



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:00 pm GMT

PDB ID : 7Q55
EMDB ID : EMD-13826
Title : Single Particle Cryo-EM structure of photosynthetic A8B8 glyceraldehyde
-3-phosphate dehydrogenase hexadecamer (major conformer) from *Spinacia
oleracea*.
Authors : Marotta, R.; Fermani, S.; Sparla, F.; Trost, P.; Del Giudice, A.
Deposited on : 2021-11-02
Resolution : 5.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

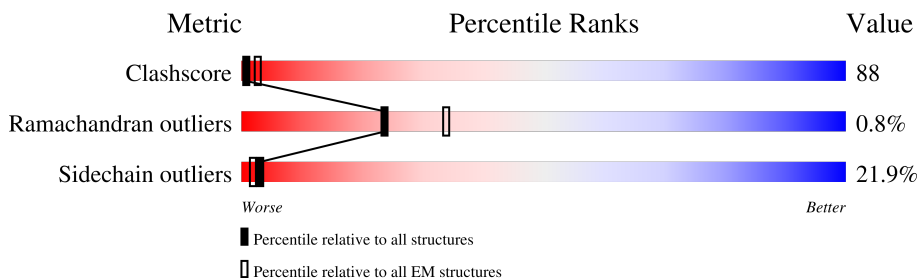
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
1	E	451	
1	G	451	
1	I	451	
1	K	451	
1	O	451	
1	Q	451	

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Mol	Chain	Length	Quality of chain				
2	B	402		8%	61%	15%	16%
2	D	402		9%	62%	12%	16%
2	F	402		6%	65%	13%	16%
2	H	402		8%	61%	14%	16%
2	J	402		8%	62%	13%	16%
2	L	402		10%	60%	14%	16%
2	P	402		8%	62%	13%	16%
2	R	402		8%	60%	15%	16%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	O	368	2694	1700	473	510	11	0	0
1	Q	368	2694	1700	473	510	11	0	0
1	A	368	2694	1700	473	510	11	0	0
1	C	368	2694	1700	473	510	11	0	0
1	E	368	2694	1700	473	510	11	0	0
1	G	368	2694	1700	473	510	11	0	0
1	I	368	2694	1700	473	510	11	0	0
1	K	368	2694	1700	473	510	11	0	0

- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	337	2544	1600	445	488	11	0	0
2	R	337	2544	1600	445	488	11	0	0
2	B	337	2544	1600	445	488	11	0	0
2	D	337	2544	1600	445	488	11	0	0
2	F	337	2544	1600	445	488	11	0	0
2	H	337	2544	1600	445	488	11	0	0
2	J	337	2544	1600	445	488	11	0	0

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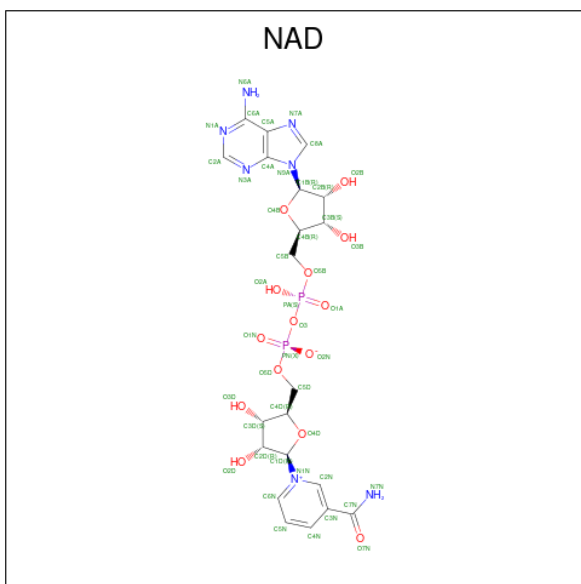
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	337	2544	1600	445	488	11	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	334	UNK	-	insertion	UNP P19866
R	334	UNK	-	insertion	UNP P19866
B	334	UNK	-	insertion	UNP P19866
D	334	UNK	-	insertion	UNP P19866
F	334	UNK	-	insertion	UNP P19866
H	334	UNK	-	insertion	UNP P19866
J	334	UNK	-	insertion	UNP P19866
L	334	UNK	-	insertion	UNP P19866

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	O	1	44	21	7	14	2	0
3	P	1	44	21	7	14	2	0
3	Q	1	44	21	7	14	2	0
3	R	1	44	21	7	14	2	0

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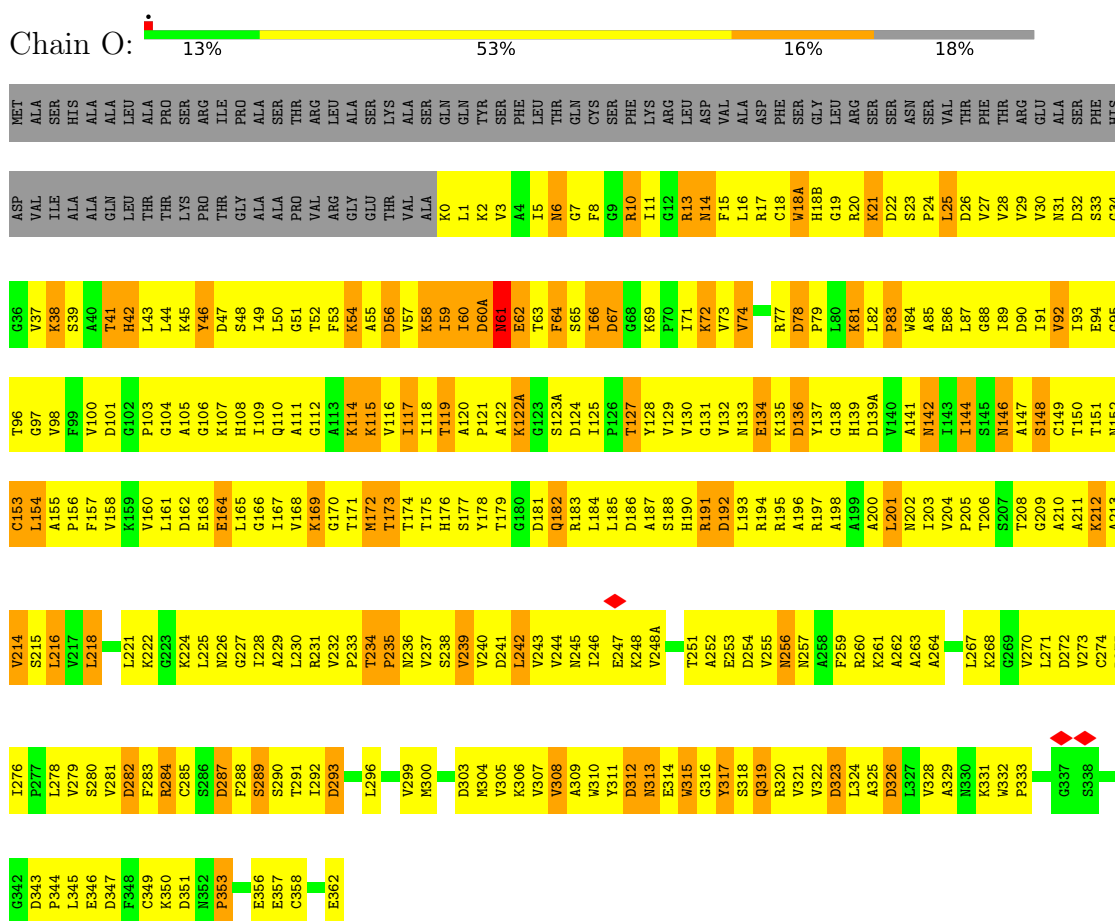
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 44	C 21	N 7	O 14	P 2	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0
3	E	1	Total 44	C 21	N 7	O 14	P 2	0
3	F	1	Total 44	C 21	N 7	O 14	P 2	0
3	G	1	Total 44	C 21	N 7	O 14	P 2	0
3	H	1	Total 44	C 21	N 7	O 14	P 2	0
3	I	1	Total 44	C 21	N 7	O 14	P 2	0
3	J	1	Total 44	C 21	N 7	O 14	P 2	0
3	K	1	Total 44	C 21	N 7	O 14	P 2	0
3	L	1	Total 44	C 21	N 7	O 14	P 2	0

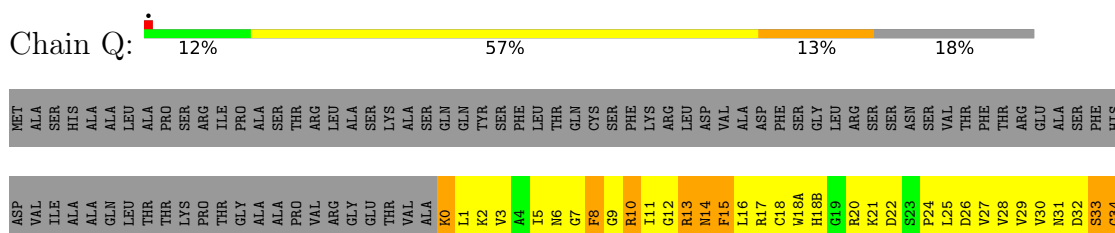
3 Residue-property plots

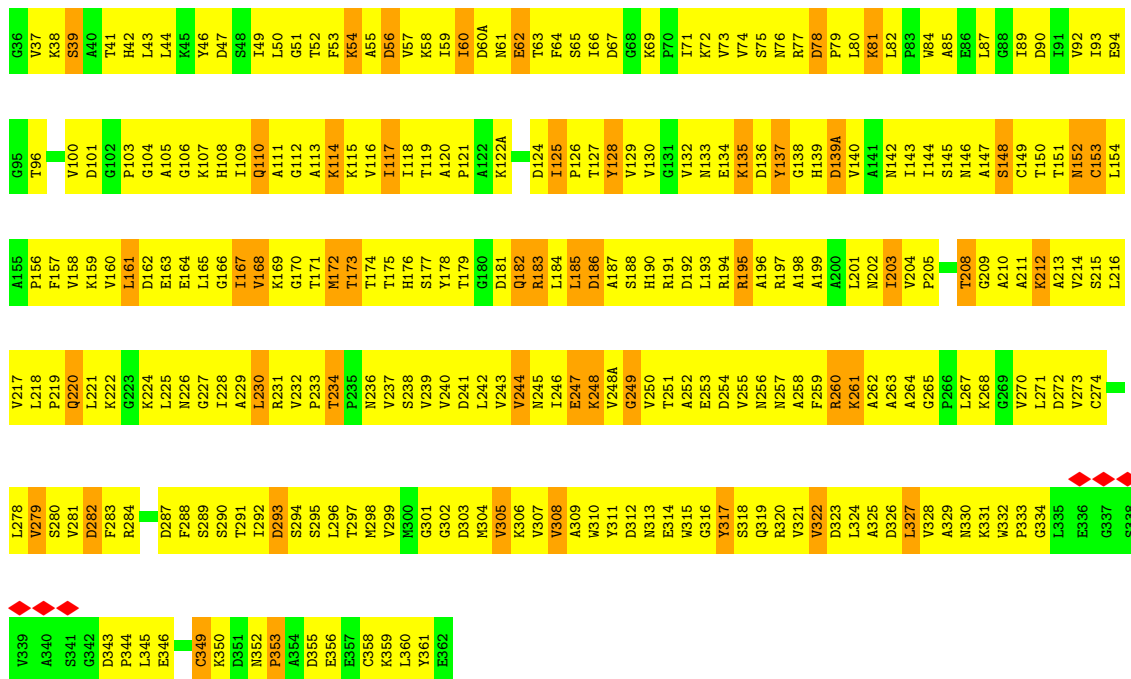
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

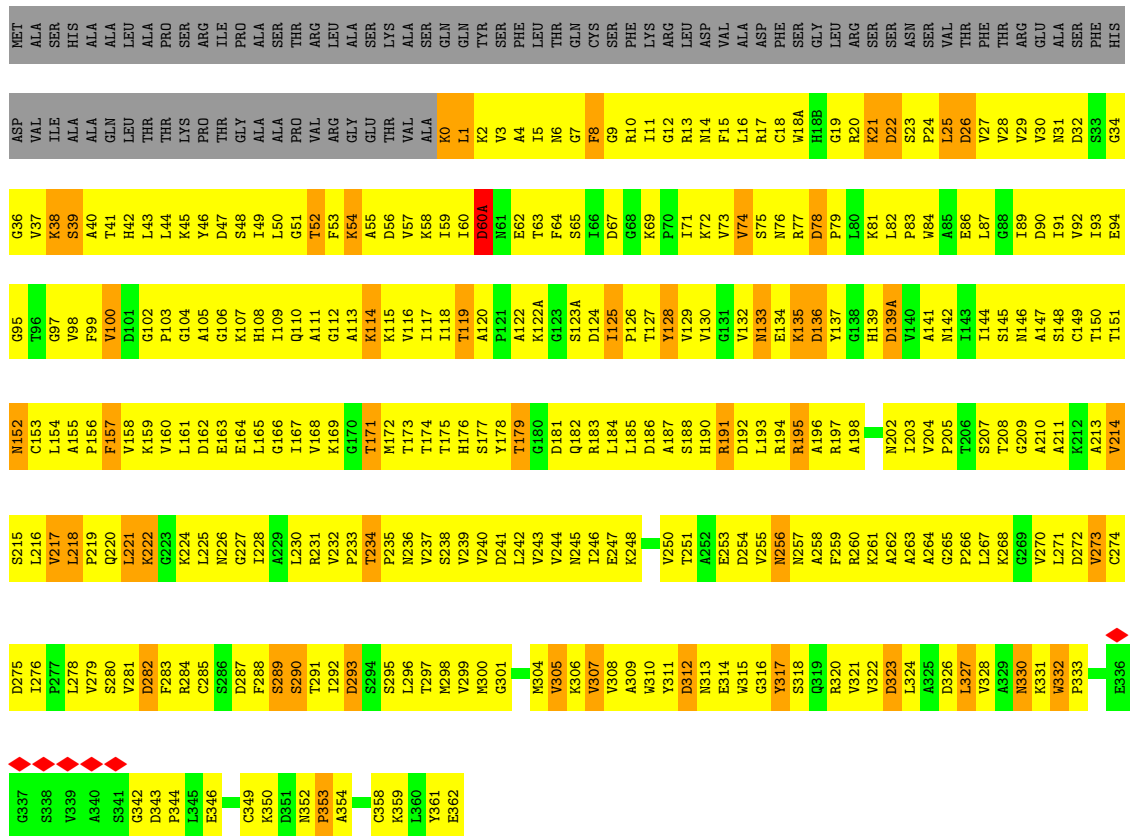
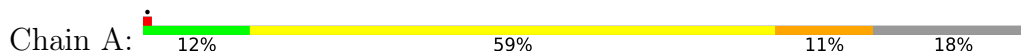


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

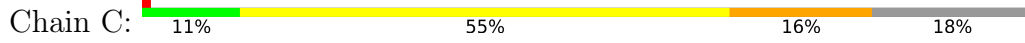




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

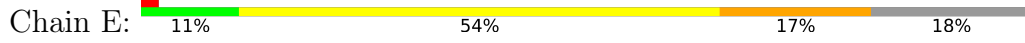


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

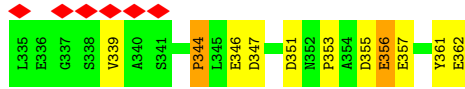


MET	ALA	SER	HIS	ALA	ALA	LEU	PRO	SER	ARG	ILE	PRO	ARG	LEU	ALA	SER	LEU	ALA	GLN	THR	THR	GLN	THR	THR	LEU	LEU	ASP	VAL	ALA	ASP	PHE	ASP	PHE	SER	GLY	LEU	ARG	ARG	SER	SER	ASN	SER	VAL	THR	PHE	THR	ARG	GLU	ALA	PHE	HIS									
ASP	VAL	ILE	ALA	ALA	GLN	LEU	THR	THR	PRO	THR	THR	VAL	VAL	ARG	GLY	GLU	THR	VAL	ALA	ALA	ALA	GLN	L1	K2	V3	I5	N6	G7	F8	G9	R10	I11	G12	R13	M14	F15	L16	ALA	C18	ASP	R18A	H18B	G19	R20	K21	D22	S23	P24	L25	D26	V27	V28	V29	N30	N31	D32	S33	G34	
G36	V37	K38	S39	A40	T41	H42	L43	L44	K45	Y46	D47	S48	I49	G51	T52	F53	K54	A55	D56	V57	K58	I59	I60	D60A	N61	E62	T63	F64	S65	I66	D67	G68	K69	I71	K72	V73	V74	S75	N76	R77	D78	P79	L80	K81	L82	P83	W84	A85	E86	L87	I89	I91	I92	I93	E94				
G95	T96	G97	V98	F99	V100	D101	G102	P103	A104	A105	G106	K107	H108	I109	Q110	A111	G112	A113	K114	V115	V116	I117	I118	T119	A120	P121	A122	K122A	I125	P126	L127	V128	V129	V130	M133	E134	K135	D136	I137	G138	H139	D139A	V140	A141	N142	I143	I144	S145	N146	A147	T151	T152	C153	L154					
A155	P156	F157	V158	K159	V160	L161	D162	E163	E164	G165	G166	I167	V168	K169	G170	M171	M172	L173	T174	T175	H176	S177	Y178	T179	G180	D181	Q182	R183	L184	L185	D186	A187	S188	H189	R191	D192	L193	R194	R195	A196	R197	A198	A199	A200	L201	N202	I203	V204	P205	T206	S207	T208	G209	A210	A211	K212	A213	V214	S215
L216	V217	L218	P219	Q220	L221	K224	L225	N226	G227	I228	A229	L230	R231	V232	P233	T234	P235	M236	S238	V239	V240	D241	L242	V243	V244	N245	I246	E247	K248	V248A	G249	V250	T251	A252	E253	D254	V255	N256	N257	A258	F259	R260	K261	A262	A263	A264	G265	P266	L267	K268	G269	V270	L271	D272	V273	C274	D275		
I276	P277	L278	V279	S280	V281	D282	F283	R284	S285	G286	D287	F288	S289	S290	T291	I292	D293	S294	S295	L296	M298	V299	M300	G301	D302	G303	M304	V305	K306	V307	V308	A309	W310	Y311	D312	M313	E314	W315	G316	Y317	S318	Q319	R320	V321	V322	D323	L324	A325	D326	V328	A329	N330	K331	W332	P333	G334			
S338	V339	A340	S341	G342	D343	P344	L345	E346	D347	F348	K349	K350	N351	P353	E356	E357	C358	K359	L360	Y361	E362																																						

