



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 7Q53 / pdb_00007q53
EMDB ID : EMD-13824
Title : Single Particle Cryo-EM structure of photosynthetic A2B2 glyceraldehyde 3-phosphate dehydrogenase from *Spinacia oleracea*
Authors : Marotta, R.; Fermani, S.; Sparla, F.; Trost, P.; Del Giudice, A.
Deposited on : 2021-11-02
Resolution : 6.30 Å(reported)
Based on initial model : 2PKQ

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

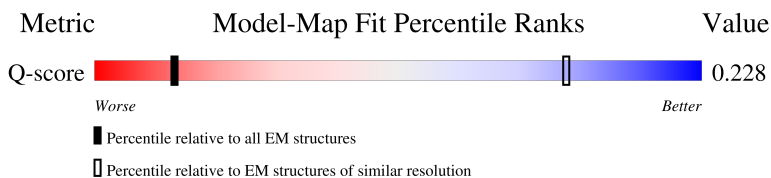
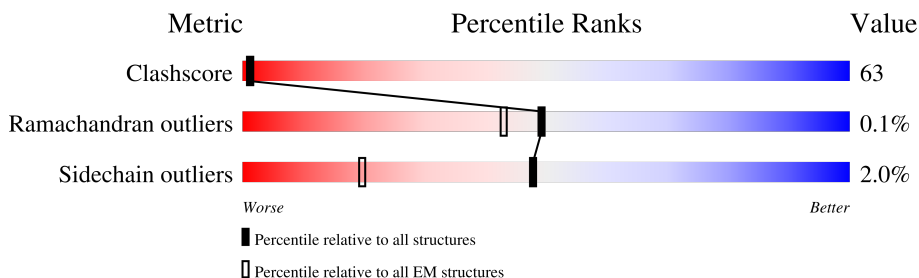
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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	O	339	24% 19% 80%
1	Q	339	24% 19% 80%
2	P	337	23% 18% 81%
2	R	337	23% 18% 81%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10362 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.

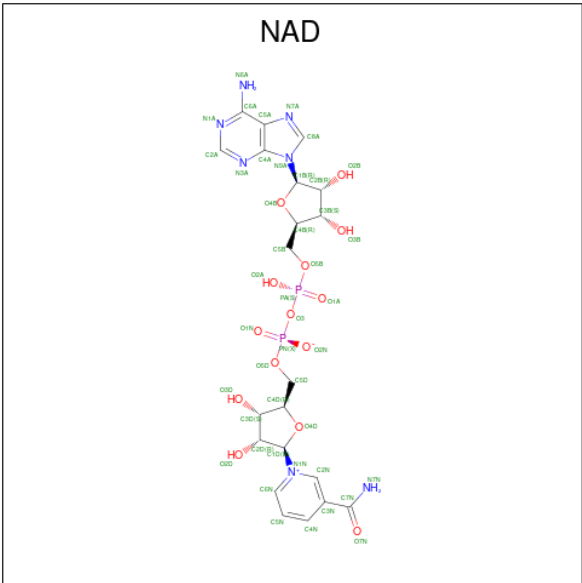
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	Q	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		

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

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

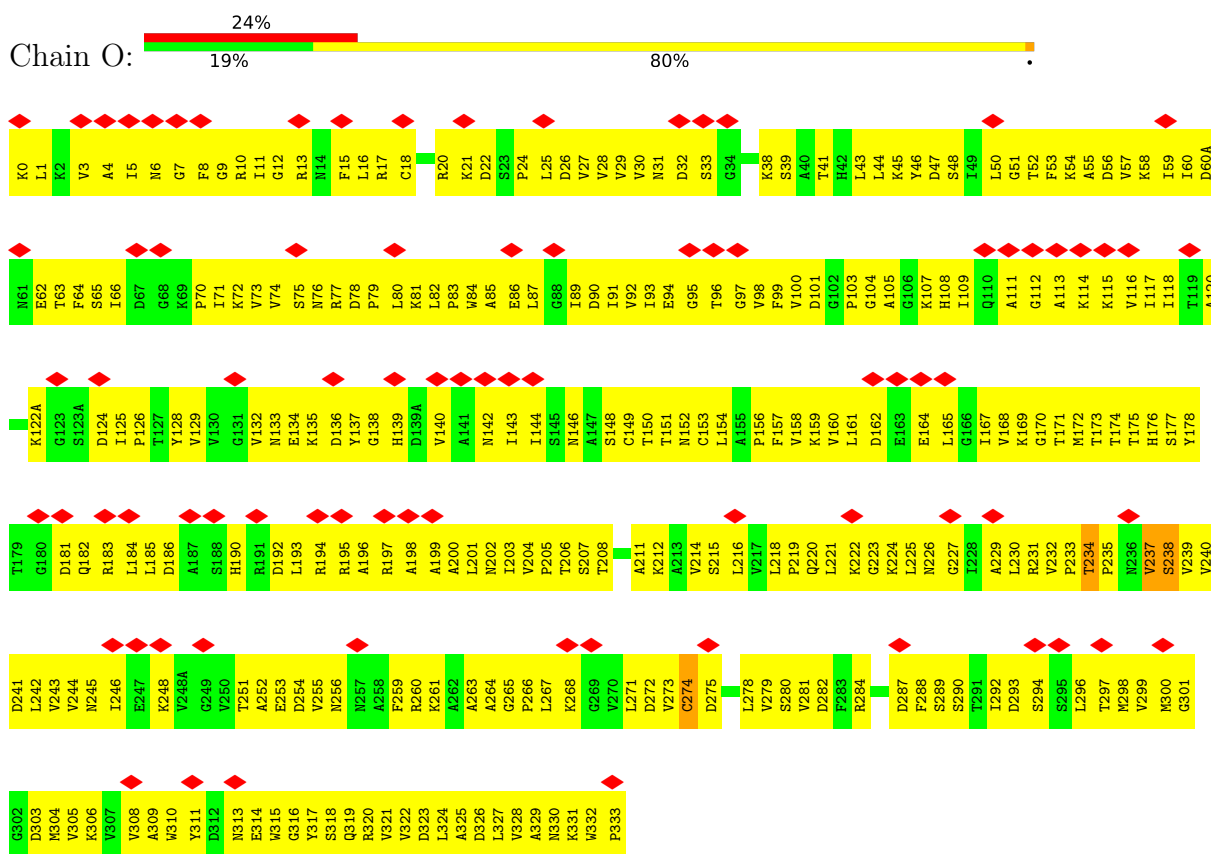


Mol	Chain	Residues	Atoms					AltConf
3	O	1	Total 44	C 21	N 7	O 14	P 2	0
3	P	1	Total 44	C 21	N 7	O 14	P 2	0
3	Q	1	Total 44	C 21	N 7	O 14	P 2	0
3	R	1	Total 44	C 21	N 7	O 14	P 2	0

