6/BRIX, CUBE, DX/DXBIN, XPLOR/CNS
- **Surface**
  - OBJ, PLY
- **General**
  - JSON, CSV, TXT, XML

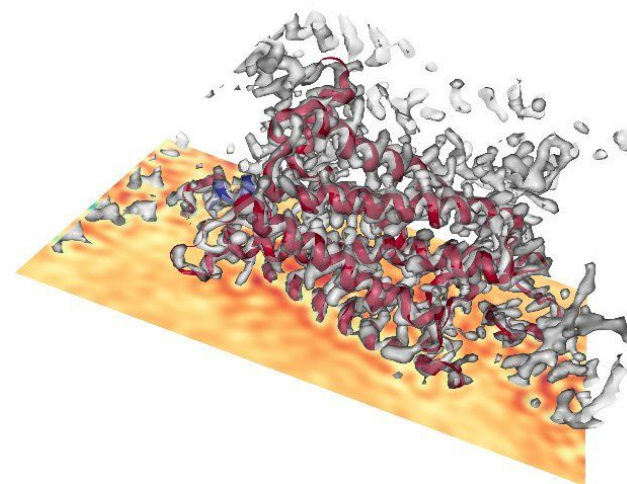


*Or add your own...*

<https://arose.github.io/ngl/api/manual/usage/file-formats.html>

# NGL - Representations

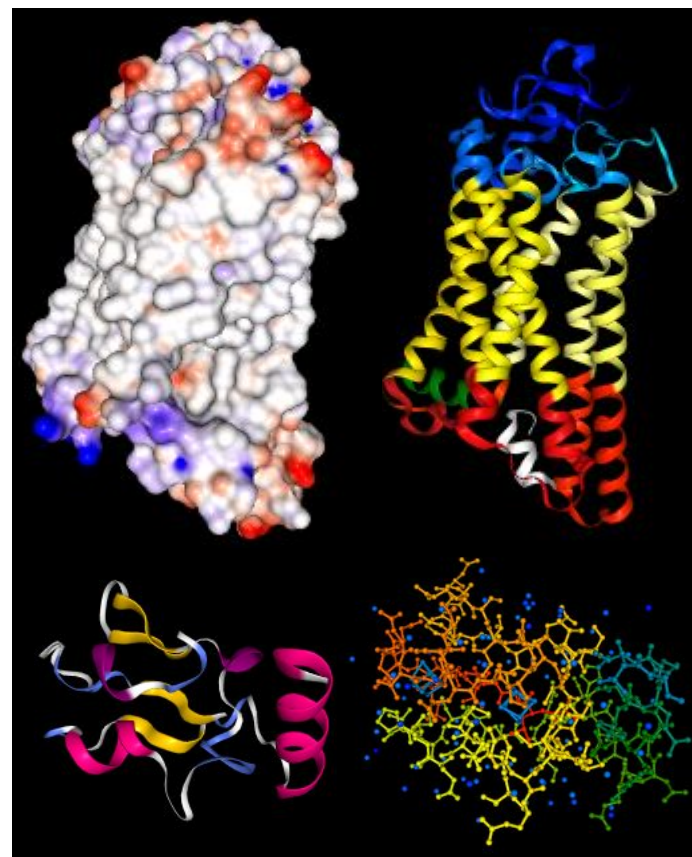
- **Structure data**
  - cartoon, ball+stick, spacefill, backbone, surface, ...
- **Volume data**
  - surface, slice, dot
- **User shapes**
  - sphere, cylinder, ellipsoid, cone, arrow, label, mesh



<https://arose.github.io/ngl/api/manual/usage/molecular-representations.html>  
<https://arose.github.io/ngl/build/docs/manual/usage/volume-representations.html>  
<https://arose.github.io/ngl/api/manual/usage/custom-geometries.html>

# NGL - Coloring

- **Predefined**
  - residue index, electrostatic, secondary structure, element, volume, B factor, ...
- **Custom**
  - Function that receives an Atom object and returns a color
- **Parameters**
  - scale, e.g. red-white-blue, also any from “ColorBrewer”
  - domain, e.g. [ 0, 1 ]
  - value: e.g. lightgreen



<https://arose.github.io/ngl/api/manual/usage/coloring.html>



# NGL - User Interaction

- **stage.mouseControls**
  - Bind actions to mouse and key combinations
- **stage.animationControls**
  - Orient the whole scene or individual components

Animate structure to align with principal axes:

```
stage.loadFile("rcsb://3pqr").then(function (o) {  
  o.addRepresentation("cartoon");  
  var pa = o.structure.getPrincipalAxes();  
  stage.animationControls.rotate(pa.getRotationQuaternion(), 1500);  
});
```