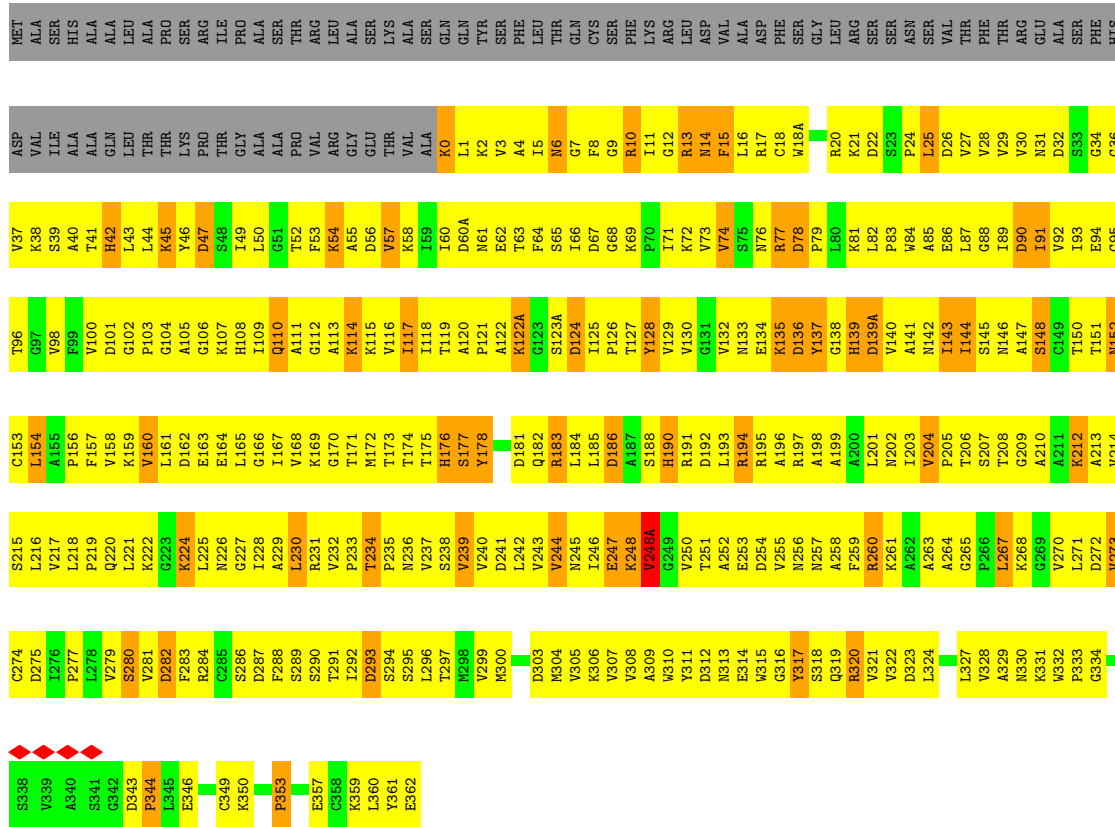
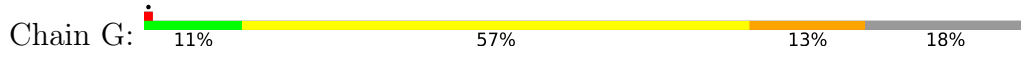
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplatic



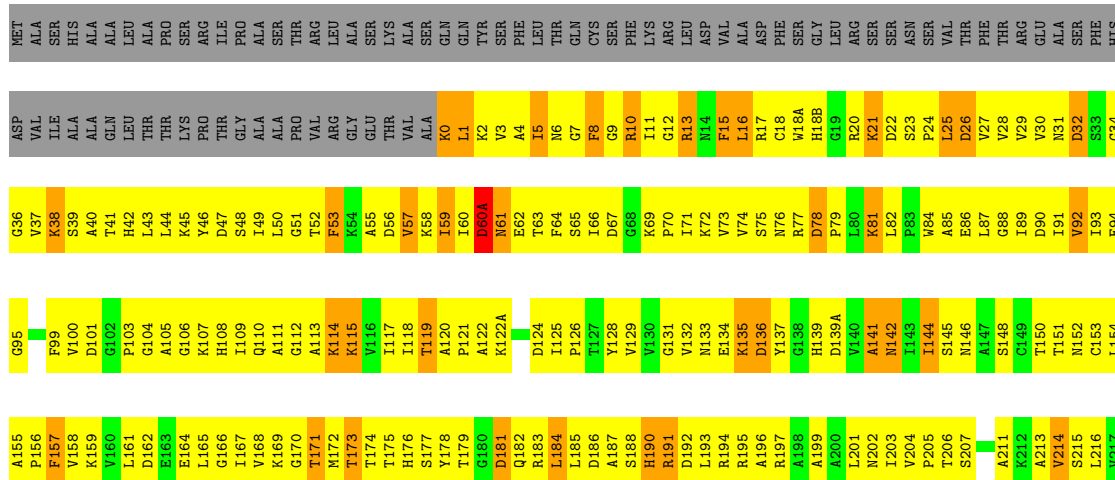
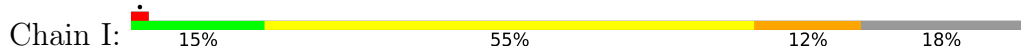
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ASP	VAL	ILE	ALA	ALA	GLN	LEU	THR	THR	PRO	THR	THR	VAL	VAL	ARG	GLY	GLU	THR	VAL	ALA	ALA	ALA	GLN	L1	K2	V3	I5	N6	G7	F8	G9	R10	I11	G12	R13	M14	F15	L16	ALA	C18	ASP	R18A	H18B	G19	R20	K21	D22	S23	P24	L25	D26	V27	V28	V29	N30	N31	D32	S33	G34
G36	V37	K38	S39	A40	T41	H42	L43	L44	K45	Y46	D47	S48	I49	G51	T52	F53	K54	A55	D56	V57	K58	I59	I60	D60A	N61	E62	T63	F64	S65	I66	D67	G68	K69	I71	K72	V73	V74	S75	N76	R77	D78	P79	L80	K81	L82	P83	W84	A85	E86	L87	I89	I91	I92	I93	E94			
G95	T96	G97	V98	F99	V100	D101	G102	P103	A104	A105	G106	K107	H108	I109	Q110	A111	G112	A113	K114	V115	V116	I117	I118	T119	A120	P121	A122	K122A	I125	P126	L127	V128	V129	V130	M133	E134	K135	D136	I137	G138	H139	D139A	V140	A141	N142	I143	I144	S145	N146	A147	T151	T152	C153	L154				
M152	C153	A155	F157	V158	K159	V160	L161	E163	D162	E164	L165	G166	I167	V168	M171	M172	L173	T174	T175	H176	S177	Y178	T179	G180	D181	Q182	R183	L184	L185	D186	A187	S188	H189	R191	D192	L193	R194	R195	A196	R197	A199	L201	N202	I203	V204	P205	T206	S207	T208	G209	A210	A211	K212	A213				
V214	S215	L216	V217	L218	P219	Q220	L221	K222	G223	I228	A229	L230	R231	V232	P233	T234	P235	M236	S238	V239	V240	D241	L242	V243	V244	N245	I246	E247	K248	V248A	T251	A252	E253	D254	V255	N256	N257	A258	F259	R260	K261	A262	A263	A264	G265	A264	G265	P266	L267	K268	G269	V270	L271	D272	V273			
C274	D275	I276	P277	L278	V279	S280	V281	D282	F283	D287	F288	S289	T291	I292	D293	S294	S295	L296	M298	V299	M300	G301	D302	G303	M304	V305	K306	K307	V308	A309	W310	Y311	D312	M313	E314	W315	G316	Y317	S318	Q319	R320	V321	V322	D323	L324	A325	D326	L327	K328	A329	N330	K331	W332	P333	G334			

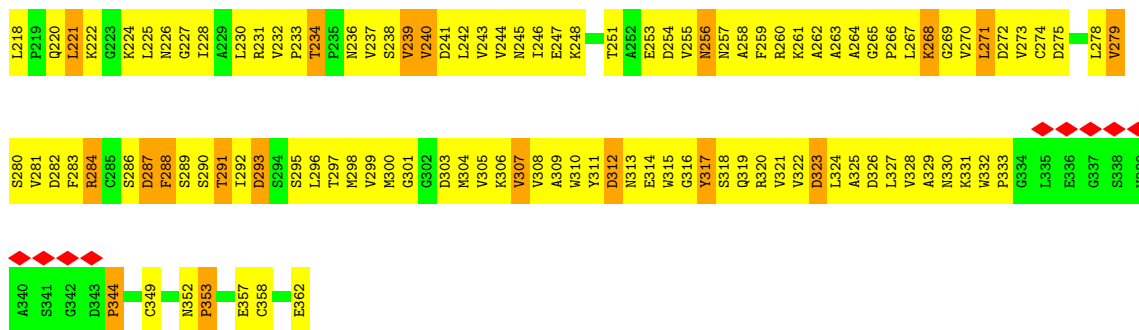


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

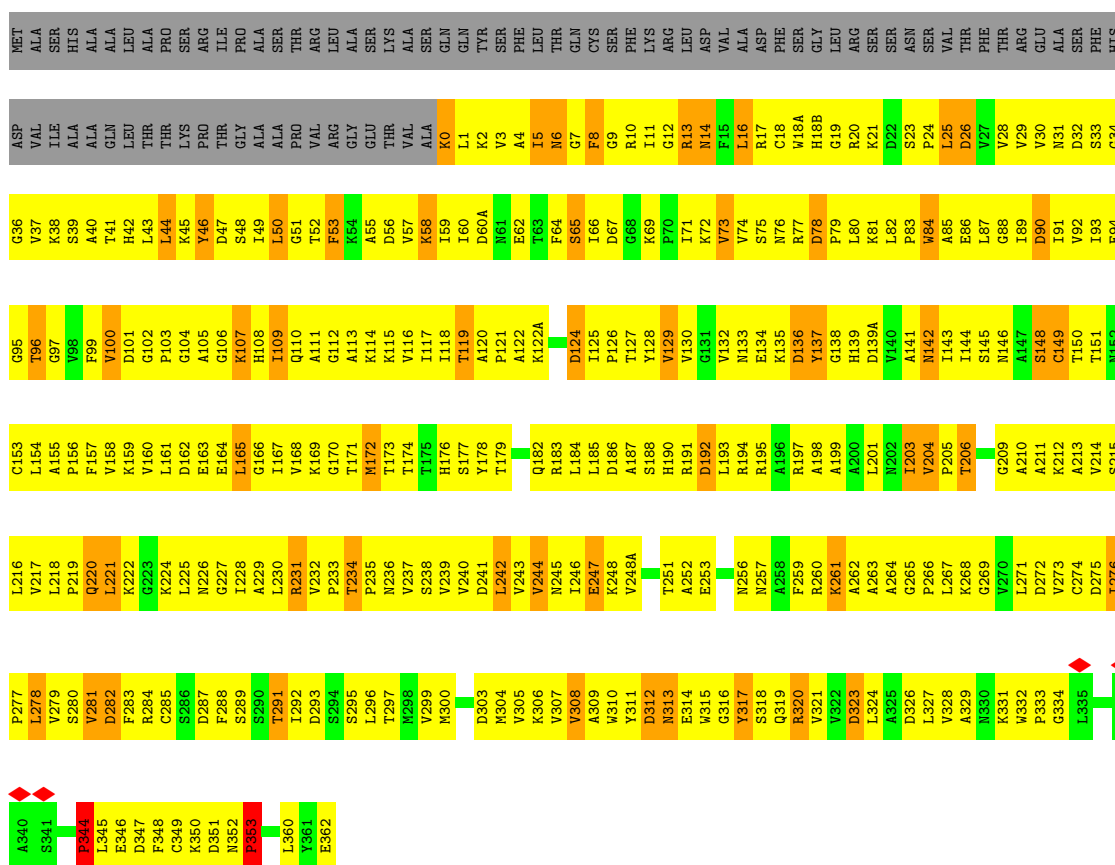
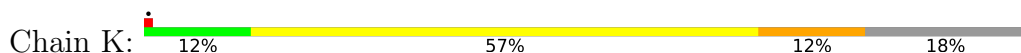


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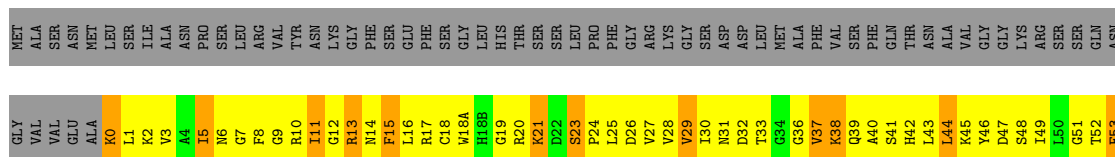
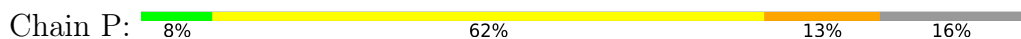


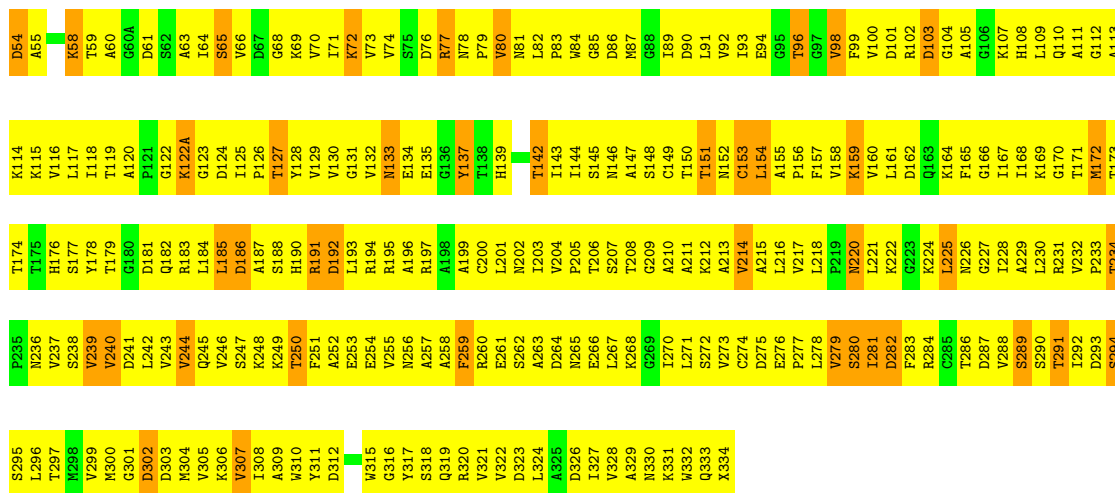


● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

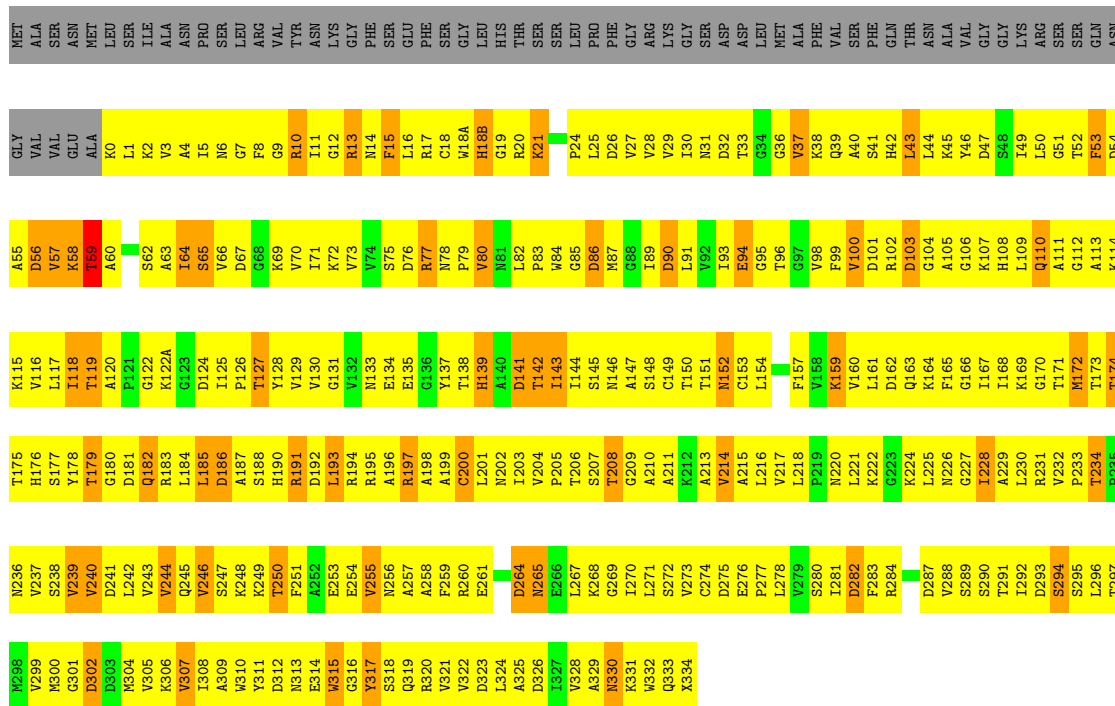
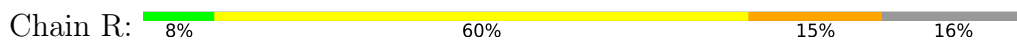


● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

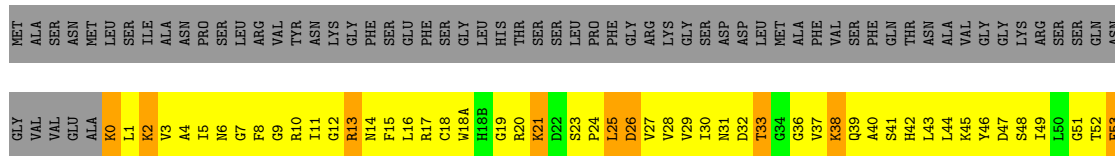
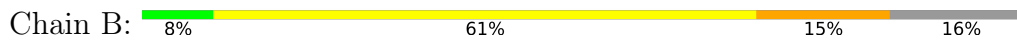


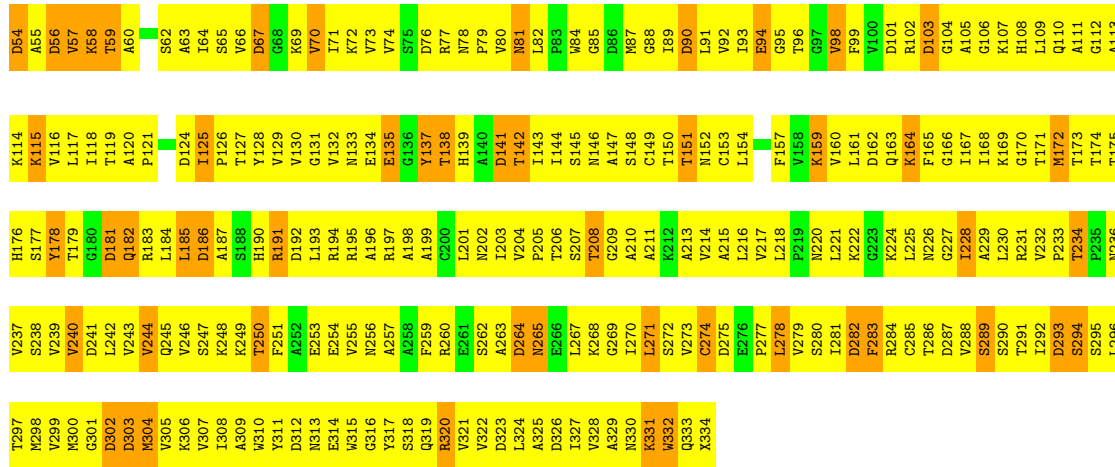


• Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplactic

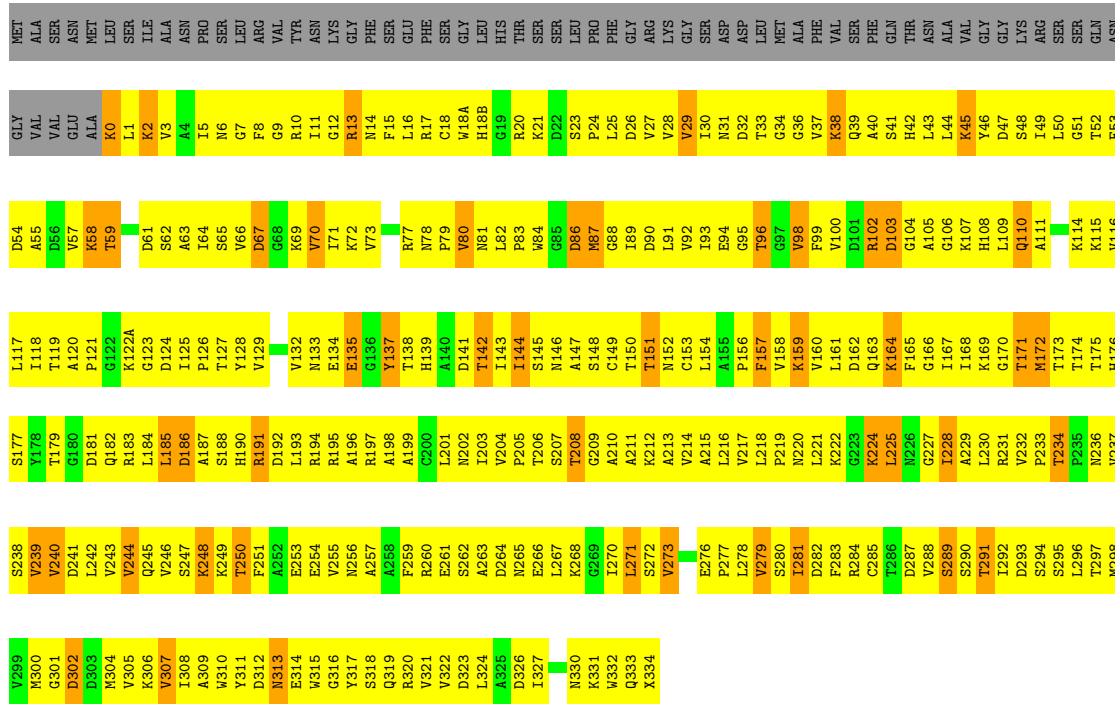
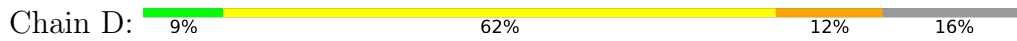


• Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplactic

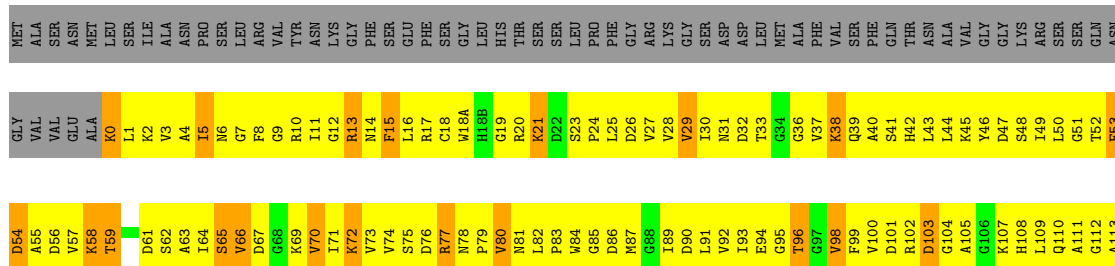
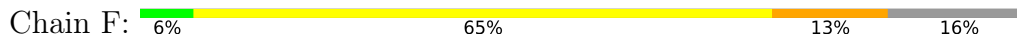




● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

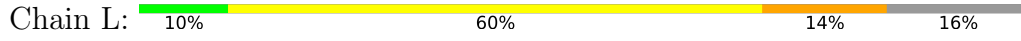


● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



S177	S238	M288	S238	M288
Y178	V239	V289	V239	V289
T179	V240	M300	V240	M300
G180	D241	D302	L242	D302
D181	L243	M304	V244	M304
Q182	Q245	K306	Q245	K306
L183	V246	A309	V246	A309
L184	S247	Y311	S247	Y311
L185	K248	W310	K248	W310
D186	S188	F251	S188	F251
A187	S188	A252	S188	A252
S188	H190	E253	H190	E253
H190	R191	E254	R191	E254
R191	D192	R195	D192	R195
D192	L193	R195	L193	R195
L193	R194	R195	R194	R195
R194	R195	N256	R195	N256
R195	A196	A257	A196	A257
A196	R197	A288	R197	A288
R197	A198	F259	A198	F259
A198	A199	R260	A199	R260
A199	C200	E261	C200	E261
C200	L201	S262	L201	S262
L201	N202	D264	N202	D264
N202	I203	N265	I203	N265
I203	V204	S266	V204	S266
V204	P205	T206	P205	T206
P205	P206	S207	P206	S207
P206	T207	K268	T207	K268
T207	G209	I270	G209	I270
G209	A210	L271	A210	L271
A210	K211	S272	K211	S272
K211	A213	W273	A213	W273
A213	V214	C274	V214	C274
V214	A215	D275	A215	D275
A215	L216	E276	L216	E276
L216	V217	P277	V217	P277
V217	L218	L278	L218	L278
L218	P219	V279	P219	V279
P219	N220	S280	N220	S280
N220	L221	F283	L221	F283
L221	K222	R284	K222	R284
K222	G223	C285	G223	C285
G223	K224	T286	K224	T286
K224	L225	S288	L225	S288
L225	N226	S290	N226	S290
N226	G227	T291	G227	T291
G227	I228	D293	I228	D293
I228	A229	S294	A229	S294
A229	L230	S295	L230	S295
L230	R231	M296	R231	M296
R231	V232	M298	V232	M298
V232	P233	V237	P233	V237
P233	T234	S238	T234	S238
T234	R235		R235	
R235	G236		G236	
G236	L237		L237	
L237	S239		S239	
S239	T297		T297	
T297	M298		M298	
M298	V297		V297	
V297				

● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



MET	GLY	V67	I118	V178	V239	M300	E276	M300
ALA	VAL	K58	T119	T179	V240	G301	P277	G301
SER	VAL	T59	P120	G180	D241	D302	L278	D302
ASN	GLU	A60	P121	D181	L242	G304	D282	G304
MET	ALA	S62	G122	Q182	V243	V305	K224	V305
LEU	KO	A63	K122A	R183	V244	K306	L225	K306
SER	L1	I64	G123	L184	Q245	T308	N226	T308
ILE	K2	S65	D124	L186	V246	I308	G227	I308
ILE	V3	V66	I125	A187	S247	W310	T286	W310
ALA	A4	D67	T126	S188	K248	Y311	S294	Y311
PRO	I5	G68	P127	H189	T250	D312	T291	D312
SER	N6	G69	Y128	R191	F251	M313	D293	M313
LEU	G7	V70	V129	D192	A252	E314	S295	E314
ARG	F8	I71		L193	E253	G316	S295	G316
VAL	G9	K72	V132	R194	E254	S318	L296	S318
TYR	R10	W73	M133	R195	E254	R320	M298	R320
ASN	I11	V74	H139	R195	V255	V322	M298	V322
ASN	E134	W75	E135	A196	N256	D323	M298	D323
LYS	G12	S75	G136	R197	A257	L324	M298	L324
GLY	R13	D76	G137	A198	A258	A325	M298	A325
PHE	M14	R77	Y137	A199	F259	D326	M298	D326
SER	R15	K78	T138	A199	R260	V328	M298	V328
GLU	TYR	N78	H139	C200	E261	K331	M298	K331
GLU	ASN	F79	A140	L201	S262	Q333	M298	Q333
PHE	ASN	W80	D141	N202	S262	X334	M298	X334
GLY	LYS	N81	T142	I203	A263		M298	
SER	GLY	L82	I143	V204	D264		M298	
LEU	LEU	P83	I144	P205	N265		M298	
HIS	HIS	W84	T145	T206	E266		M298	
THR	THR	G85	N146	S207	K268		M298	
SER	SER	D86	A147	T208	L267		M298	
SER	SER	G87	S148	G209	G269		M298	
LEU	LEU	M87	C149	A210	I270		M298	
PRO	PRO	G88	C149	A210	L271		M298	
PHE	PHE	I89	T150	A211	S272		M298	
PHE	PHE	D90	T151	K212	S272		M298	
GLY	GLY	L91	M152	A213	V273		M298	
ARG	ARG	V92	C153	V214	V273		M298	
LYS	LYS	I93	L154	A215	P277		M298	
GLY	GLY	E94	A155	L216	L278		M298	
SER	SER	G95	F156	V217	V279		M298	
ASP	ASP	T96	F157	L218	L278		M298	
LEU	LEU	G97	V158	L218	V279		M298	
MET	MET	V98	K159	P219	S280		M298	
ALA	ALA	F99	V160	N220	L281		M298	
PHE	PHE	V100	L161	L221	D282		M298	
VAL	VAL	D101	D162	K222	F283		M298	
SER	SER	R102	Q163	G223	R284		M298	
PHE	PHE	D103	K164	K224	C285		M298	
GLN	GLN	G104	F165	L225	T286		M298	
THR	THR	A105	G166	N226	D287		M298	
ASN	ASN	G106	I167	G227	V288		M298	
ALA	ALA	K107	I168	I228	S288		M298	
VAL	VAL	H108	I168	A229	S290		M298	
GLY	GLY	I49	G170	L230	T291		M298	
GLY	GLY	L109	T171	R231	I292		M298	
LYS	LYS	Q110	M172	V232	D293		M298	
ARG	ARG	A111	T173	P233	S294		M298	
SER	SER	K114	T174	T234	S295		M298	
GLN	GLN	K115	T175	P235	L296		M298	
ASN	ASN	V116	H176	M236	T297		M298	
		L117	S177	V237	M298		M298	
				S238	V299		M298	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	363.0, 363.0, 363.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.21, 1.21, 1.21	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2739	0.56	2/3726 (0.1%)
1	C	0.44	0/2739	0.56	2/3726 (0.1%)
1	E	0.43	0/2739	0.58	2/3726 (0.1%)
1	G	0.44	0/2739	0.56	2/3726 (0.1%)
1	I	0.42	0/2739	0.57	2/3726 (0.1%)
1	K	0.43	0/2739	0.58	2/3726 (0.1%)
1	O	0.42	0/2739	0.56	2/3726 (0.1%)
1	Q	0.44	0/2739	0.55	2/3726 (0.1%)
2	B	0.39	0/2579	0.52	0/3502
2	D	0.39	0/2579	0.53	0/3502
2	F	0.38	0/2579	0.52	0/3502
2	H	0.40	0/2579	0.53	0/3502
2	J	0.39	0/2579	0.52	0/3502
2	L	0.39	0/2579	0.53	0/3502
2	P	0.38	0/2579	0.52	0/3502
2	R	0.40	0/2579	0.54	0/3502
All	All	0.41	0/42544	0.55	16/57824 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	344	PRO	N-CA-CB	7.13	111.86	103.30
1	A	344	PRO	N-CA-CB	6.72	111.36	103.30
1	I	344	PRO	N-CA-CB	6.70	111.34	103.30
1	K	353	PRO	N-CA-CB	6.26	110.81	103.30
1	E	344	PRO	N-CA-CB	6.10	110.62	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	248	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2694	0	2681	479	0
1	C	2694	0	2681	536	0
1	E	2694	0	2681	515	0
1	G	2694	0	2681	547	0
1	I	2694	0	2681	461	0
1	K	2694	0	2681	479	0
1	O	2694	0	2681	565	0
1	Q	2694	0	2681	476	0
2	B	2544	0	2577	492	0
2	D	2544	0	2577	459	0
2	F	2544	0	2577	504	0
2	H	2544	0	2577	485	0
2	J	2544	0	2577	494	0
2	L	2544	0	2577	454	0
2	P	2544	0	2577	457	0
2	R	2544	0	2577	477	0
3	A	44	0	26	7	0
3	B	44	0	25	11	0
3	C	44	0	25	12	0
3	D	44	0	25	12	0
3	E	44	0	25	9	0
3	F	44	0	25	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	44	0	25	16	0
3	H	44	0	25	11	0
3	I	44	0	26	9	0
3	J	44	0	26	9	0
3	K	44	0	26	11	0
3	L	44	0	25	10	0
3	O	44	0	26	10	0
3	P	44	0	26	14	0
3	Q	44	0	25	12	0
3	R	44	0	26	13	0
All	All	42608	0	42471	7484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 88.

The worst 5 of 7484 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:VAL:HB	1:O:59:ILE:CG2	1.27	1.55
2:F:10:ARG:NH2	1:G:185:LEU:HD13	1.32	1.42
1:Q:37:VAL:CG1	1:Q:59:ILE:HG23	1.55	1.35
2:F:10:ARG:CZ	1:G:185:LEU:HD13	1.58	1.33
1:E:17:ARG:CD	1:E:44:LEU:HG	1.60	1.32

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	366/451 (81%)	278 (76%)	85 (23%)	3 (1%)	19 60
1	C	366/451 (81%)	262 (72%)	100 (27%)	4 (1%)	14 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	366/451 (81%)	286 (78%)	71 (19%)	9 (2%)	5	32
1	G	366/451 (81%)	257 (70%)	104 (28%)	5 (1%)	11	46
1	I	366/451 (81%)	268 (73%)	94 (26%)	4 (1%)	14	51
1	K	366/451 (81%)	264 (72%)	100 (27%)	2 (0%)	29	69
1	O	366/451 (81%)	265 (72%)	94 (26%)	7 (2%)	8	38
1	Q	366/451 (81%)	273 (75%)	87 (24%)	6 (2%)	9	43
2	B	335/402 (83%)	263 (78%)	72 (22%)	0	100	100
2	D	335/402 (83%)	254 (76%)	80 (24%)	1 (0%)	41	76
2	F	335/402 (83%)	251 (75%)	82 (24%)	2 (1%)	25	65
2	H	335/402 (83%)	259 (77%)	76 (23%)	0	100	100
2	J	335/402 (83%)	263 (78%)	72 (22%)	0	100	100
2	L	335/402 (83%)	256 (76%)	78 (23%)	1 (0%)	41	76
2	P	335/402 (83%)	248 (74%)	86 (26%)	1 (0%)	41	76
2	R	335/402 (83%)	257 (77%)	77 (23%)	1 (0%)	41	76
All	All	5608/6824 (82%)	4204 (75%)	1358 (24%)	46 (1%)	24	60

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	18(A)	TRP
1	O	61	ASN
1	Q	60	ILE
1	Q	352	ASN
1	A	352	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/370 (76%)	228 (81%)	54 (19%)	1	8
1	C	282/370 (76%)	210 (74%)	72 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	282/370 (76%)	212 (75%)	70 (25%)	0	4
1	G	282/370 (76%)	219 (78%)	63 (22%)	1	6
1	I	282/370 (76%)	224 (79%)	58 (21%)	1	7
1	K	282/370 (76%)	222 (79%)	60 (21%)	1	6
1	O	282/370 (76%)	211 (75%)	71 (25%)	0	3
1	Q	282/370 (76%)	226 (80%)	56 (20%)	1	8
2	B	279/332 (84%)	217 (78%)	62 (22%)	1	6
2	D	279/332 (84%)	223 (80%)	56 (20%)	1	7
2	F	279/332 (84%)	222 (80%)	57 (20%)	1	7
2	H	279/332 (84%)	218 (78%)	61 (22%)	1	6
2	J	279/332 (84%)	221 (79%)	58 (21%)	1	7
2	L	279/332 (84%)	218 (78%)	61 (22%)	1	6
2	P	279/332 (84%)	220 (79%)	59 (21%)	1	6
2	R	279/332 (84%)	214 (77%)	65 (23%)	1	4
All	All	4488/5616 (80%)	3505 (78%)	983 (22%)	3	6

5 of 983 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	151	THR
1	K	119	THR
2	F	53	PHE
1	K	73	VAL
2	L	144	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	108	HIS
1	I	14	ASN
2	F	190	HIS
1	G	18(B)	HIS
1	I	226	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	P	401	-	42,48,48	0.64	1 (2%)	50,73,73	0.75	2 (4%)
3	NAD	J	401	-	42,48,48	0.63	1 (2%)	50,73,73	0.78	3 (6%)
3	NAD	R	401	-	42,48,48	0.64	1 (2%)	50,73,73	0.83	4 (8%)
3	NAD	O	401	-	42,48,48	0.67	1 (2%)	50,73,73	0.69	2 (4%)
3	NAD	C	401	-	42,48,48	3.82	15 (35%)	50,73,73	2.33	10 (20%)
3	NAD	E	401	-	42,48,48	3.80	16 (38%)	50,73,73	2.34	10 (20%)
3	NAD	B	401	-	42,48,48	3.85	18 (42%)	50,73,73	2.29	9 (18%)
3	NAD	G	401	-	42,48,48	3.85	17 (40%)	50,73,73	2.15	7 (14%)
3	NAD	Q	401	-	42,48,48	3.84	17 (40%)	50,73,73	2.31	9 (18%)
3	NAD	H	401	-	42,48,48	3.84	17 (40%)	50,73,73	2.24	7 (14%)
3	NAD	I	401	-	42,48,48	0.65	1 (2%)	50,73,73	0.75	2 (4%)
3	NAD	K	401	-	42,48,48	0.67	1 (2%)	50,73,73	0.92	4 (8%)
3	NAD	D	401	-	42,48,48	3.88	18 (42%)	50,73,73	2.28	8 (16%)
3	NAD	F	401	-	42,48,48	3.86	18 (42%)	50,73,73	2.28	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	L	401	-	42,48,48	3.88	19 (45%)	50,73,73	2.28	7 (14%)
3	NAD	A	401	-	42,48,48	0.65	0	50,73,73	0.81	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	P	401	-	-	14/26/62/62	0/5/5/5
3	NAD	J	401	-	-	9/26/62/62	0/5/5/5
3	NAD	R	401	-	-	15/26/62/62	0/5/5/5
3	NAD	O	401	-	-	15/26/62/62	0/5/5/5
3	NAD	C	401	-	-	11/26/62/62	0/5/5/5
3	NAD	E	401	-	-	10/26/62/62	0/5/5/5
3	NAD	B	401	-	-	12/26/62/62	0/5/5/5
3	NAD	G	401	-	-	12/26/62/62	0/5/5/5
3	NAD	Q	401	-	-	9/26/62/62	0/5/5/5
3	NAD	H	401	-	-	13/26/62/62	0/5/5/5
3	NAD	I	401	-	-	13/26/62/62	0/5/5/5
3	NAD	K	401	-	-	14/26/62/62	0/5/5/5
3	NAD	D	401	-	-	12/26/62/62	0/5/5/5
3	NAD	F	401	-	-	12/26/62/62	0/5/5/5
3	NAD	L	401	-	-	12/26/62/62	0/5/5/5
3	NAD	A	401	-	-	15/26/62/62	0/5/5/5

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAD	O4D-C1D	-10.40	1.26	1.41
3	L	401	NAD	O4D-C1D	-10.39	1.26	1.41
3	B	401	NAD	O4D-C1D	-10.20	1.26	1.41
3	F	401	NAD	O4D-C1D	-10.19	1.26	1.41
3	H	401	NAD	O4D-C1D	-10.05	1.27	1.41

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAD	C1B-N9A-C4A	-9.63	109.73	126.64
3	E	401	NAD	C1B-N9A-C4A	-9.49	109.96	126.64
3	L	401	NAD	C1B-N9A-C4A	-9.43	110.06	126.64
3	D	401	NAD	C1B-N9A-C4A	-9.43	110.08	126.64
3	H	401	NAD	C1B-N9A-C4A	-9.20	110.47	126.64

There are no chirality outliers.