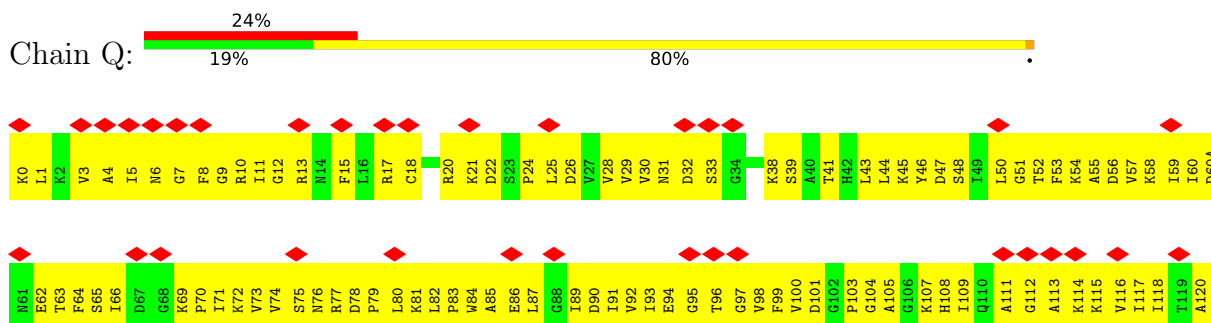
3 Residue-property plots

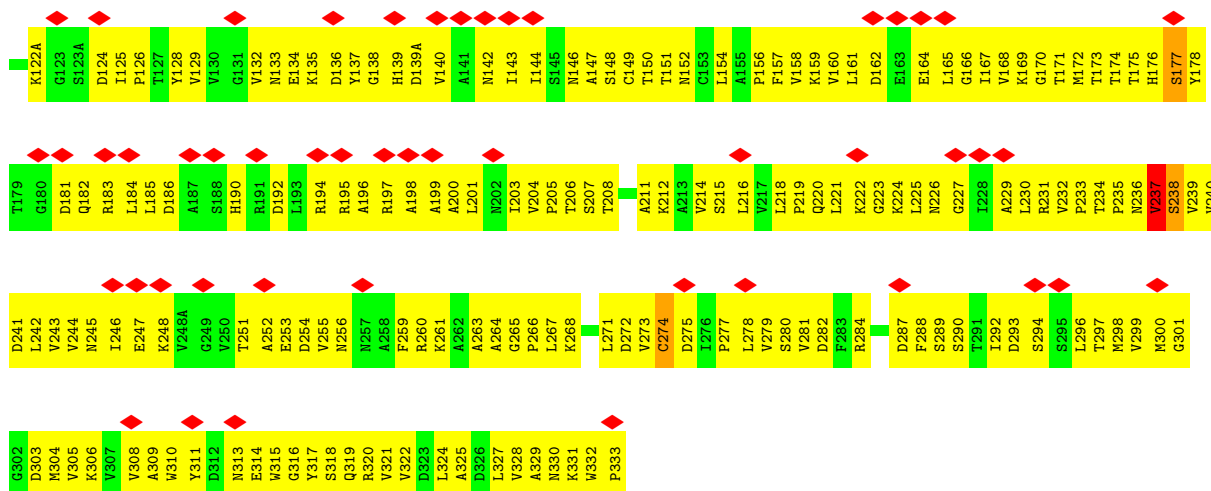
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



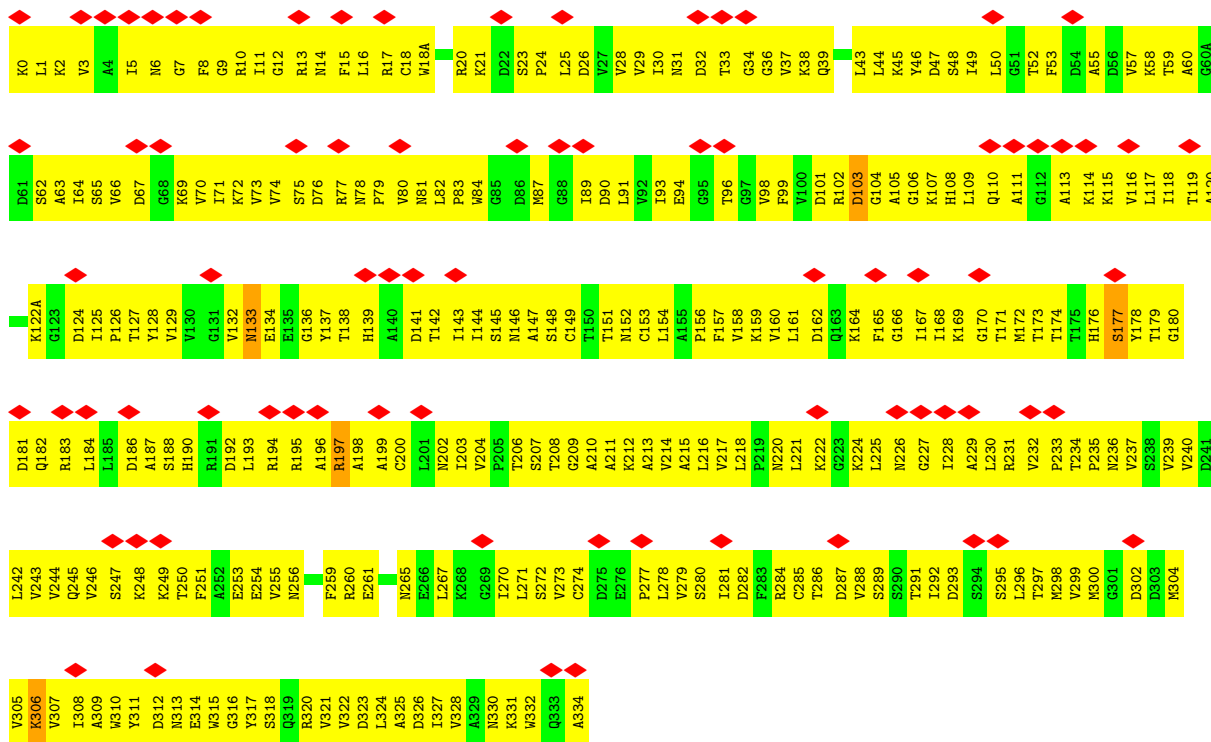
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic





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

Chain P: 23%
18% 81%



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

Chain R: 23%
18% 81%

V305	K306	V307	I308	A309	W310	D312	N313	E314	W315	G316	Y317	S318	G319	R320	V321	V322	D323	L324	A325	D326	I327	V328	A329	N330	K331	W332	Q333	A334																															
L242	V243	V244	Q245	V246	S247	K248	K249	T250	F251	A252	E253	E254	V255	N256	F259	R260	E261	N265	E266	L267	K268	G269	I270	L271	S272	V273	C274	D275	E276	P277	L278	V279	S280	I281	D282	F283	R284	C285	T286	D287	V288	S289	S290	T291	I292	D293	S294	S295	L296	T297	M298	V299	M300	G301	D302	B303	M304		
D181	Q182	R183	L184	L185	D186	A187	S188	H190	R191	D192	L193	R194	R195	A196	A197	A198	A199	C200	L201	N202	I203	V204	P205	T206	S207	T208	G209	A210	A211	K212	A213	V214	A215	L216	V217	L218	P219	N220	L221	K222	G223	K224	L225	N226	G227	I228	A229	L230	R231	V232	P233	T234	P235	N236	V237	V239	V240	D241	
D61	S62	A63	I64	S65	V66	D67	G68	K69	V70	I71	K72	V73	V74	S75	D76	R77	N78	P79	V80	N81	L82	P83	W84	G85	D86	M87	G88	I89	D90	L91	V92	I93	E94	G95	T96	G97	V98	F99	V100	D101	R102	D103	G104	A105	G106	K107	H108	L109	Q110	A111	G112	A113	K114	K115	V116	L117	T118	T119	A120
K0	L1	K2	V3	A4	I5	N6	G7	F8	G9	R10	I11	G12	R13	N14	F15	L16	C18	W18A	R20	K21	D22	S23	P24	L25	D26	V27	V28	V29	I30	N31	D32	T33	G34	G36	V37	K38	Q39	L43	L44	K45	Y46	D47	S48	I49	L50	G51	T52	F53	D54	A55	D56	V57	K58	T59	A60	G60A			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	19636	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	0.107	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0312	Depositor
Map size (Å)	181.5, 181.5, 181.5	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	O	0.40	0/2594	0.69	0/3527
1	Q	0.41	0/2594	0.69	0/3527
2	P	0.38	0/2585	0.65	0/3509
2	R	0.38	0/2585	0.64	0/3509
All	All	0.39	0/10358	0.67	0/14072

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	O	2549	0	2612	345	0
1	Q	2549	0	2612	341	0
2	P	2544	0	2580	341	0
2	R	2544	0	2580	340	0
3	O	44	0	26	2	0
3	P	44	0	26	0	0
3	Q	44	0	26	2	0
3	R	44	0	26	0	0
All	All	10362	0	10488	1312	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 63.

The worst 5 of 1312 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)
2:R:281:ILE:HA	2:R:284:ARG:HE	1.32	0.94
2:P:281:ILE:HA	2:P:284:ARG:HE	1.32	0.93
1:O:259:PHE:HB3	1:O:273:VAL:HG21	1.51	0.92
1:Q:259:PHE:HB3	1:Q:273:VAL:HG21	1.51	0.92
1:Q:301:GLY:HA3	1:Q:304:MET:HE3	1.55	0.89

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	O	337/339 (99%)	269 (80%)	67 (20%)	1 (0%)	36	72
1	Q	337/339 (99%)	268 (80%)	68 (20%)	1 (0%)	36	72
2	P	335/337 (99%)	288 (86%)	47 (14%)	0	100	100
2	R	335/337 (99%)	288 (86%)	47 (14%)	0	100	100
All	All	1344/1352 (99%)	1113 (83%)	229 (17%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	237	VAL
1	O	235	PRO

5.3.2 Protein sidechains ⓘ

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	O	280/280 (100%)	275 (98%)	5 (2%)	51	68
1	Q	280/280 (100%)	274 (98%)	6 (2%)	47	65
2	P	279/279 (100%)	273 (98%)	6 (2%)	45	64
2	R	279/279 (100%)	274 (98%)	5 (2%)	51	68
All	All	1118/1118 (100%)	1096 (98%)	22 (2%)	48	66

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	238	SER
2	R	103	ASP
1	Q	289	SER
2	R	133	ASN
2	P	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	139	HIS
2	R	108	HIS
1	Q	319	GLN
2	R	202	ASN
2	P	108	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	Q	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	O	401	-	46,48,48	0.58	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	R	401	-	46,48,48	0.62	1 (2%)	64,73,73	0.55	1 (1%)
3	NAD	P	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.53	1 (1%)

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	Q	401	-	-	20/30/62/62	0/5/5/5
3	NAD	O	401	-	-	19/30/62/62	0/5/5/5
3	NAD	R	401	-	-	13/30/62/62	0/5/5/5
3	NAD	P	401	-	-	12/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	401	NAD	C2N-N1N	2.48	1.37	1.35
3	P	401	NAD	C2N-N1N	2.46	1.37	1.35
3	Q	401	NAD	C2N-N1N	2.37	1.37	1.35
3	O	401	NAD	C2N-N1N	2.30	1.37	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	401	NAD	C6N-N1N-C2N	-2.85	119.45	121.88
3	Q	401	NAD	C6N-N1N-C2N	-2.84	119.46	121.88
3	R	401	NAD	C6N-N1N-C2N	-2.70	119.58	121.88
3	P	401	NAD	C6N-N1N-C2N	-2.61	119.66	121.88