<https://arose.github.io/ngl/api/manual/usage/interaction-controls.html>

# NGL - Working with Molecules

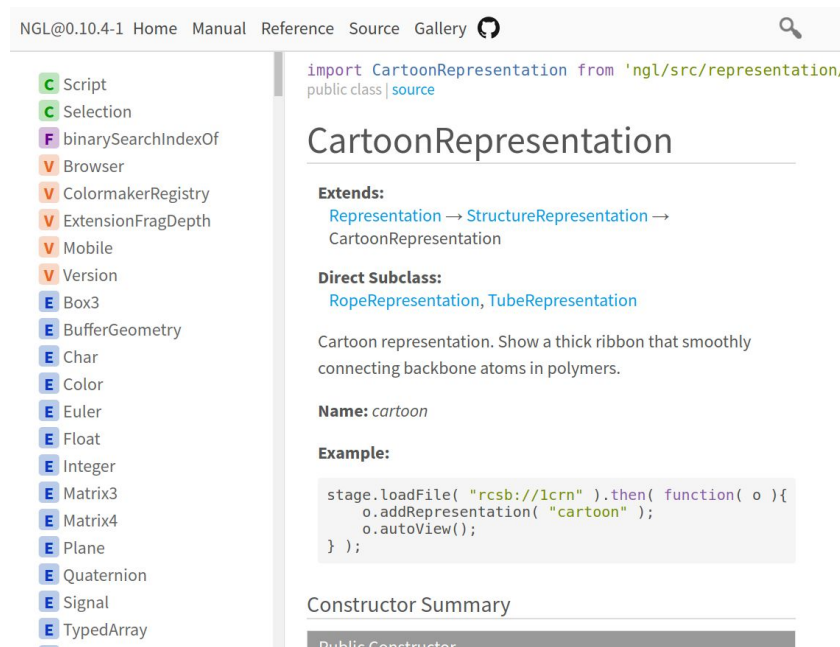
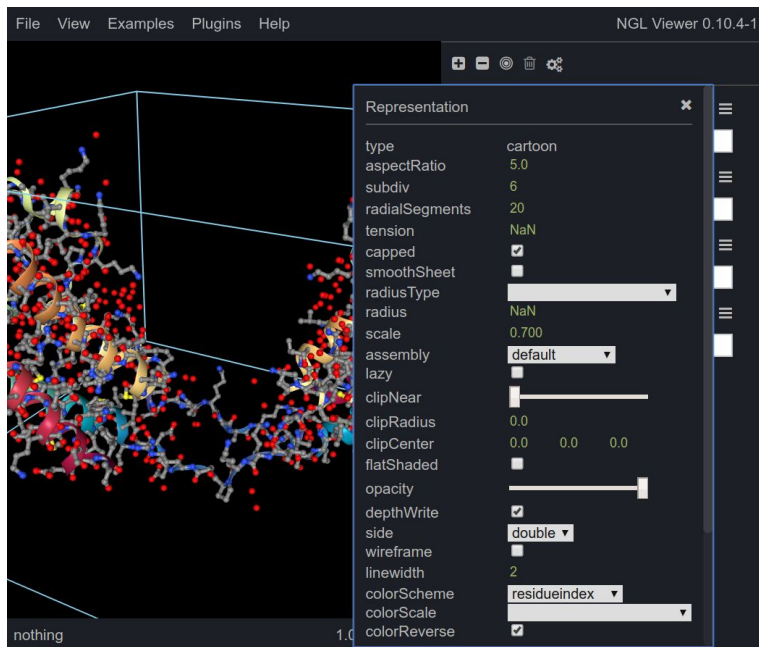
- **Structure data**
  - Iterate over the hierarchy model/chain/residue/atom
- **Selection language**
  - Concisely specify a set of atoms to work with

```
// Calculate B-factor statistics
stage.loadFile("rcsb://1crn").then(function(component) {
  var bfactorSum = 0
  var bfactorMin = +Infinity
  var bfactorMax = -Infinity
  component.structure.eachAtom(function(atom) {
    bfactorSum += atom.bfactor;
    if (bfactorMin > atom.bfactor) bfactorMin = atom.bfactor
    if (bfactorMax < atom.bfactor) bfactorMax = atom.bfactor
  });
  var bfactorAvg = bfactorSum / component.structure.atomCount
  console.log(bfactorSum, bfactorMin, bfactorMax, bfactorAvg)
});
```

<http://arose.github.io/ngl/api/manual/usage/selection-language.html>

<http://arose.github.io/ngl/api/manual/usage/structure-data.html>

# NGL - Discover Parameters



Webapp: <http://arose.github.io/ngl/>

Docs: <http://arose.github.io/ngl/api/>

# NGL Viewer/Library - Resources

- **Github repository**
  - <https://github.com/arose/ngl>
- **API docs & manual**
  - <http://arose.github.io/ngl/api/>
- **Examples Gallery**
  - <https://arose.github.io/ngl/gallery/>
- **CDN**
  - <https://unpkg.com/ngl> (latest release)
  - <https://unpkg.com/ngl@0.10.3>



# Hands-on exercises

- **MMTF JavaScript API**

- Play around with examples on CodePen
- Change examples to use `MMTF.fetch()`
- Write your own callback functions for `MMTF.traverse()`

- **NGL Library/Viewer**

- Play around with examples from gallery on CodePen
- Load your favorite structure and add your favorite representations
- Iterate over the atoms in a structure and print a label
- Calculate B-factor statistics for backbone atoms only
- Print the distance between two clicked-on atoms

# Funding

This workshop was supported by the National Cancer Institute of the National Institutes of Health under Award Number U01CA198942. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.