5 of 198 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	401	NAD	C5B-O5B-PA-O2A
3	O	401	NAD	C5B-O5B-PA-O3
3	O	401	NAD	O4B-C4B-C5B-O5B
3	O	401	NAD	C3B-C4B-C5B-O5B
3	O	401	NAD	C5D-O5D-PN-O3

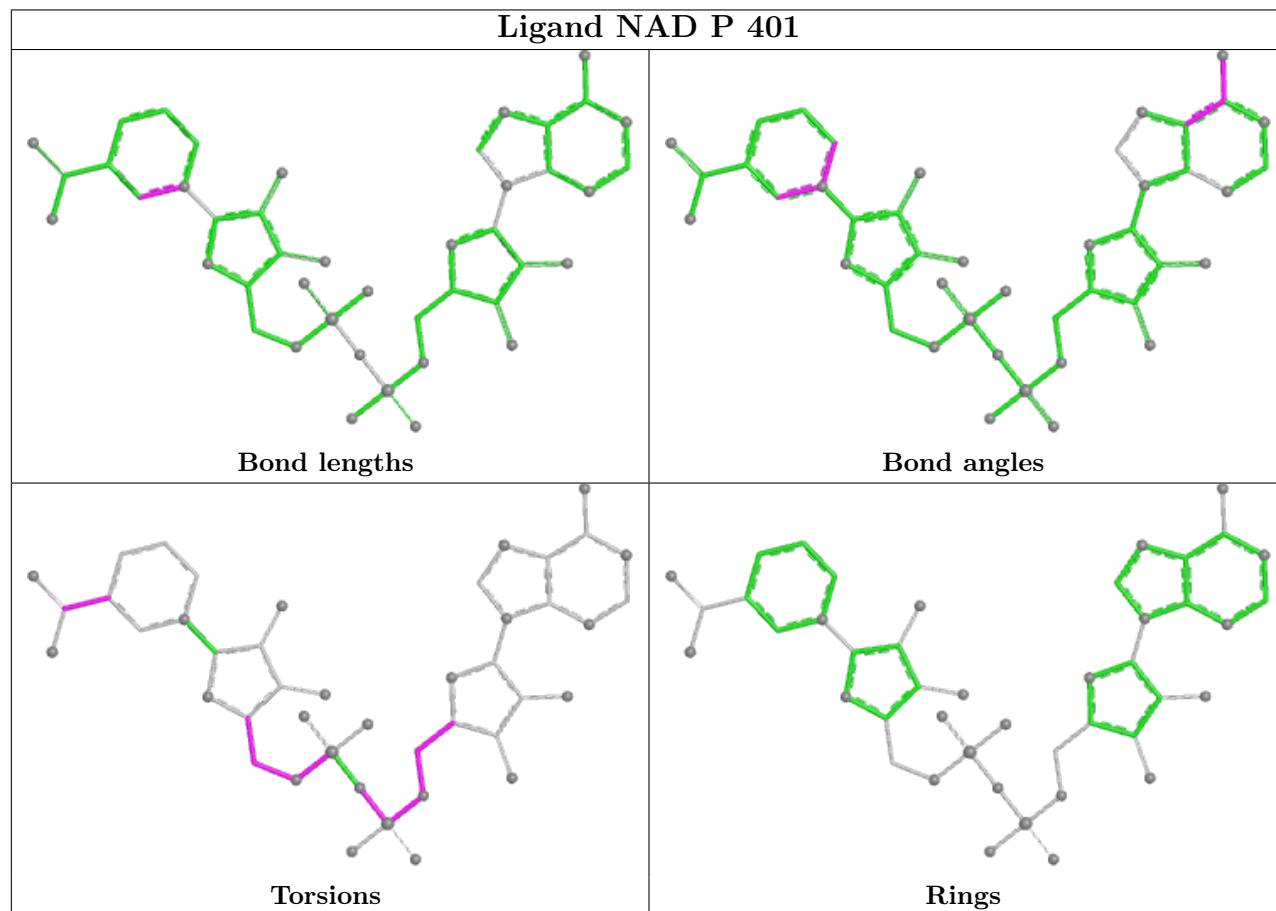
There are no ring outliers.

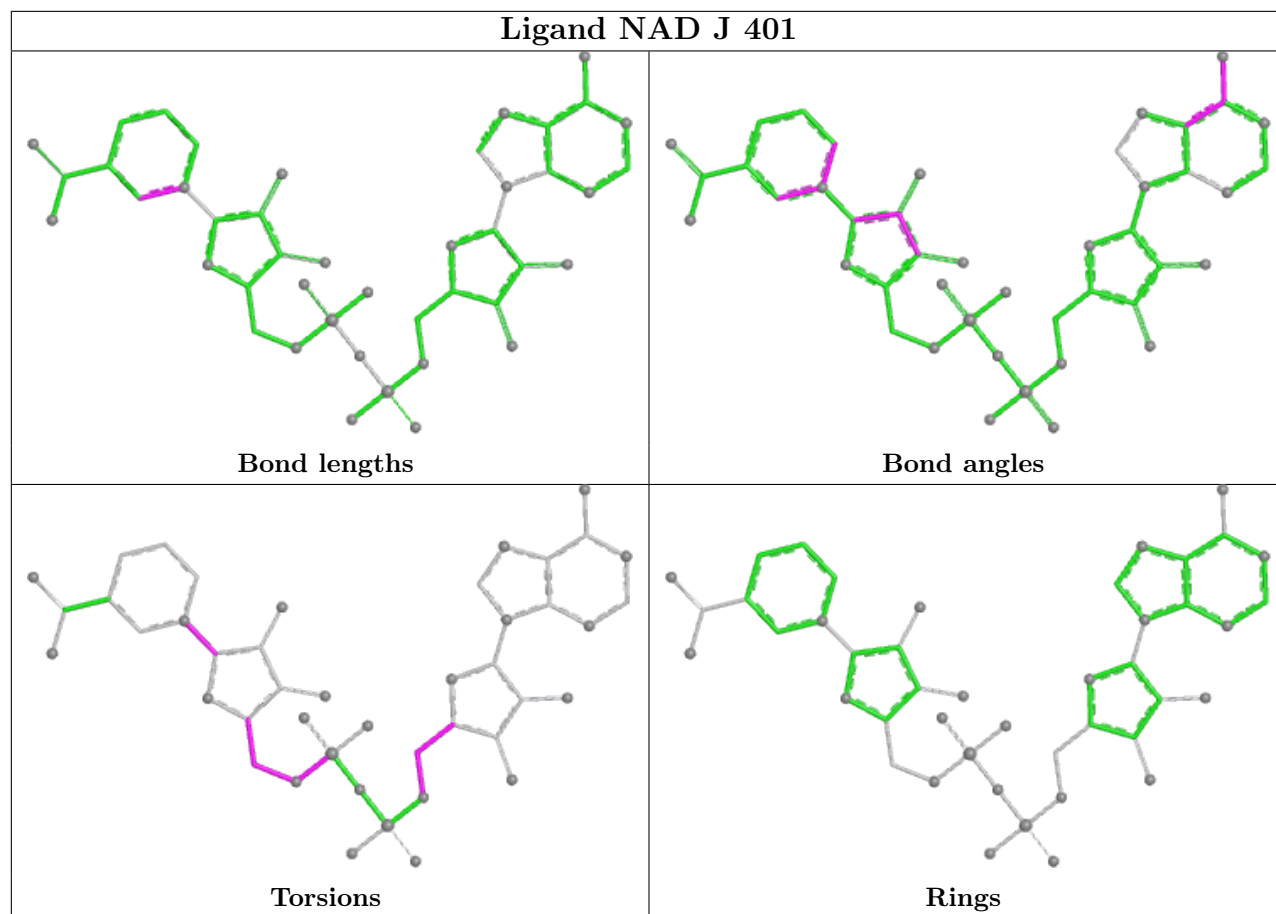
16 monomers are involved in 176 short contacts:

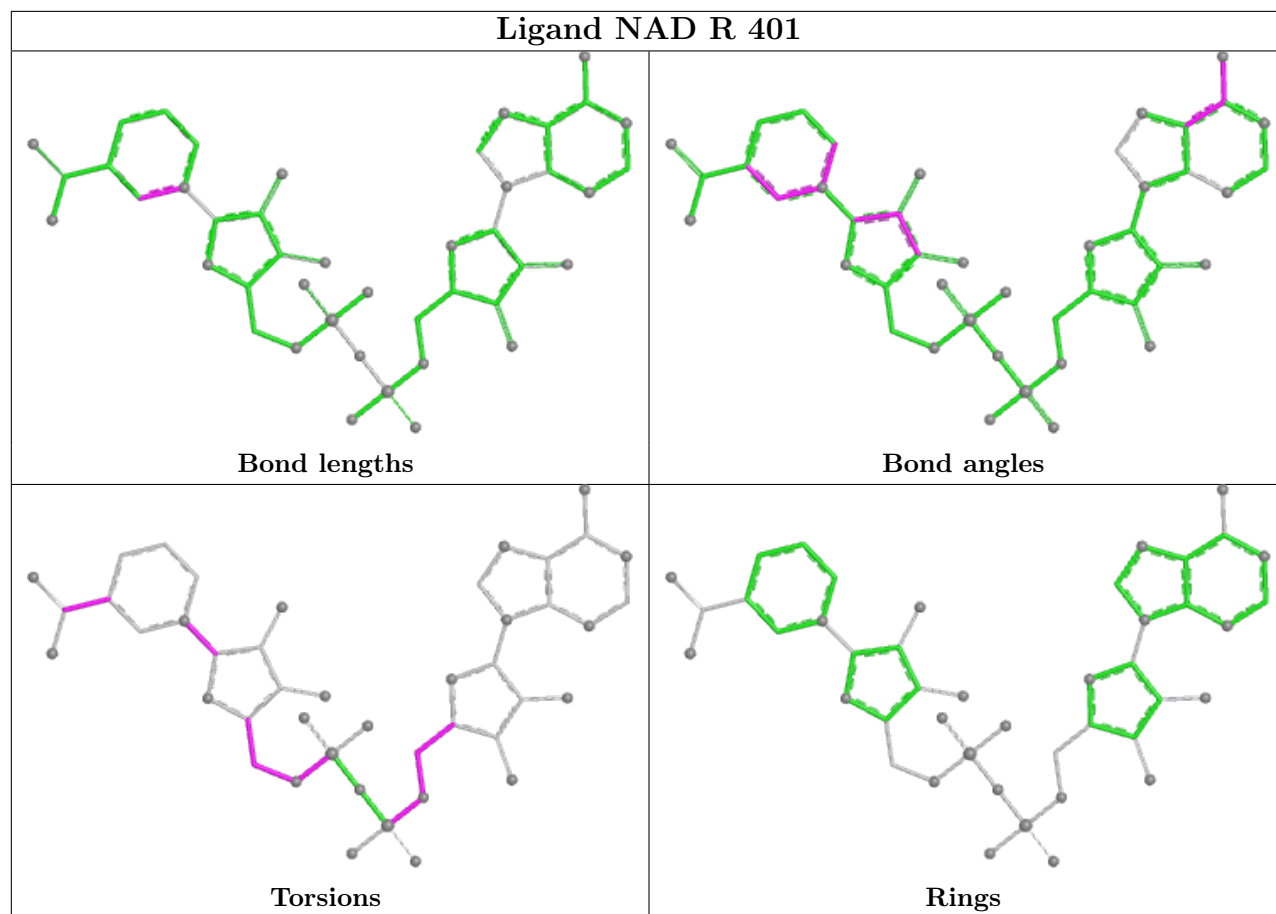
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	401	NAD	14	0
3	J	401	NAD	9	0
3	R	401	NAD	13	0
3	O	401	NAD	10	0
3	C	401	NAD	12	0
3	E	401	NAD	9	0
3	B	401	NAD	11	0
3	G	401	NAD	16	0
3	Q	401	NAD	12	0
3	H	401	NAD	11	0
3	I	401	NAD	9	0
3	K	401	NAD	11	0
3	D	401	NAD	12	0
3	F	401	NAD	10	0
3	L	401	NAD	10	0
3	A	401	NAD	7	0

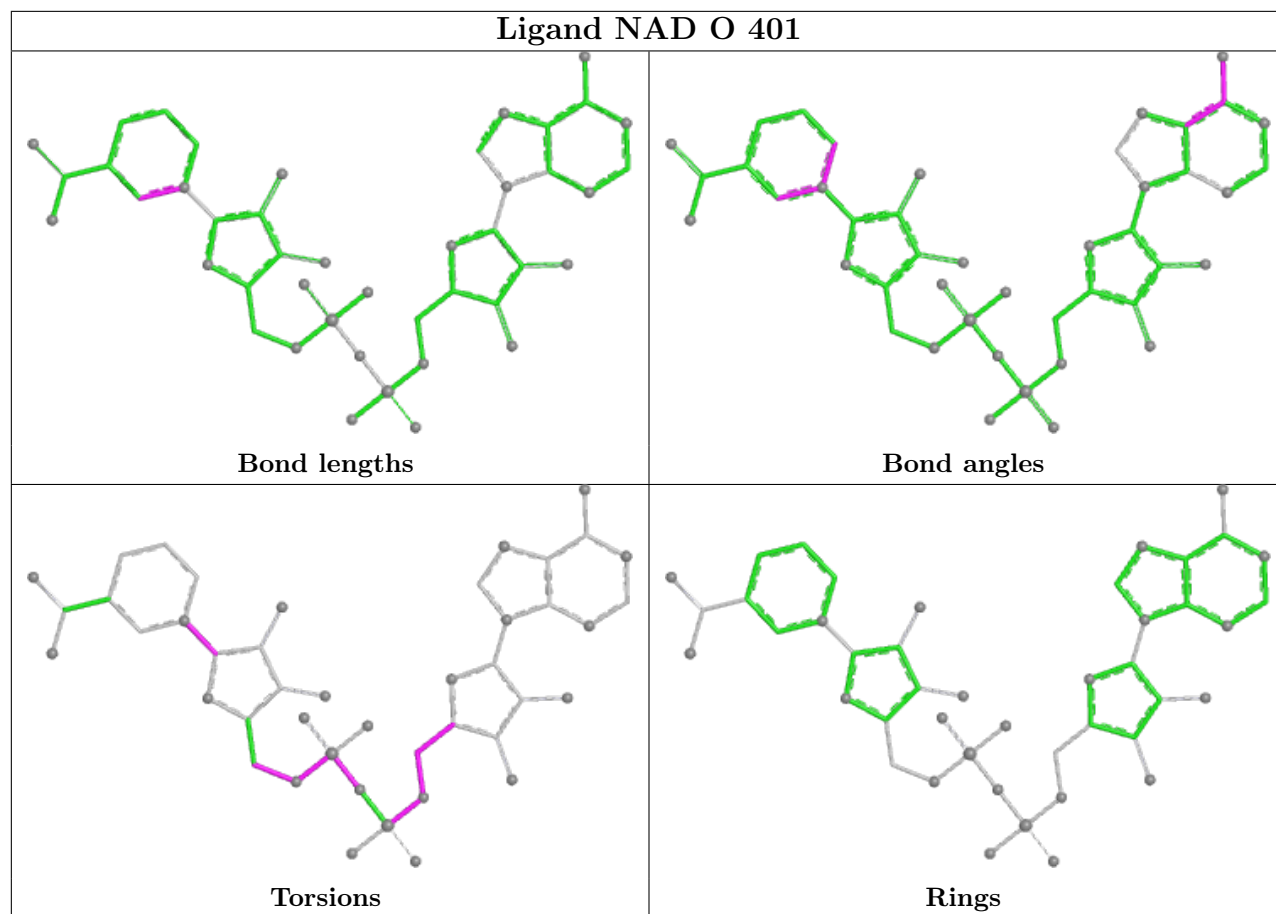
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

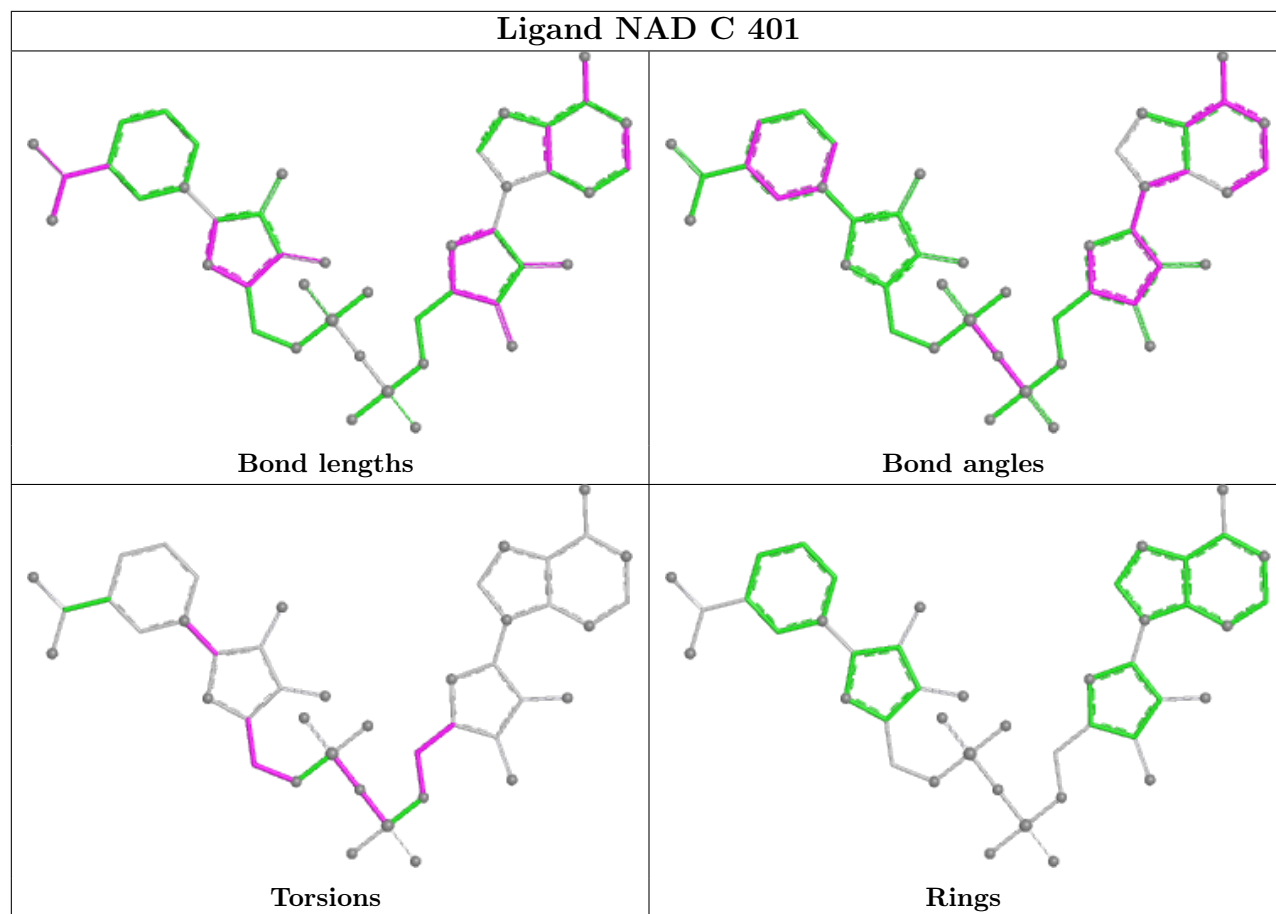
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