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

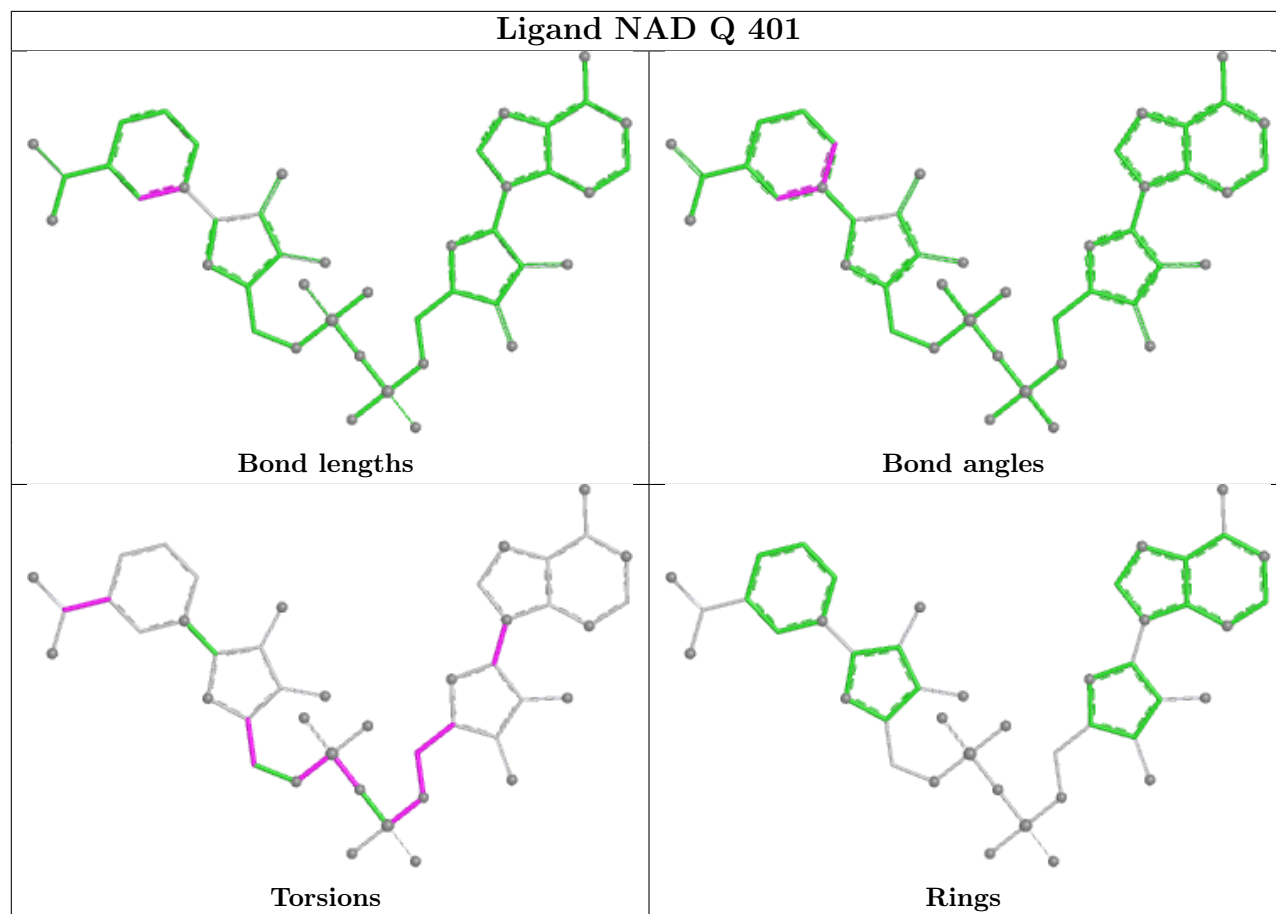
Mol	Chain	Res	Type	Atoms
3	O	401	NAD	C5B-O5B-PA-O1A
3	O	401	NAD	C5B-O5B-PA-O2A
3	O	401	NAD	C5B-O5B-PA-O3
3	O	401	NAD	C5D-O5D-PN-O3
3	O	401	NAD	C5D-O5D-PN-O1N

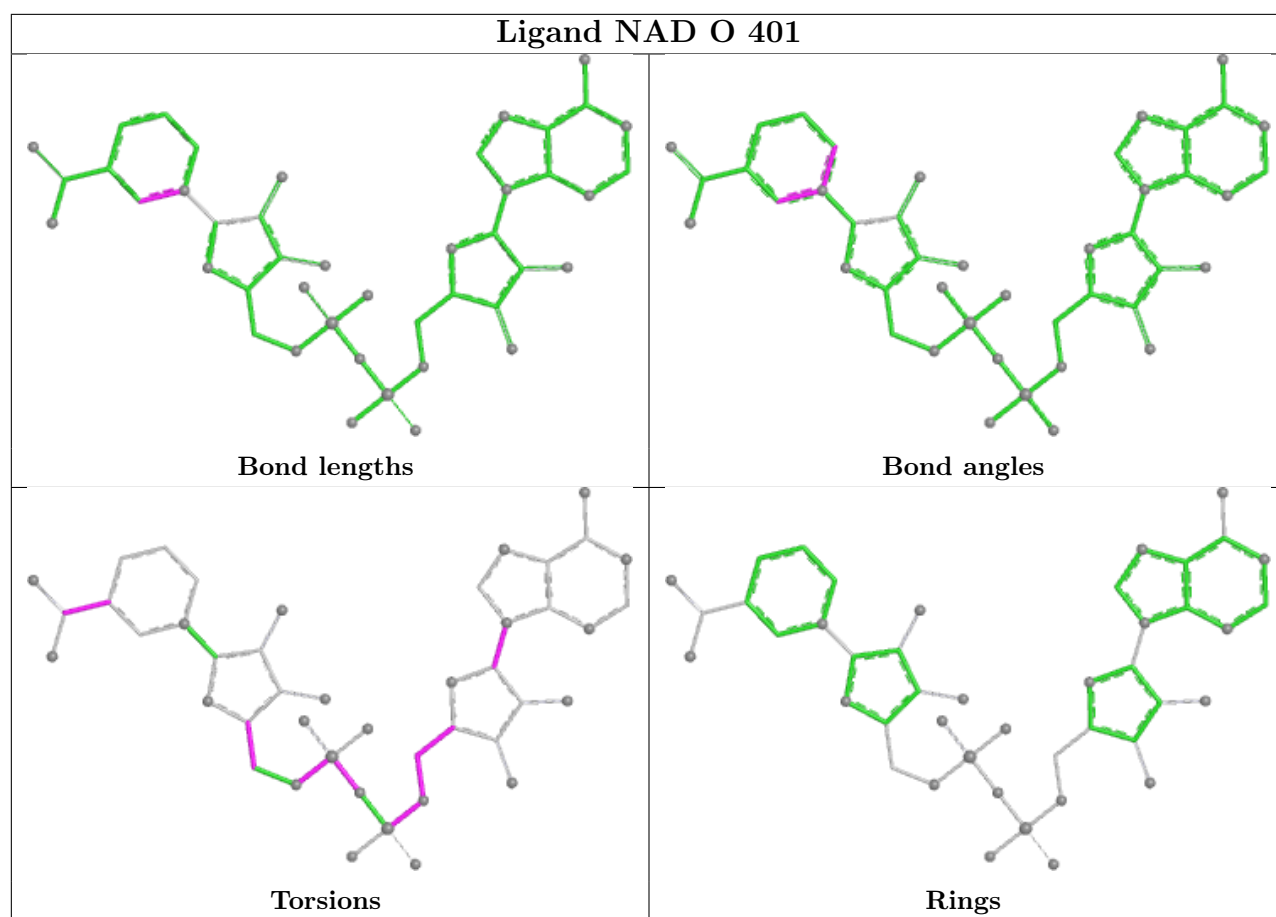
There are no ring outliers.

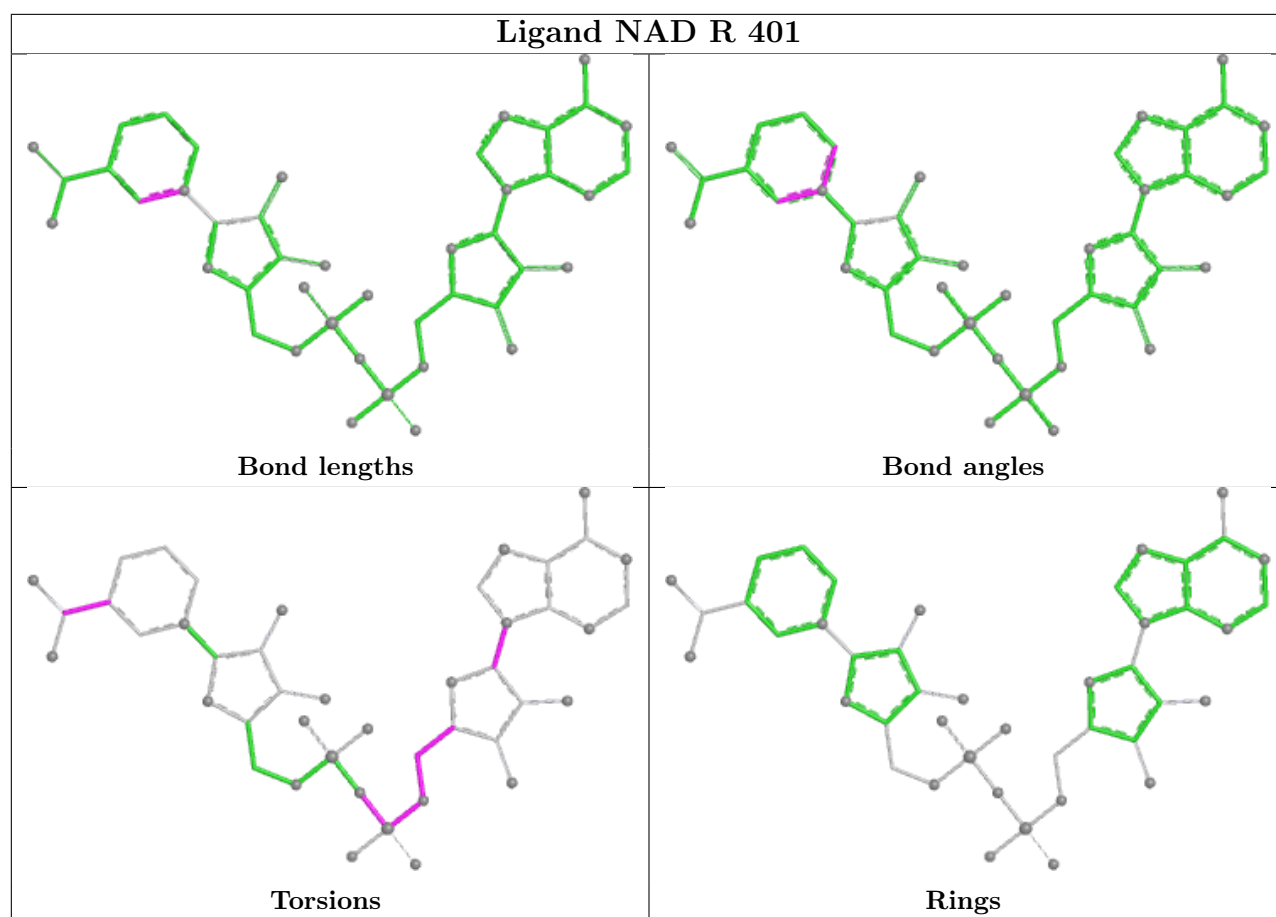
2 monomers are involved in 4 short contacts:

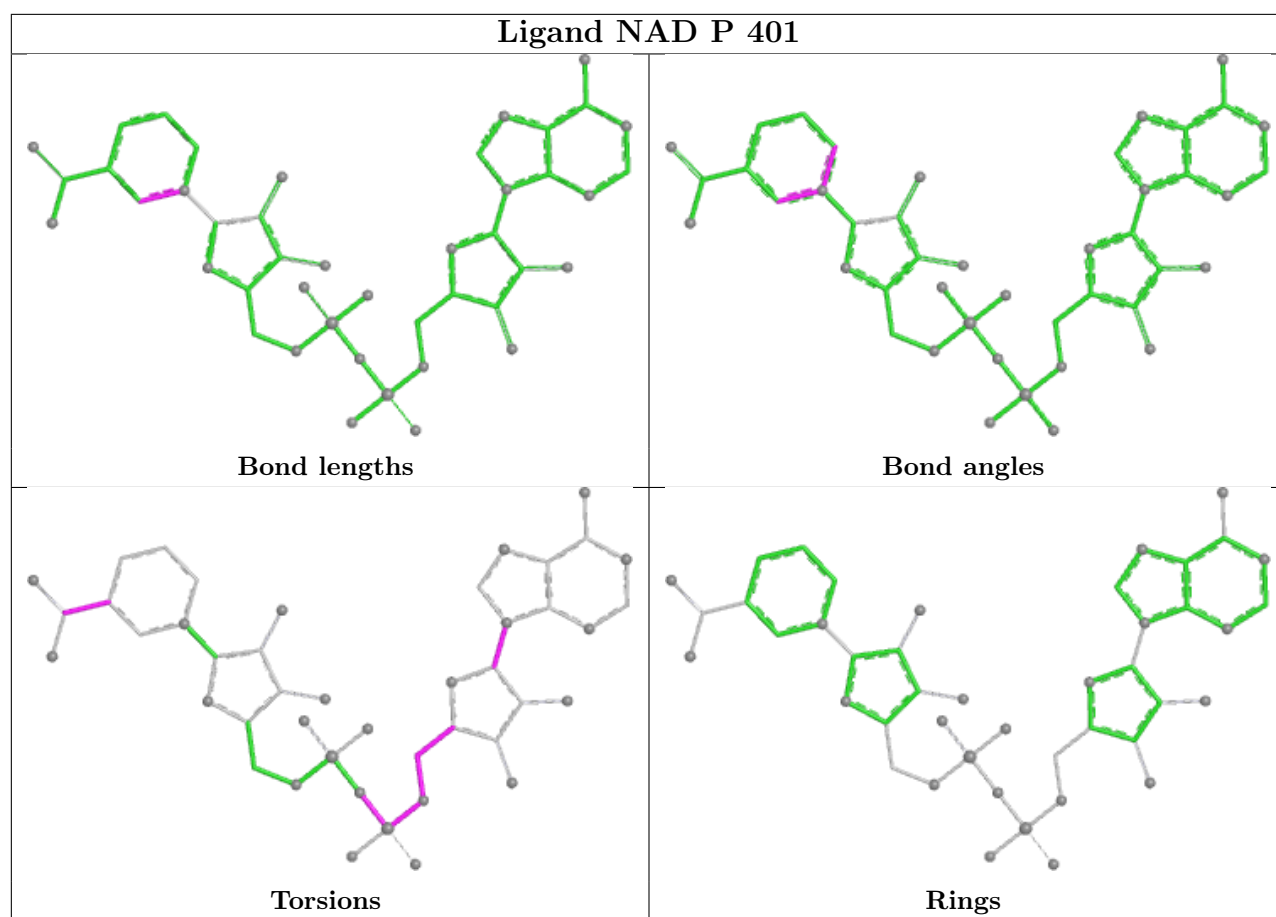
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	401	NAD	2	0
3	O	401	NAD	2	0

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-13824. These allow visual inspection of the internal detail of the map and identification of artifacts.