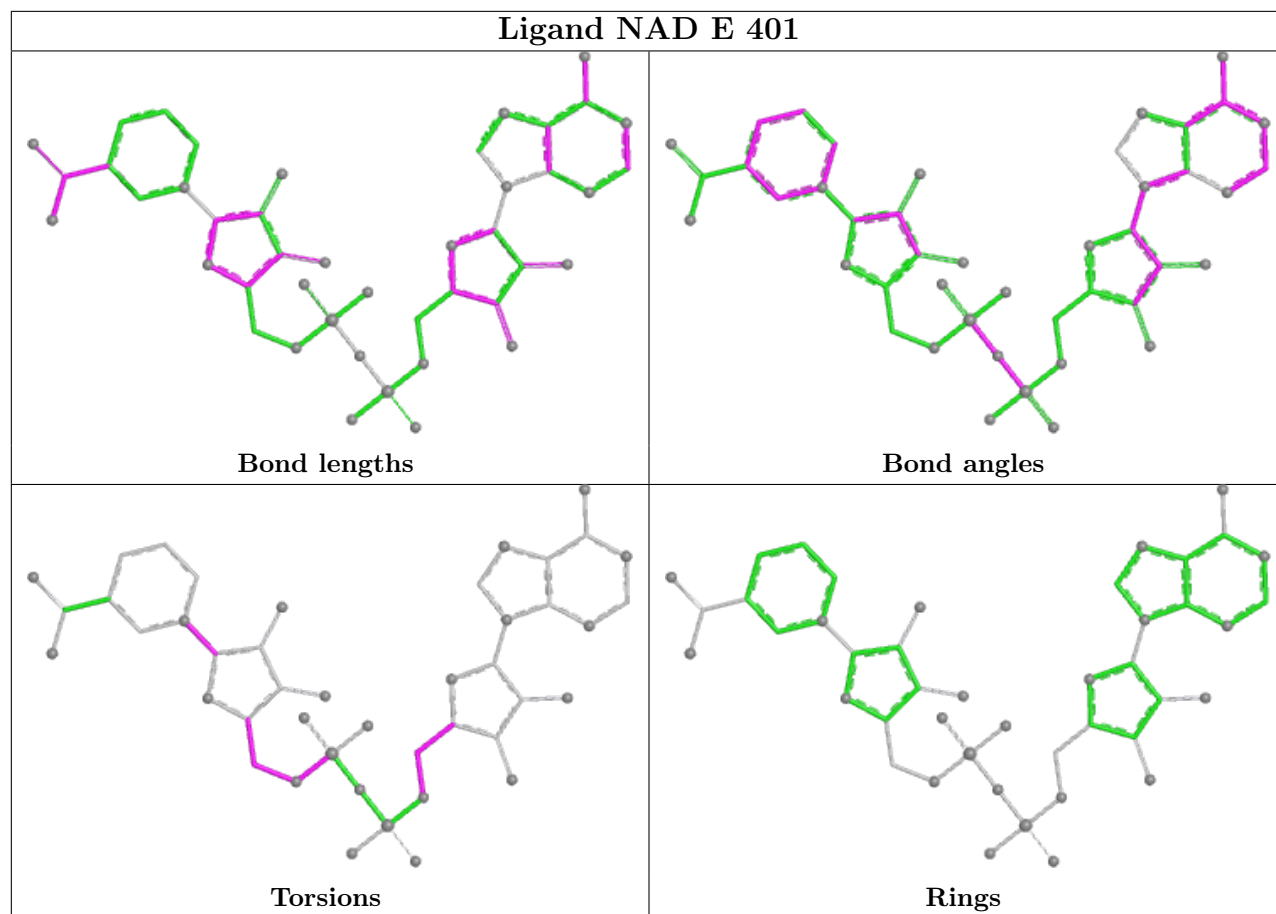


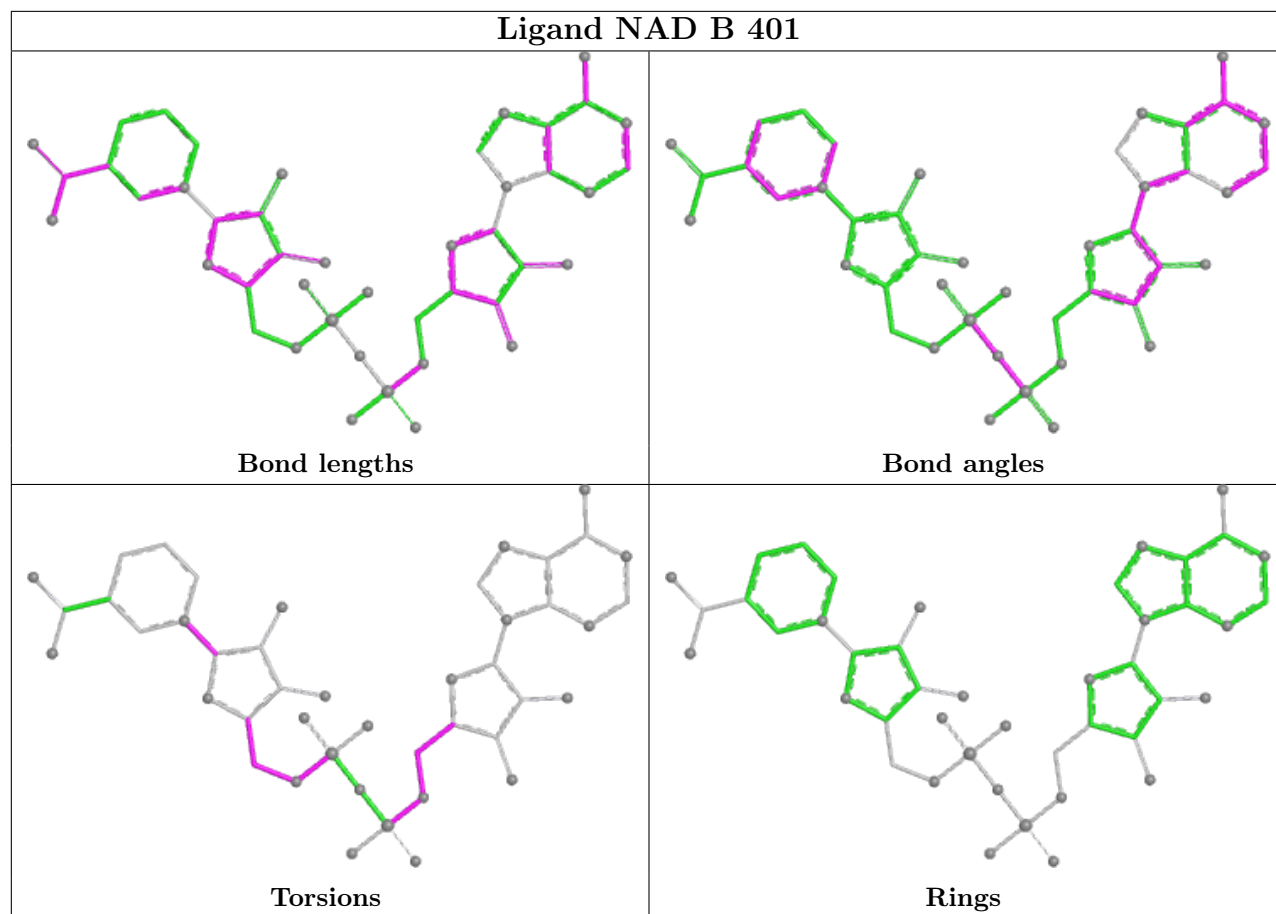


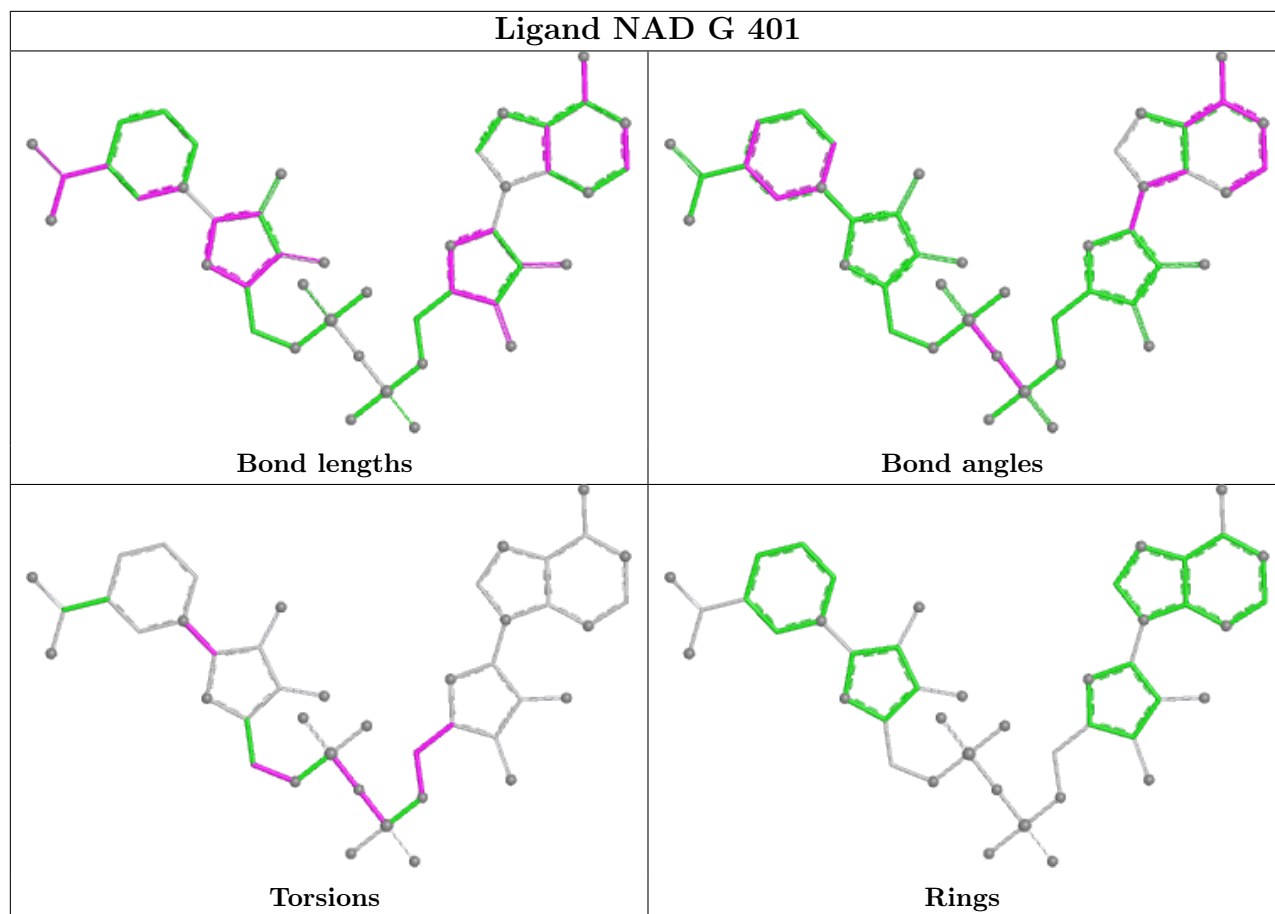


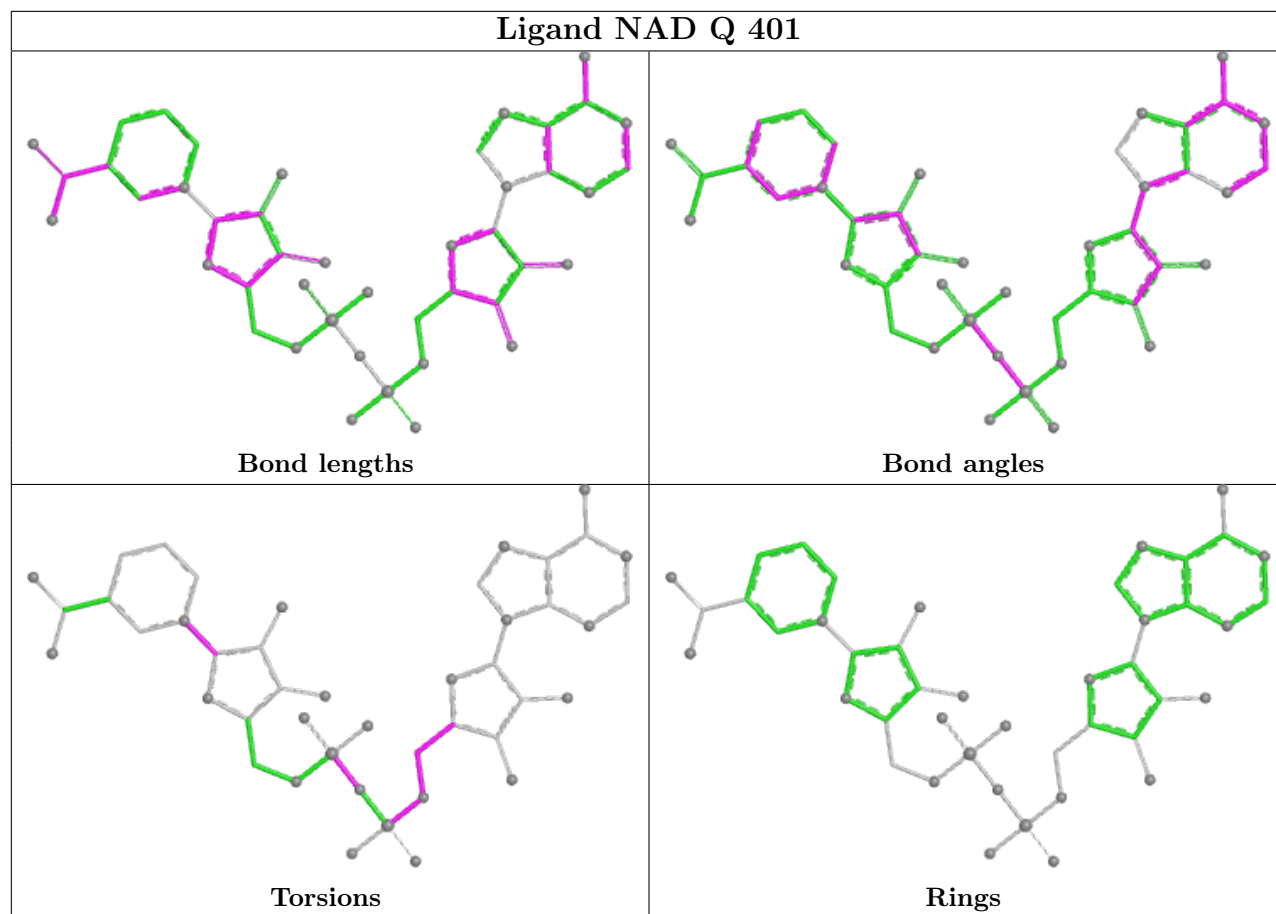


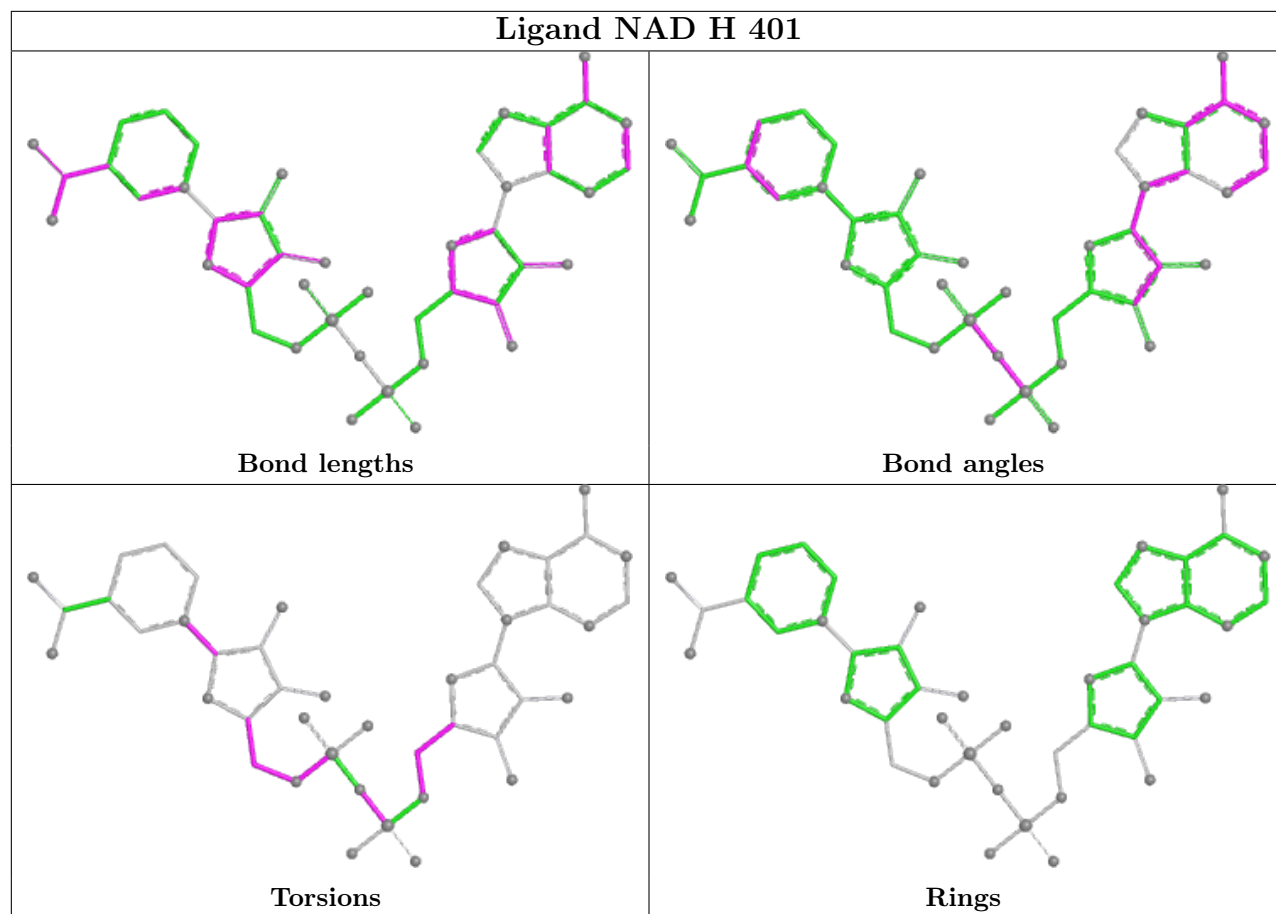


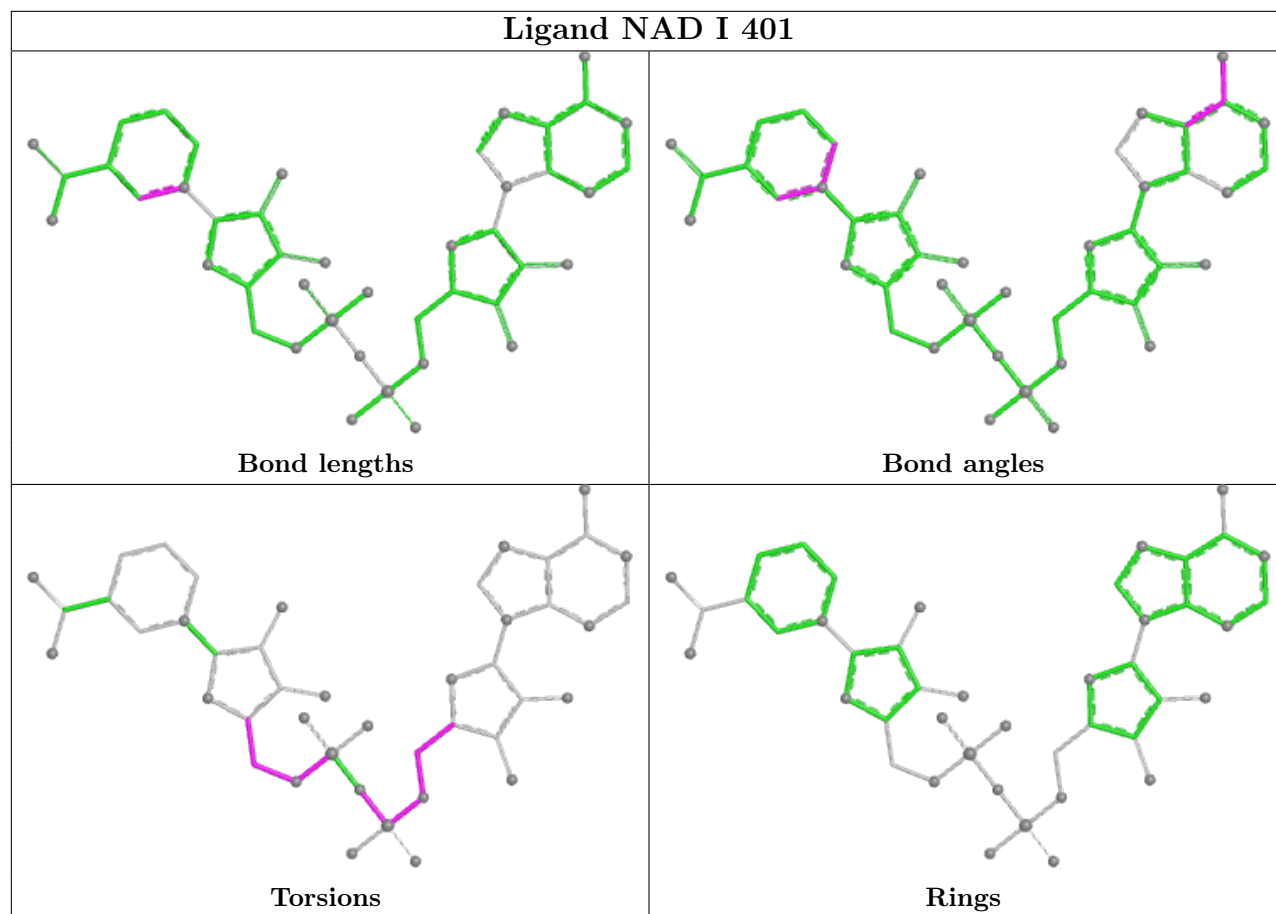


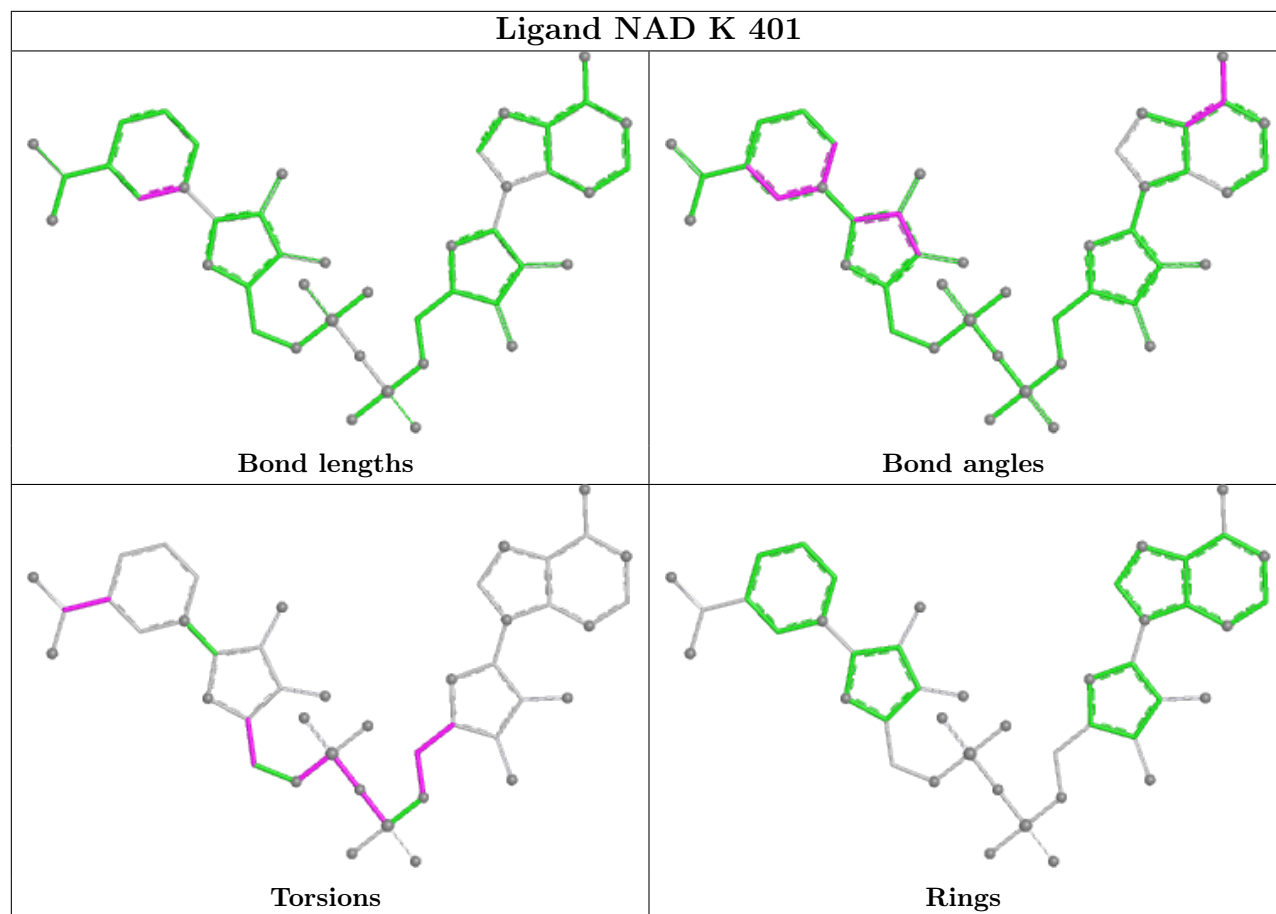


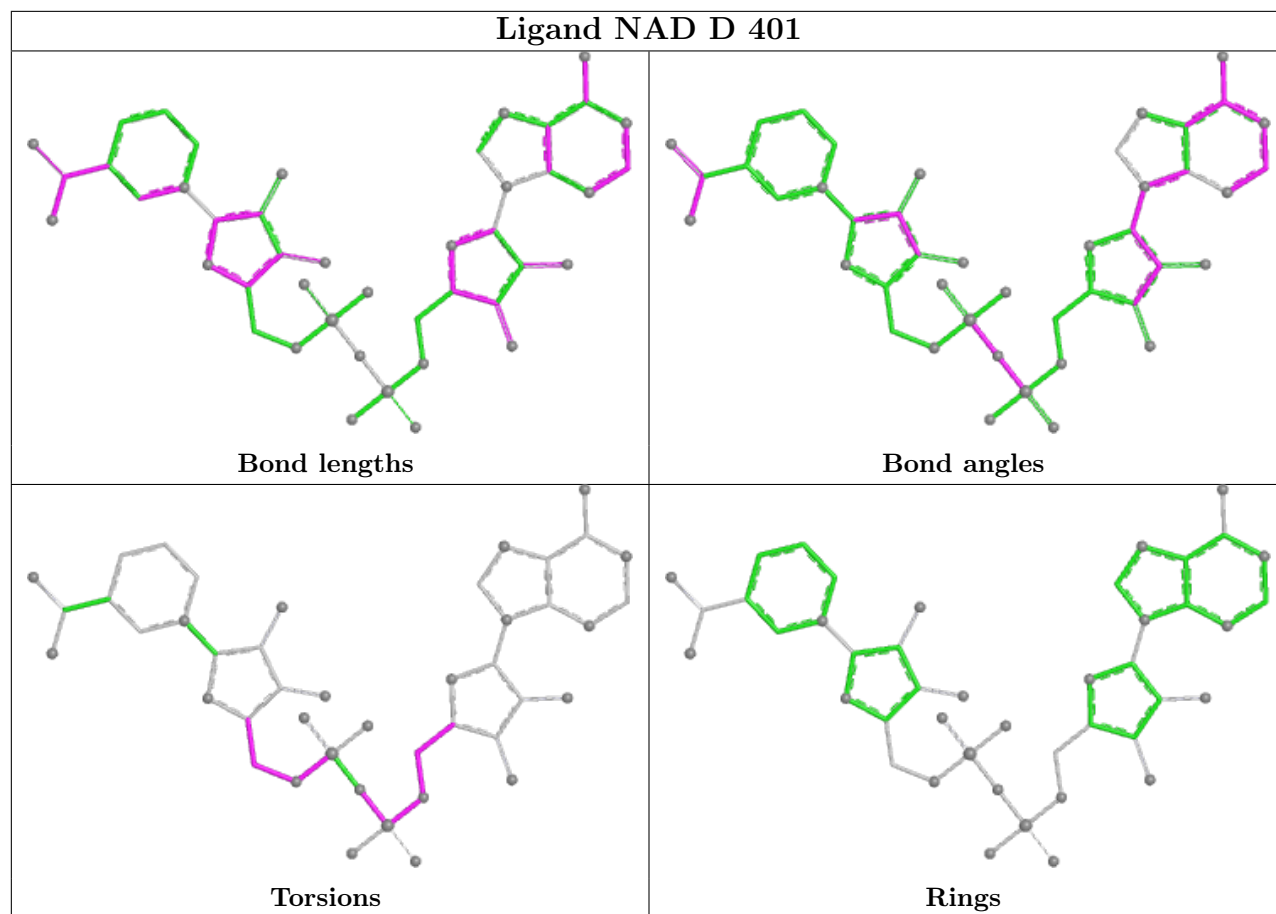


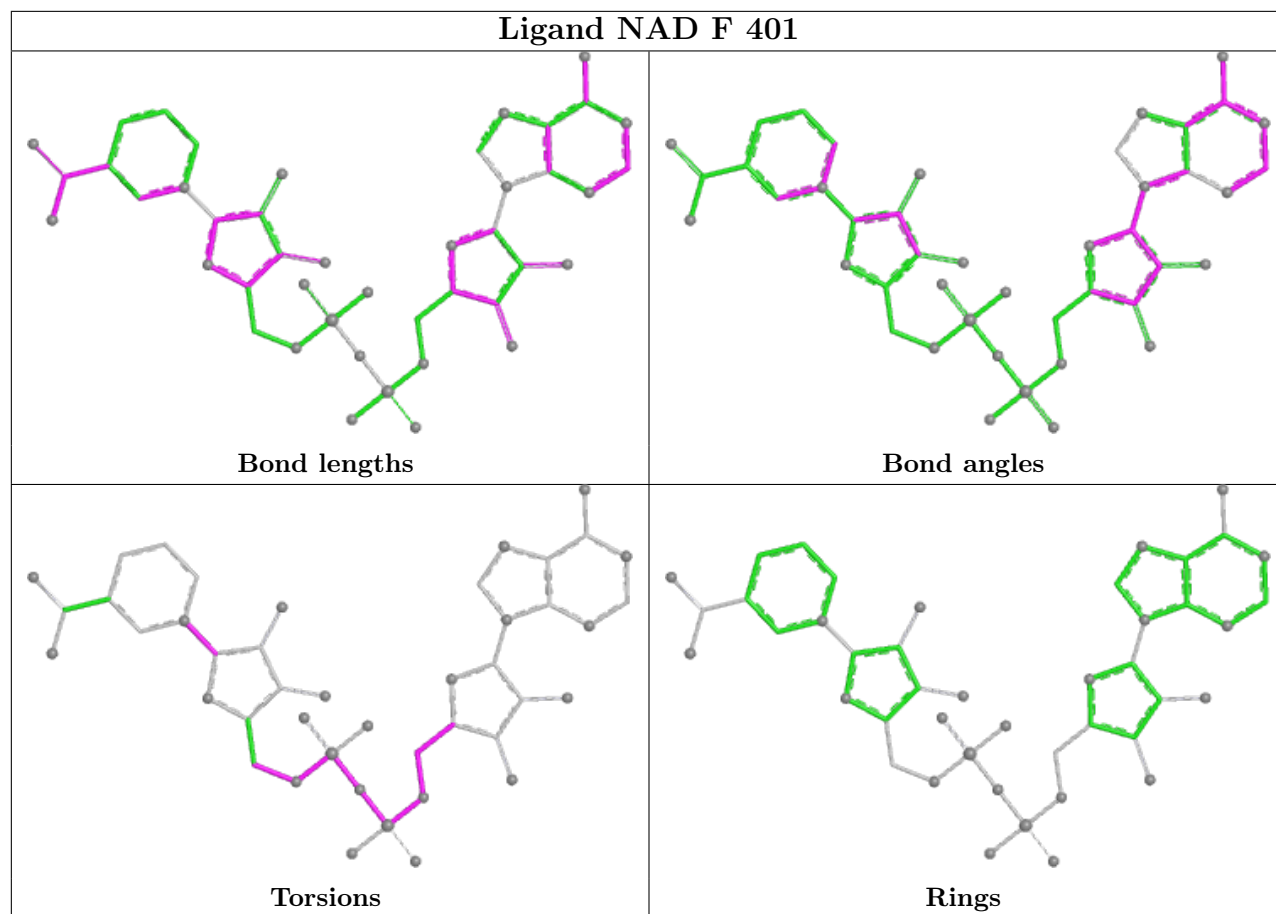