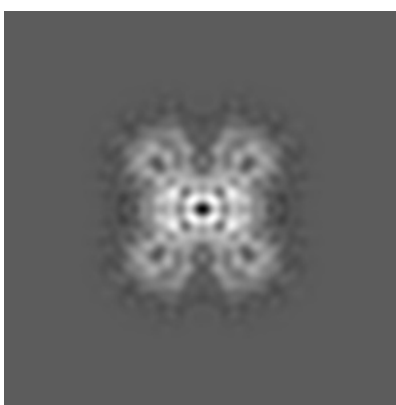
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 75



Y Index: 75



Z Index: 75

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: 71



Y Index: 79



Z Index: 87

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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

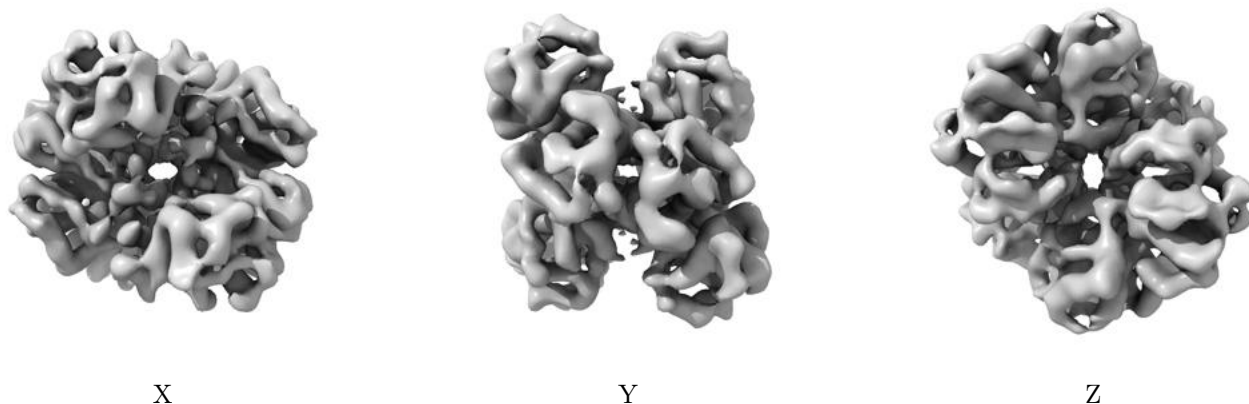


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0312. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

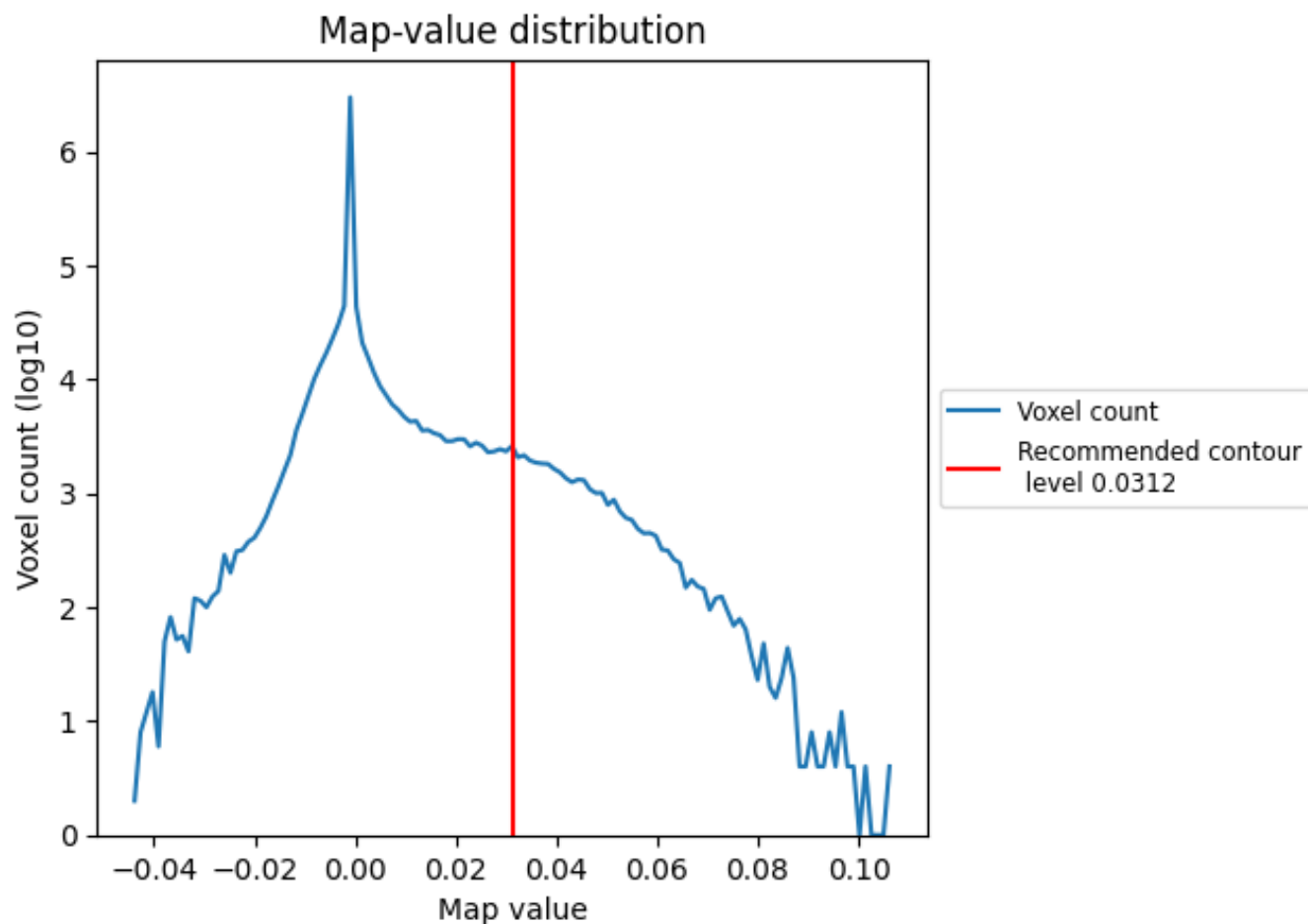
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