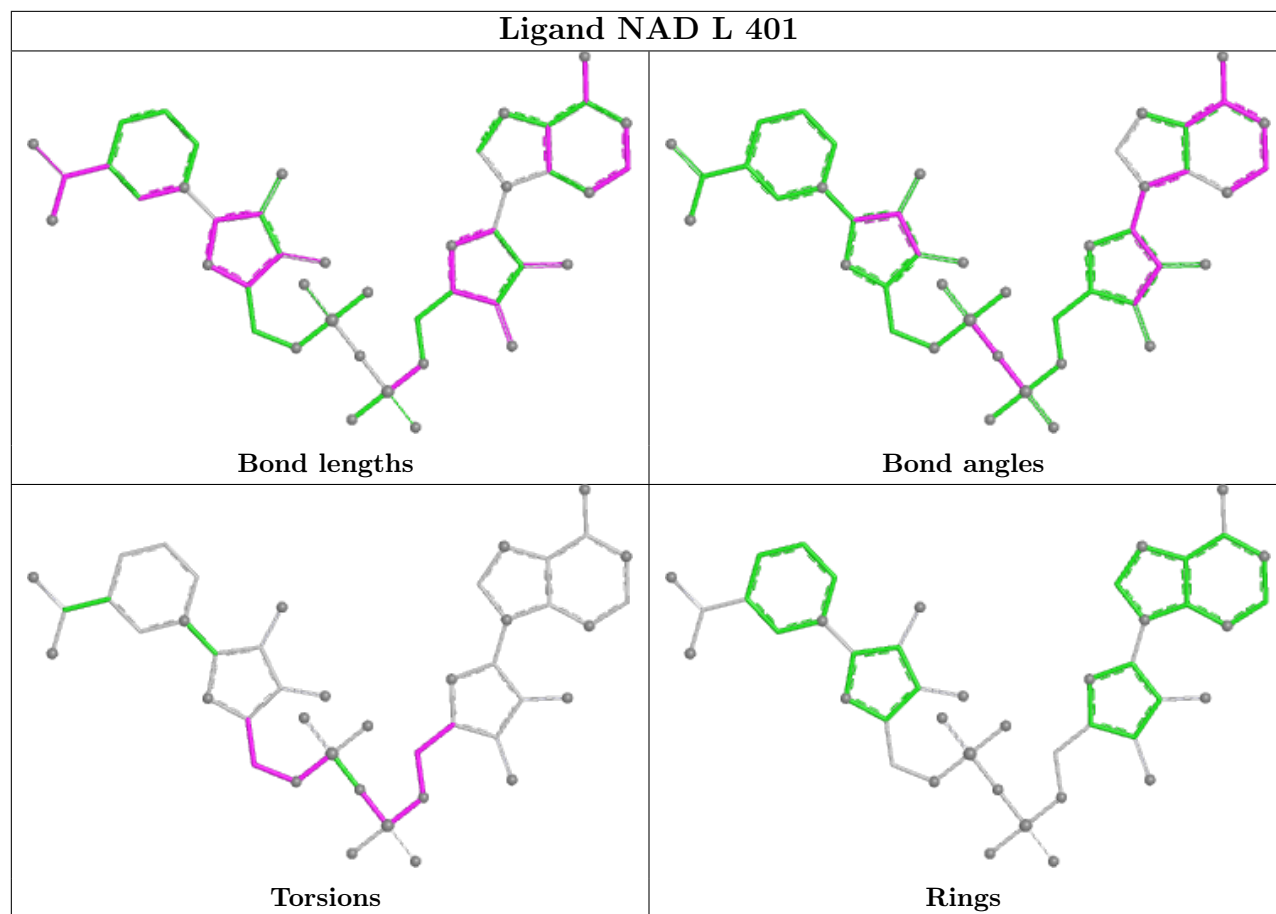


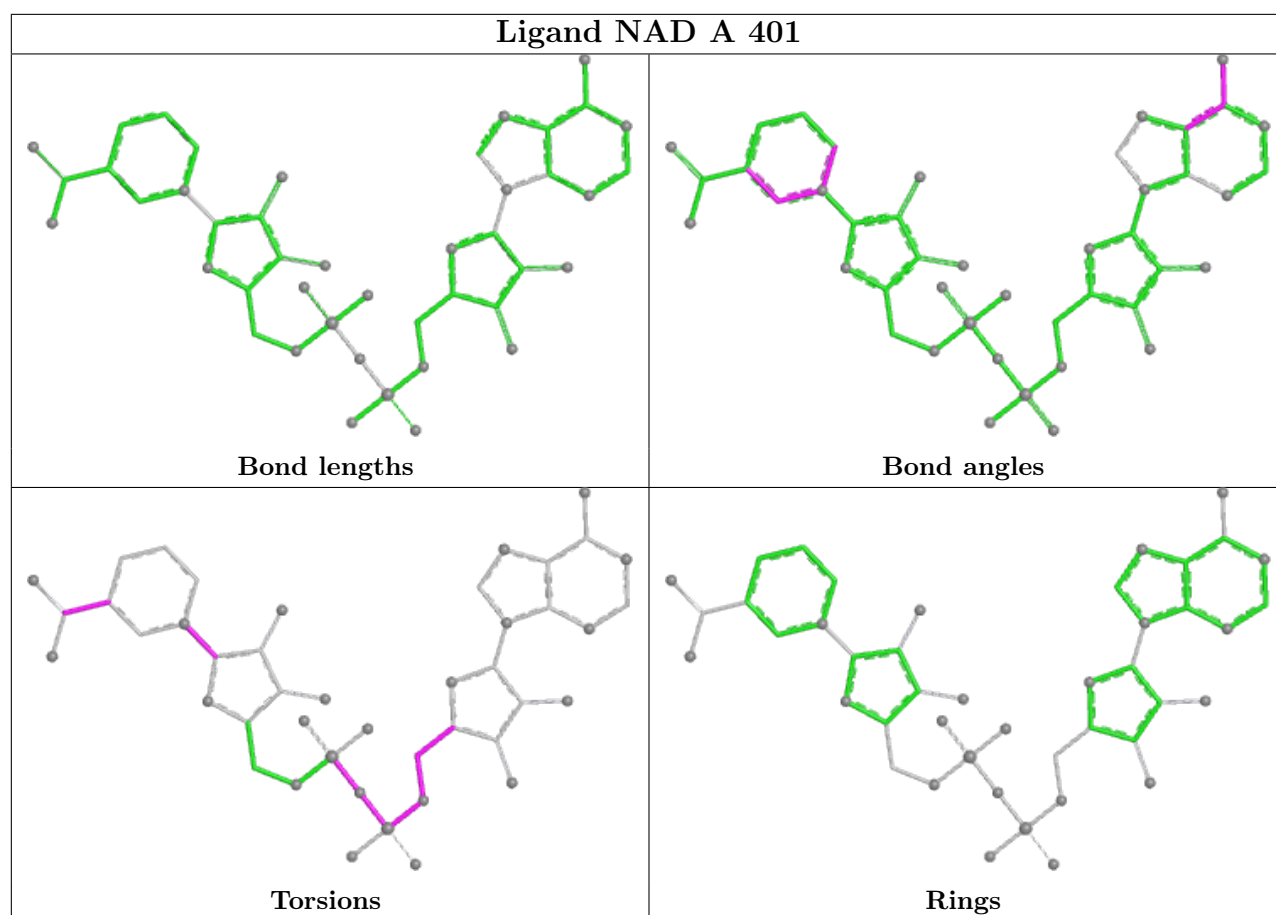












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

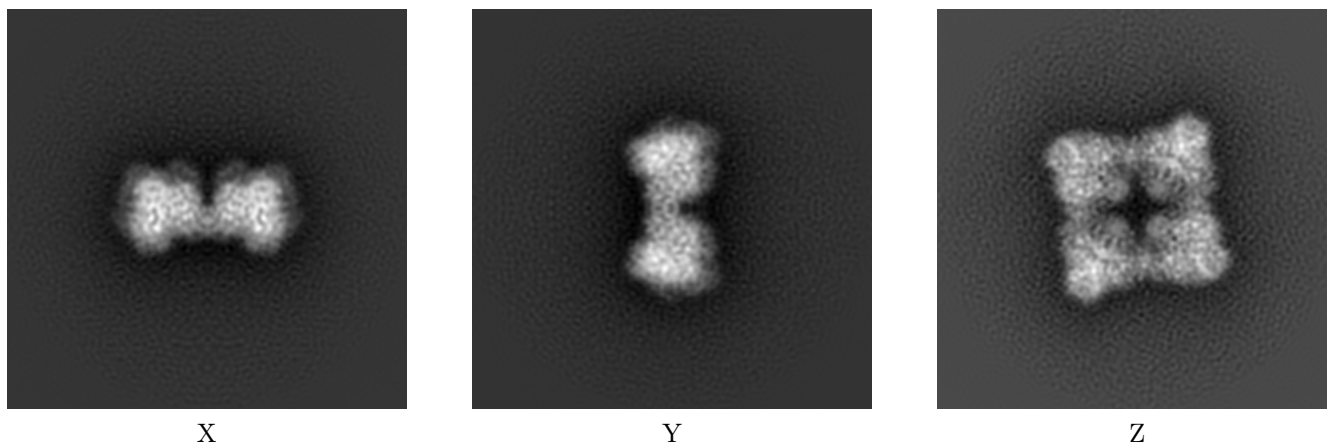
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13826. These allow visual inspection of the internal detail of the map and identification of artifacts.