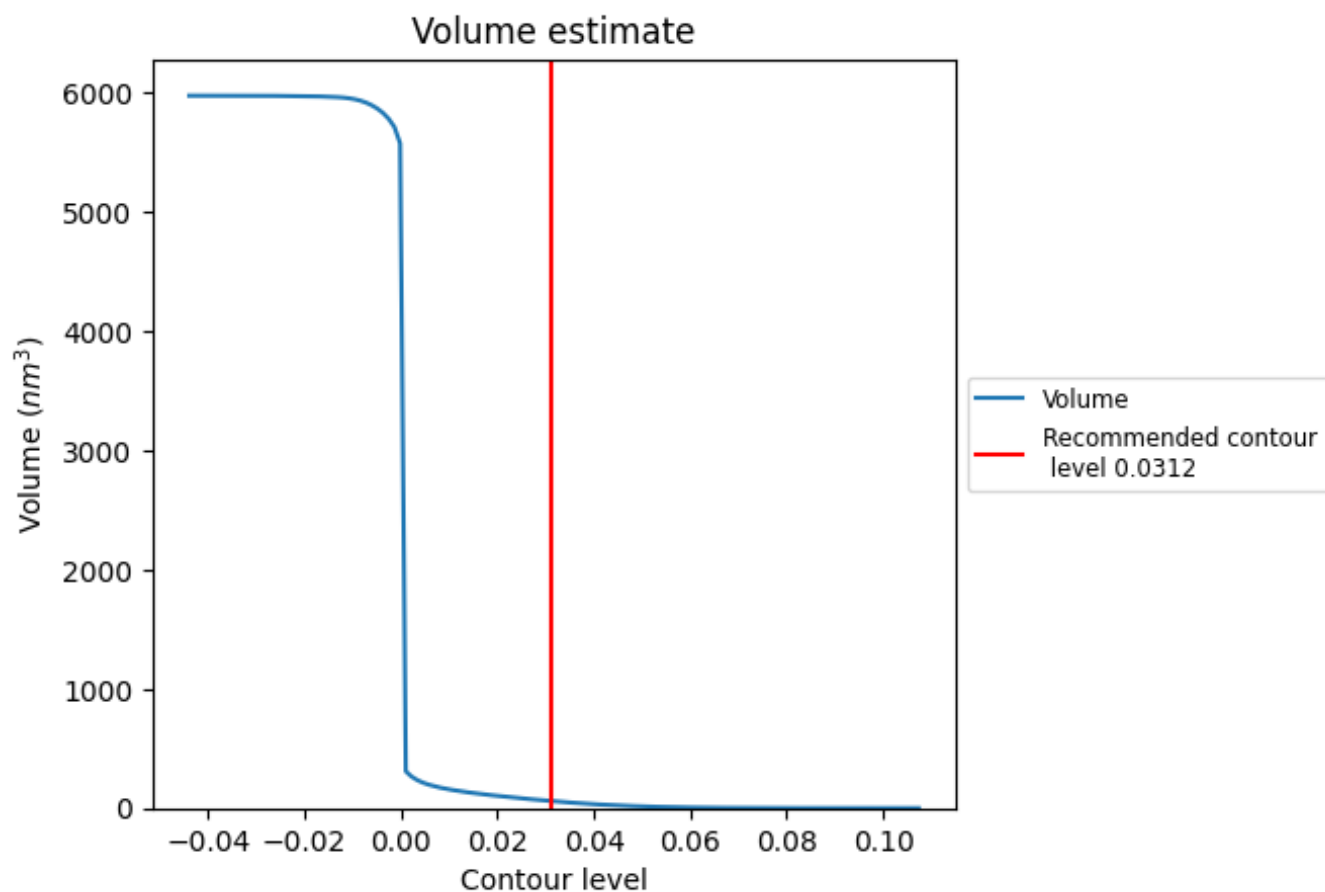
This section contains the results of statistical analysis of the map.

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.

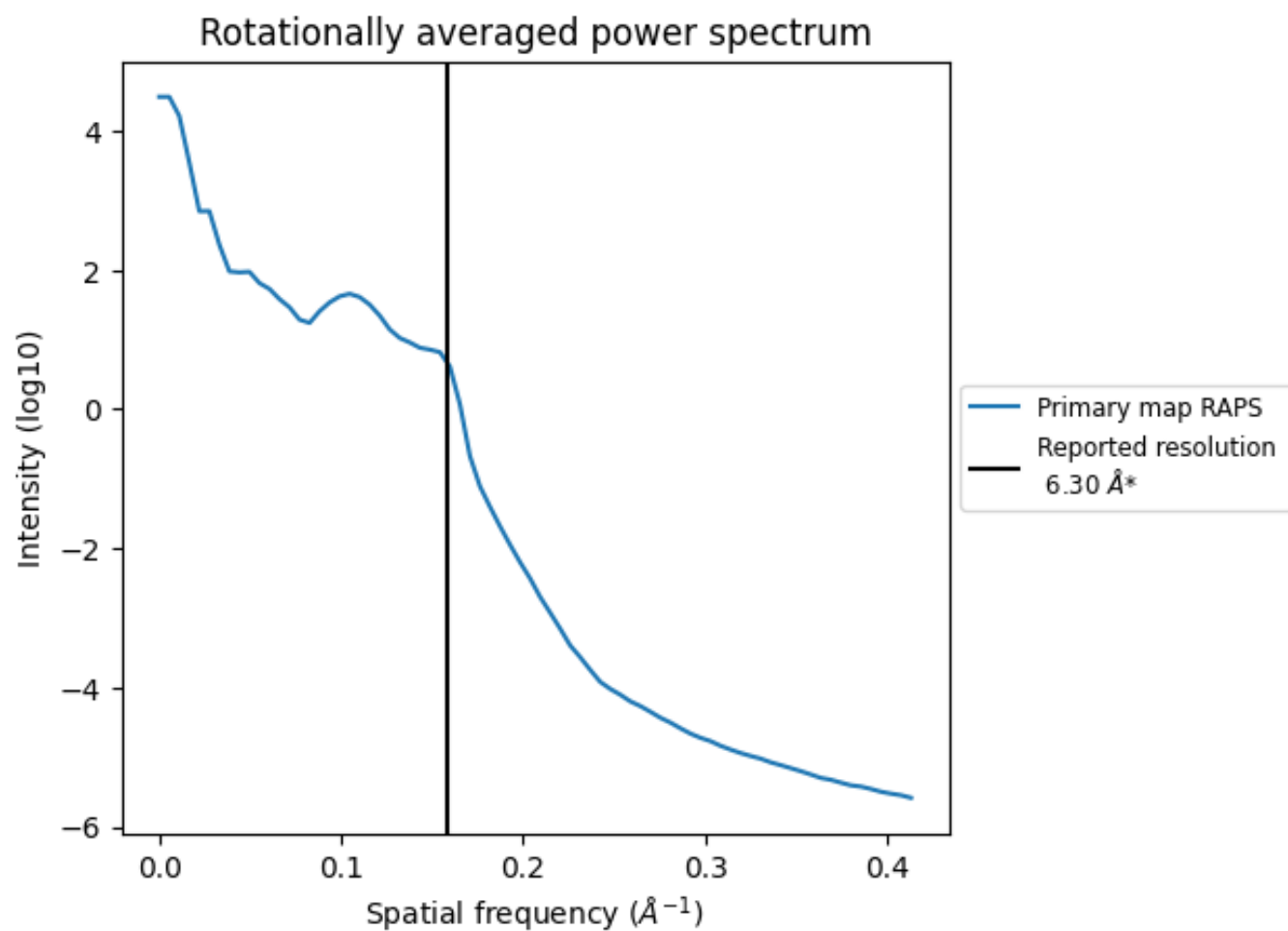
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 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 ⓘ