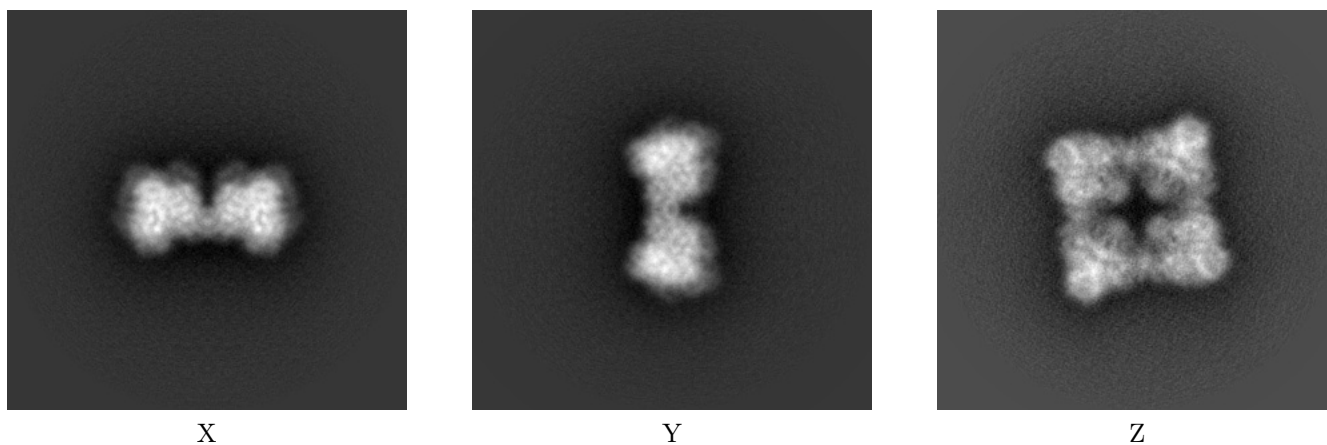
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



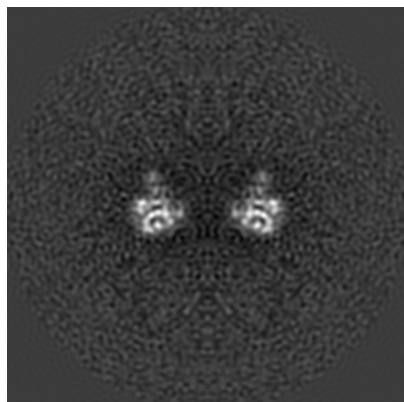
6.1.2 Raw map



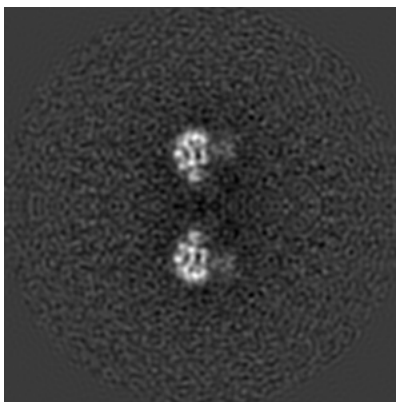
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

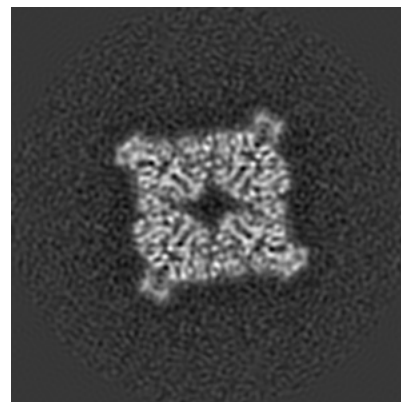
6.2.1 Primary map



X Index: 150

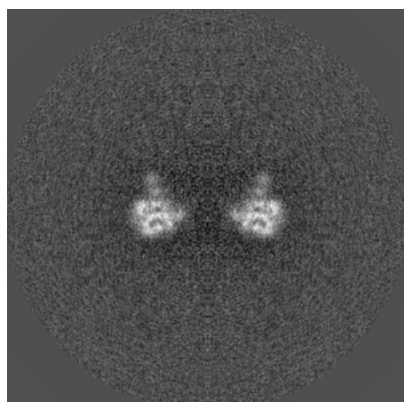


Y Index: 150

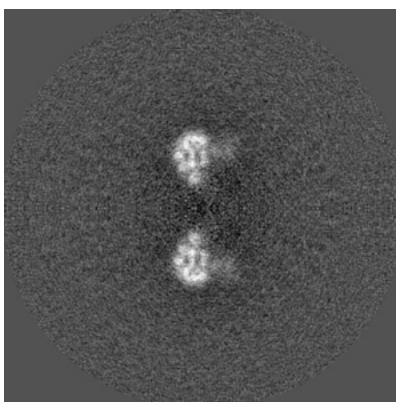


Z Index: 150

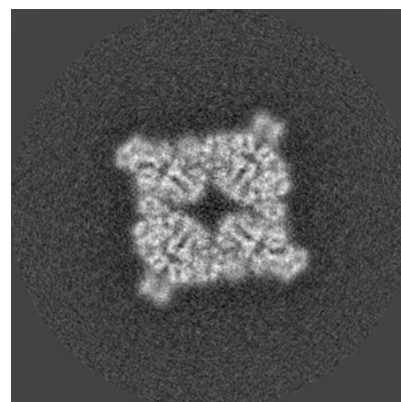
6.2.2 Raw map



X Index: 150



Y Index: 150

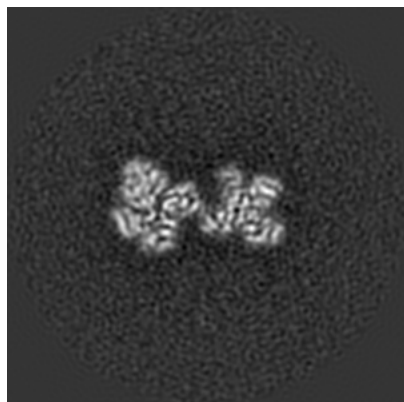


Z Index: 150

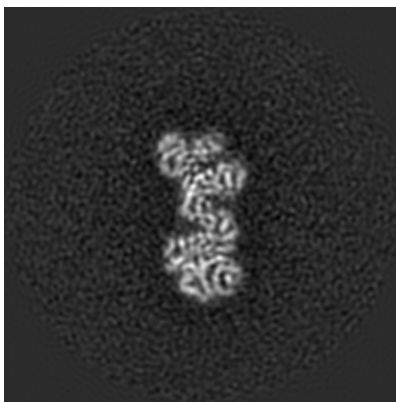
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

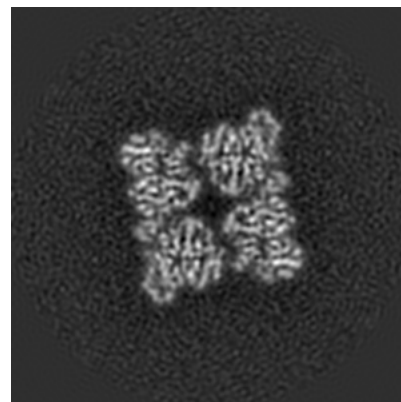
6.3.1 Primary map



X Index: 119

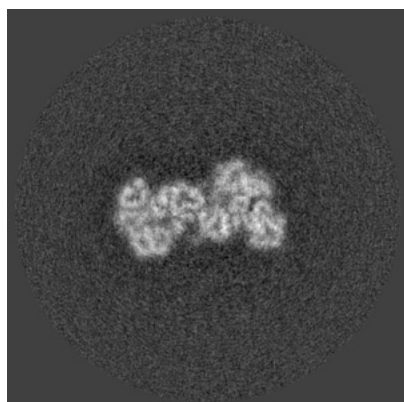


Y Index: 186

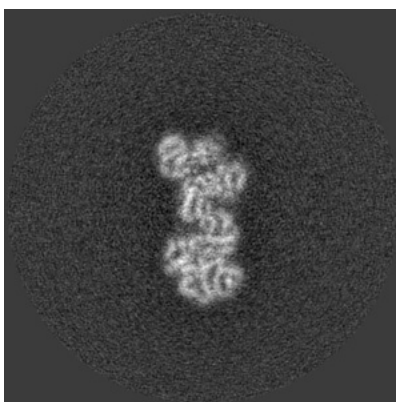


Z Index: 143

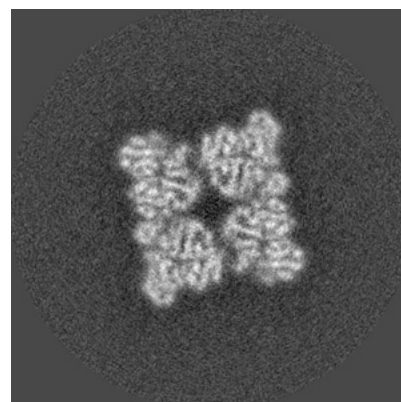
6.3.2 Raw map



X Index: 105



Y Index: 187

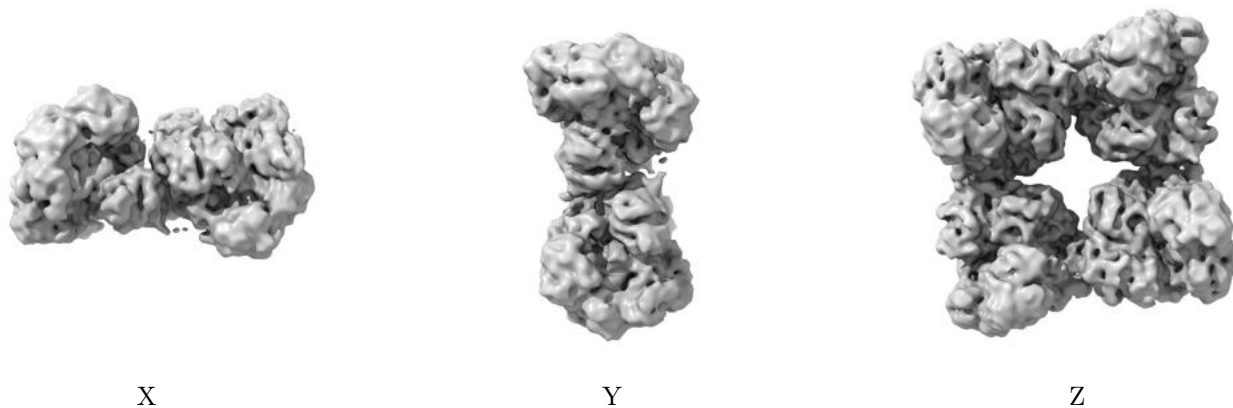


Z Index: 144

The images above show the largest variance slices of the map in three orthogonal directions.

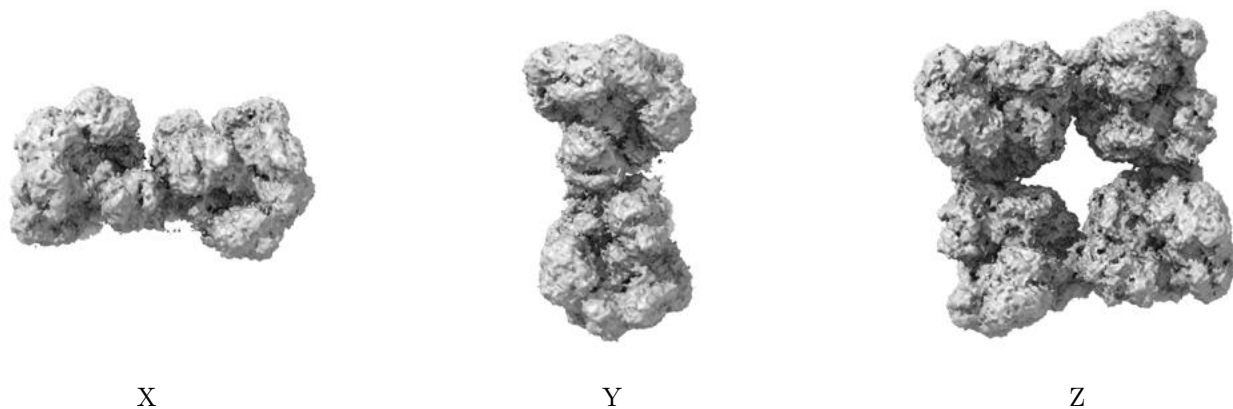
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

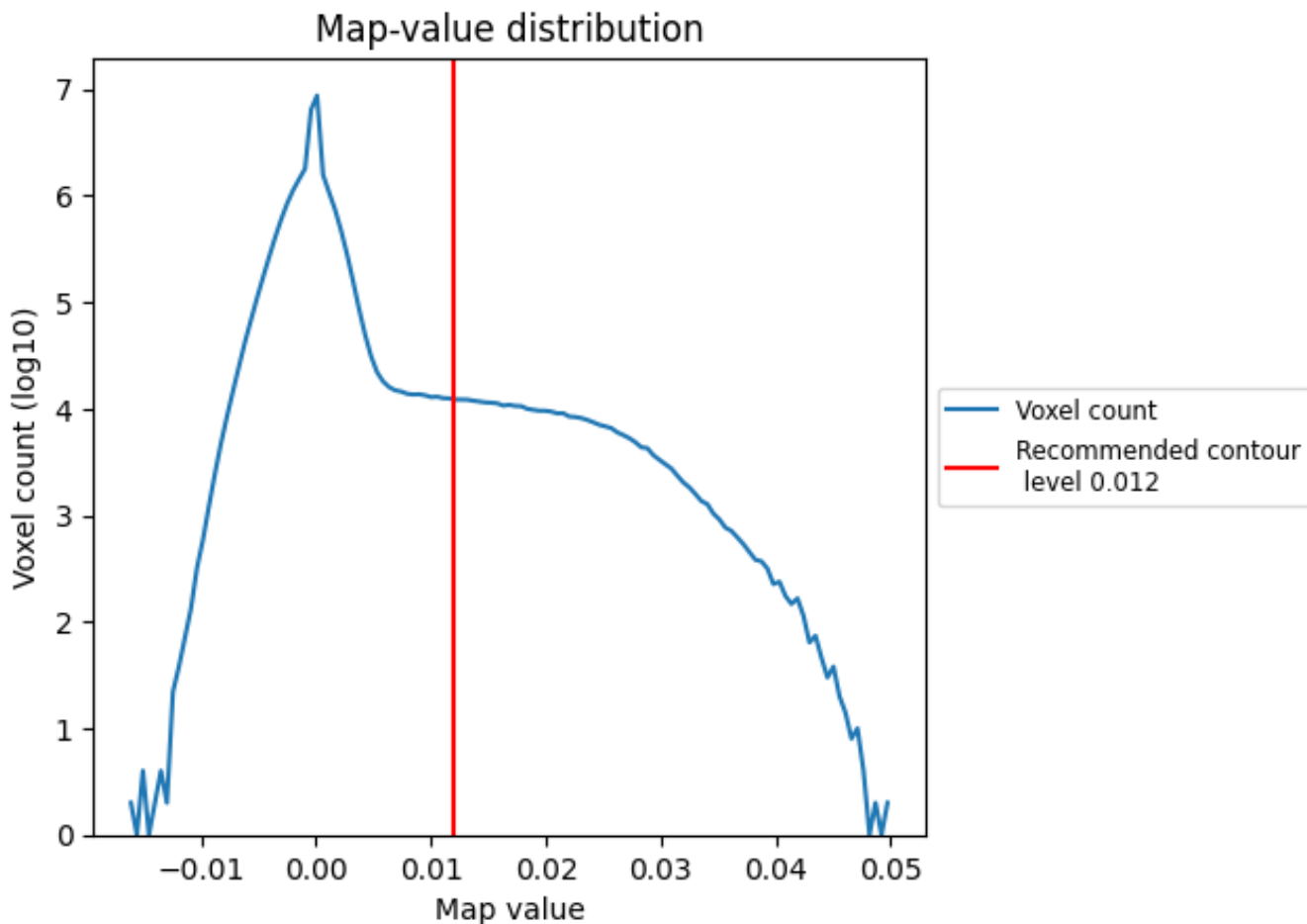
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

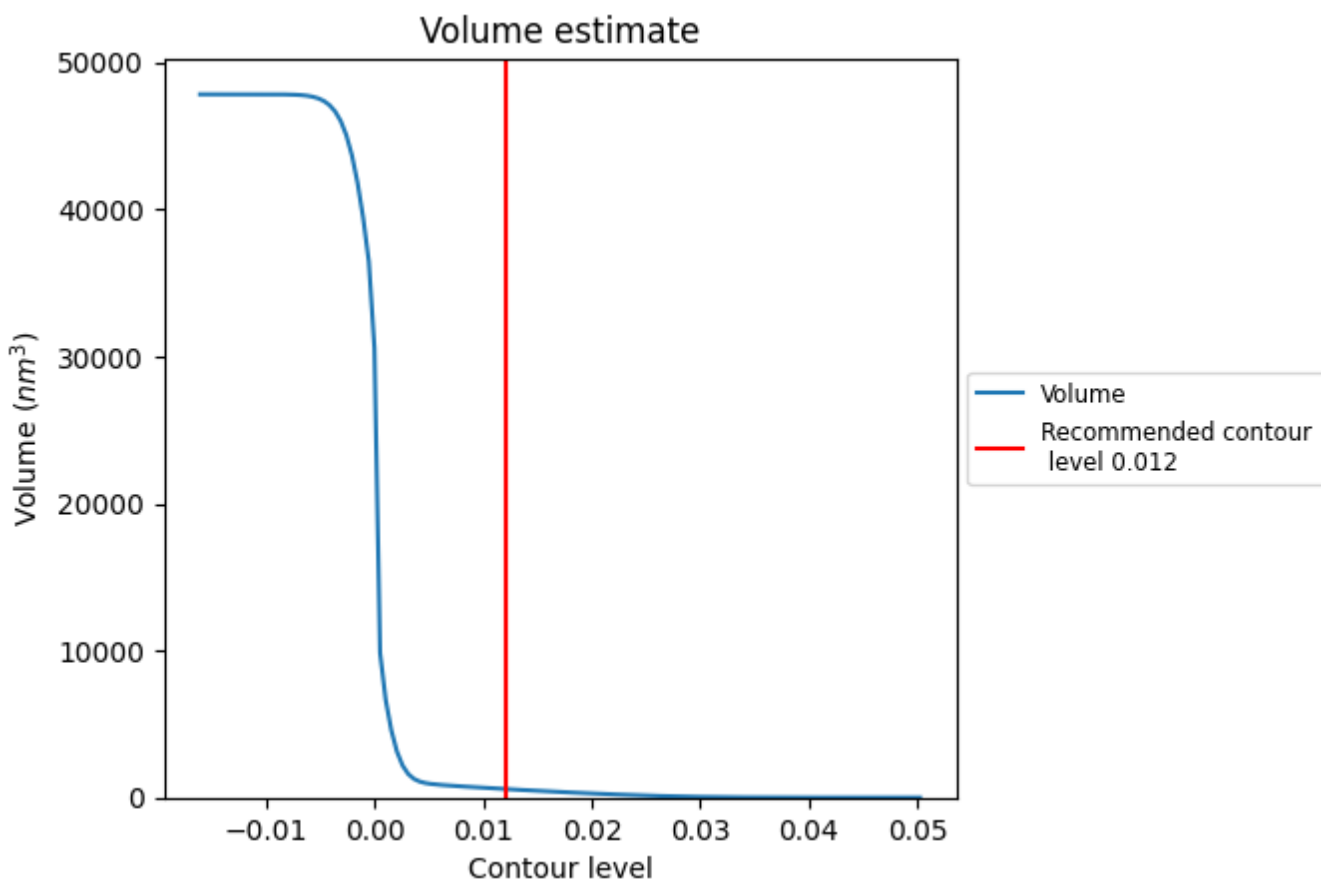
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

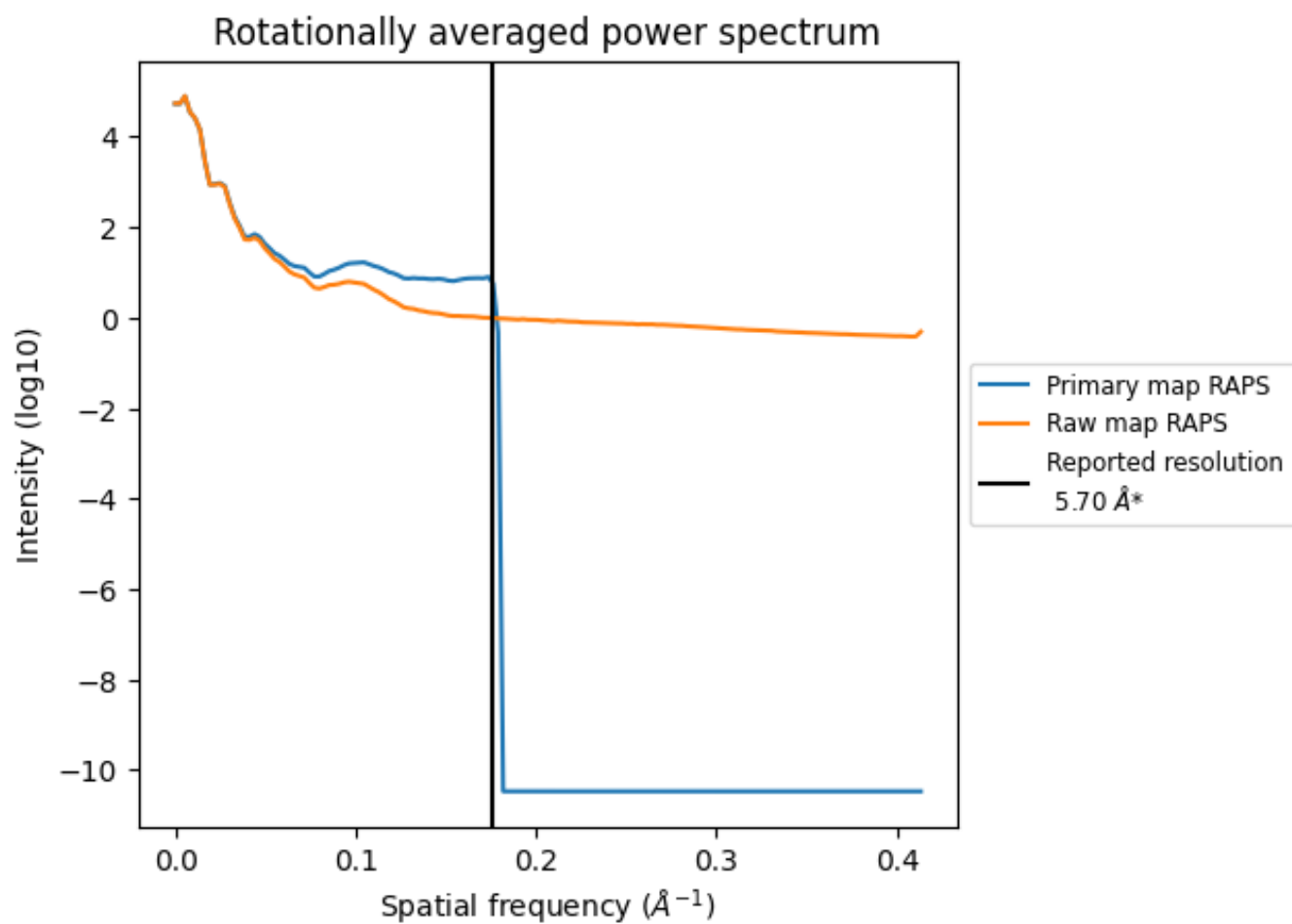
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

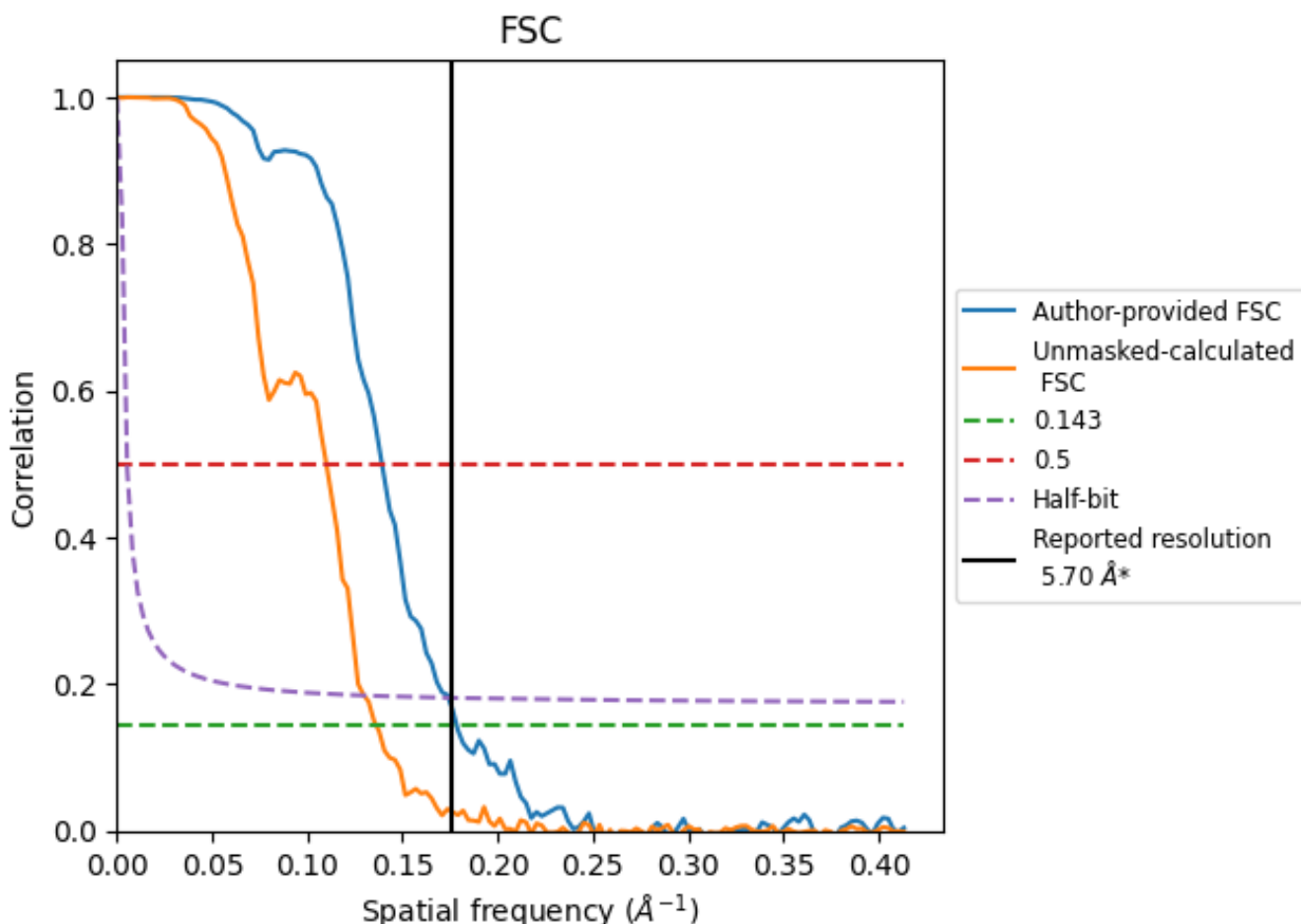


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8.2 Resolution estimates [i](#)

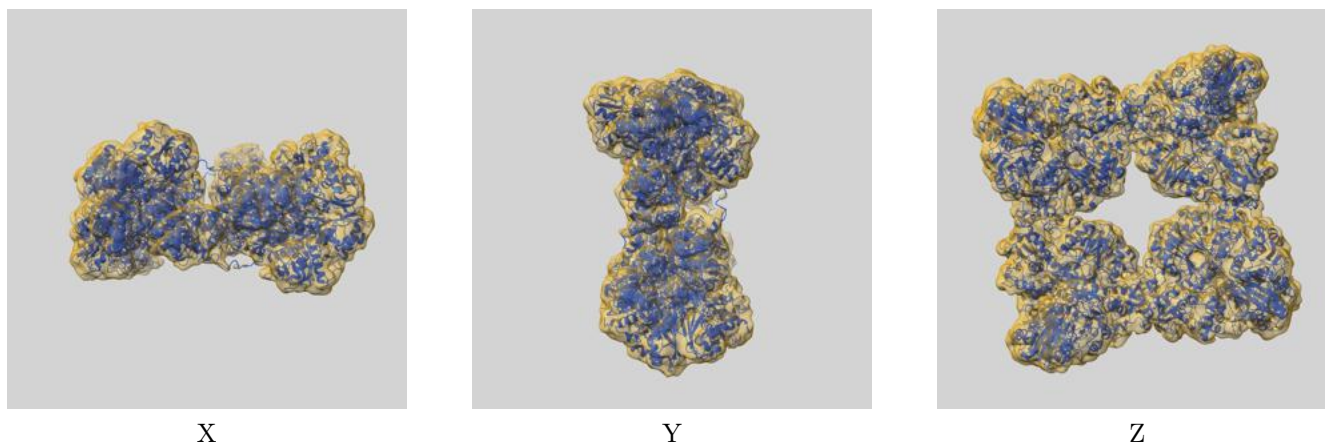
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.61	7.18	5.74
Unmasked-calculated*	7.34	9.09	7.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 5.7 by more than 10 %

9 Map-model fit [i](#)

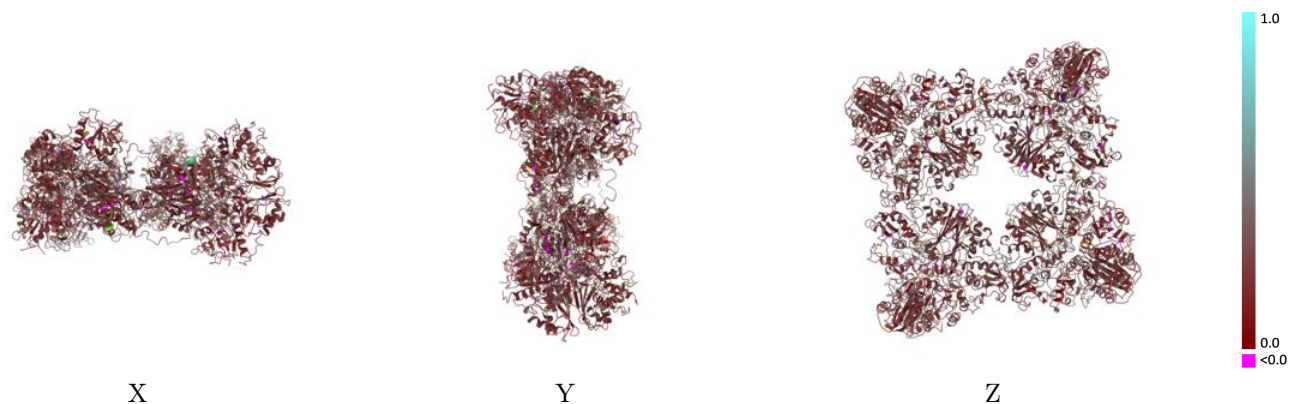
This section contains information regarding the fit between EMDB map EMD-13826 and PDB model 7Q55. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



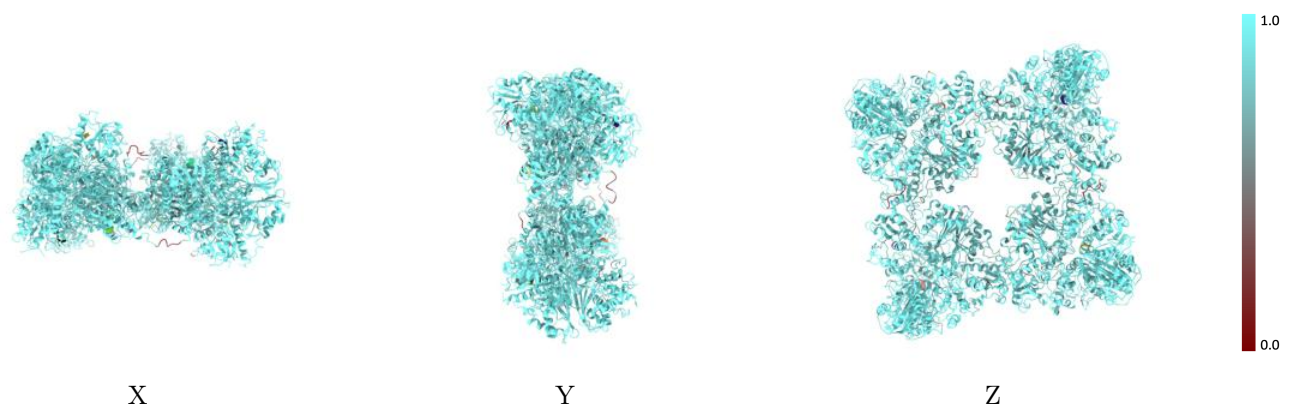
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



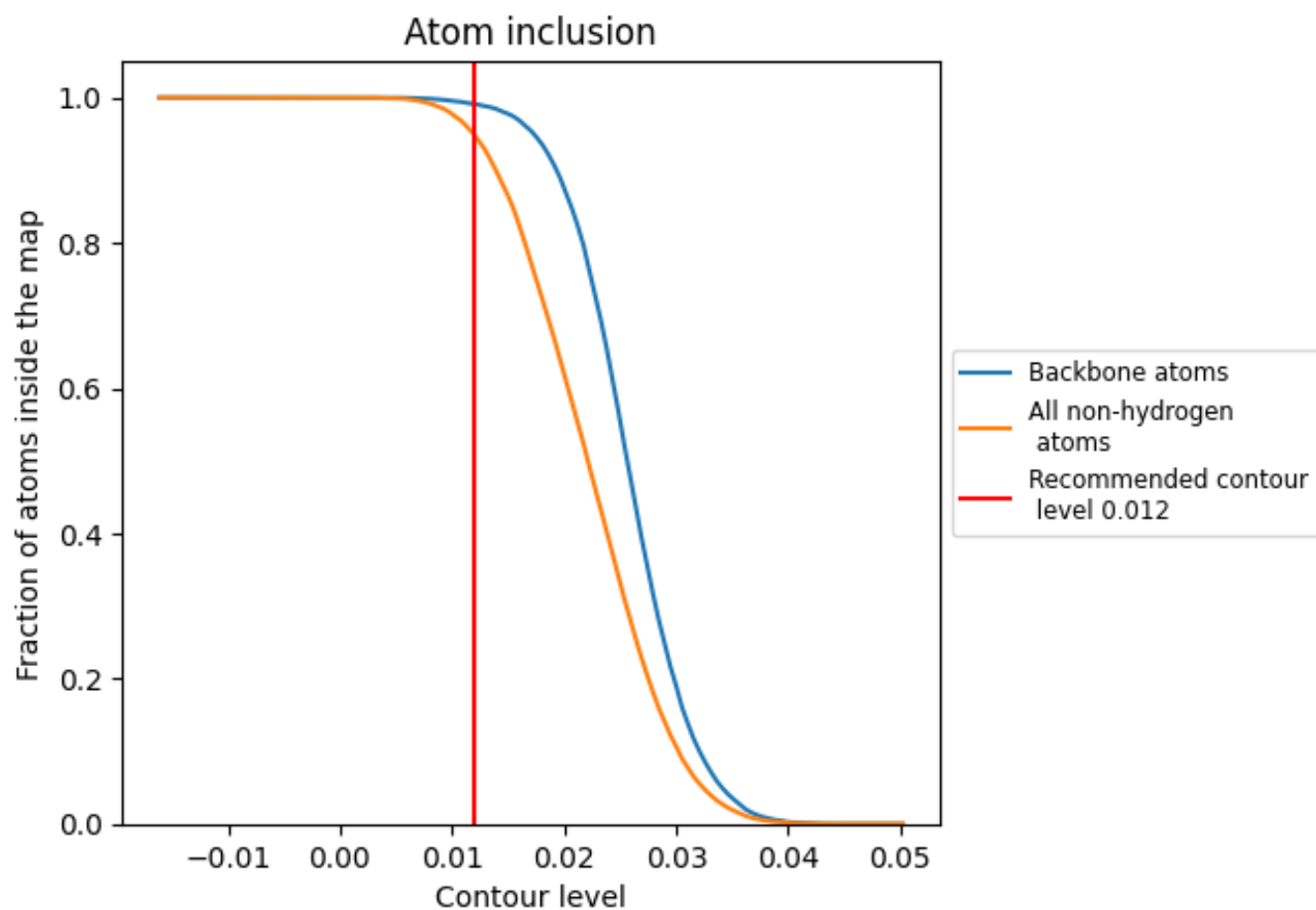
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9489	 0.2620
A	 0.9370	 0.2700
B	 0.9658	 0.2560
C	 0.9326	 0.2690
D	 0.9670	 0.2510
E	 0.9315	 0.2700
F	 0.9623	 0.2550
G	 0.9381	 0.2690
H	 0.9631	 0.2600
I	 0.9296	 0.2680
J	 0.9678	 0.2540
K	 0.9359	 0.2710
L	 0.9682	 0.2520
O	 0.9322	 0.2680
P	 0.9651	 0.2520
Q	 0.9296	 0.2670
R	 0.9647	 0.2610