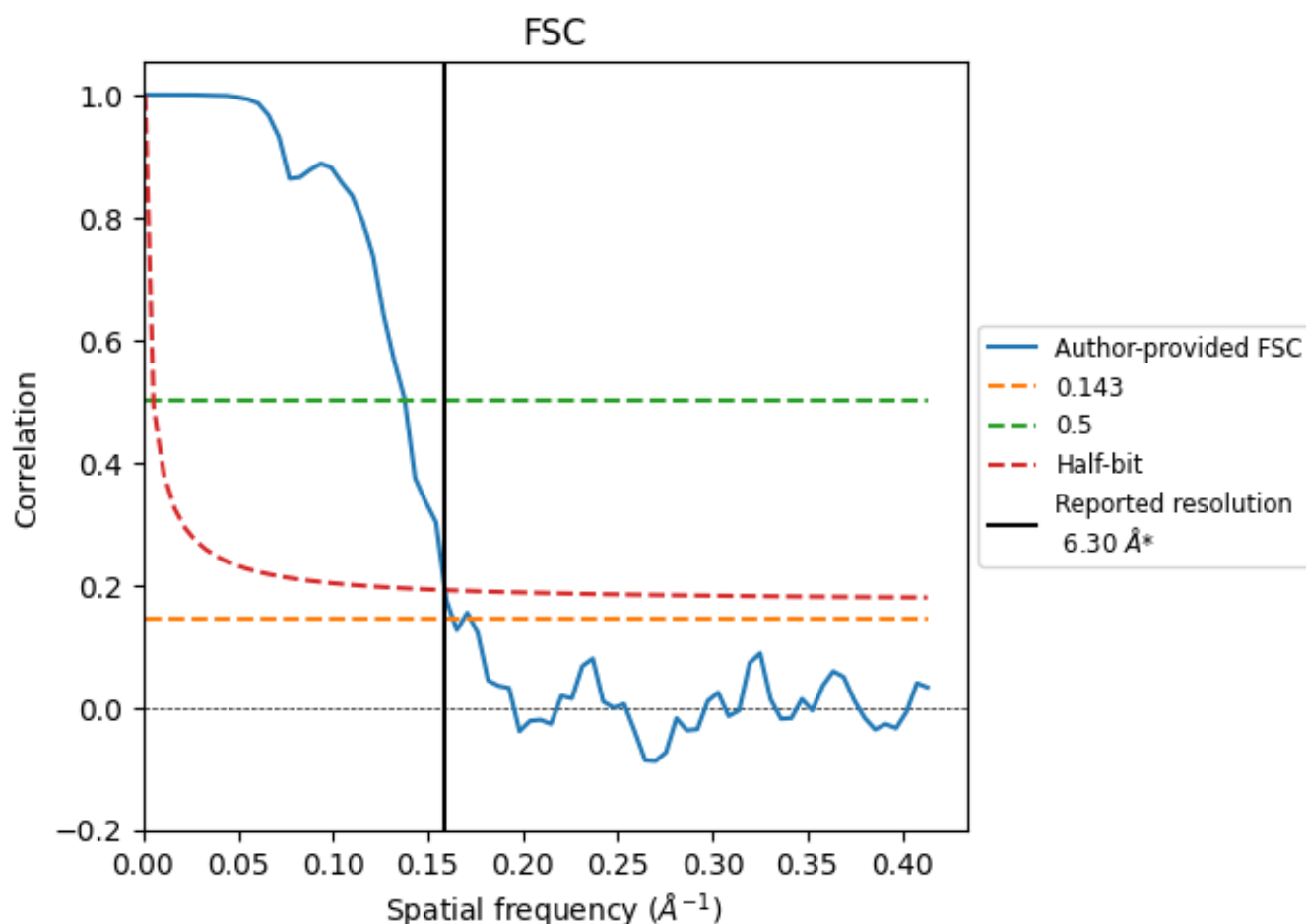


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

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 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

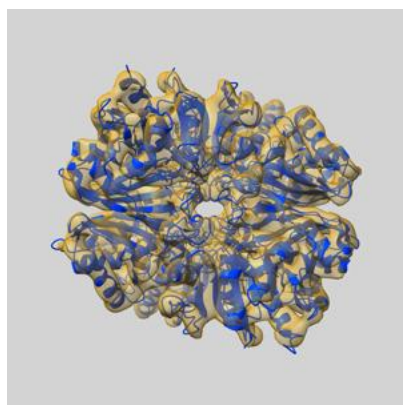
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.12	7.25	6.29
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

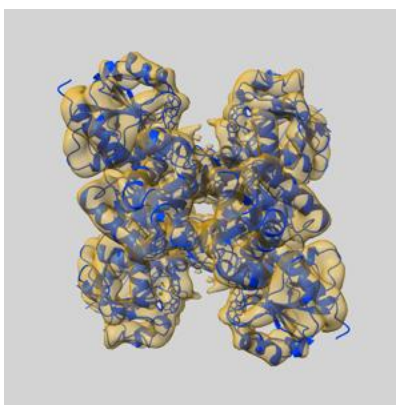
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13824 and PDB model 7Q53. Per-residue inclusion information can be found in section [3](#) on page [5](#).

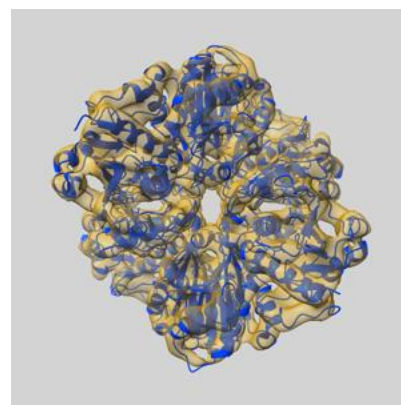
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0312 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](#)

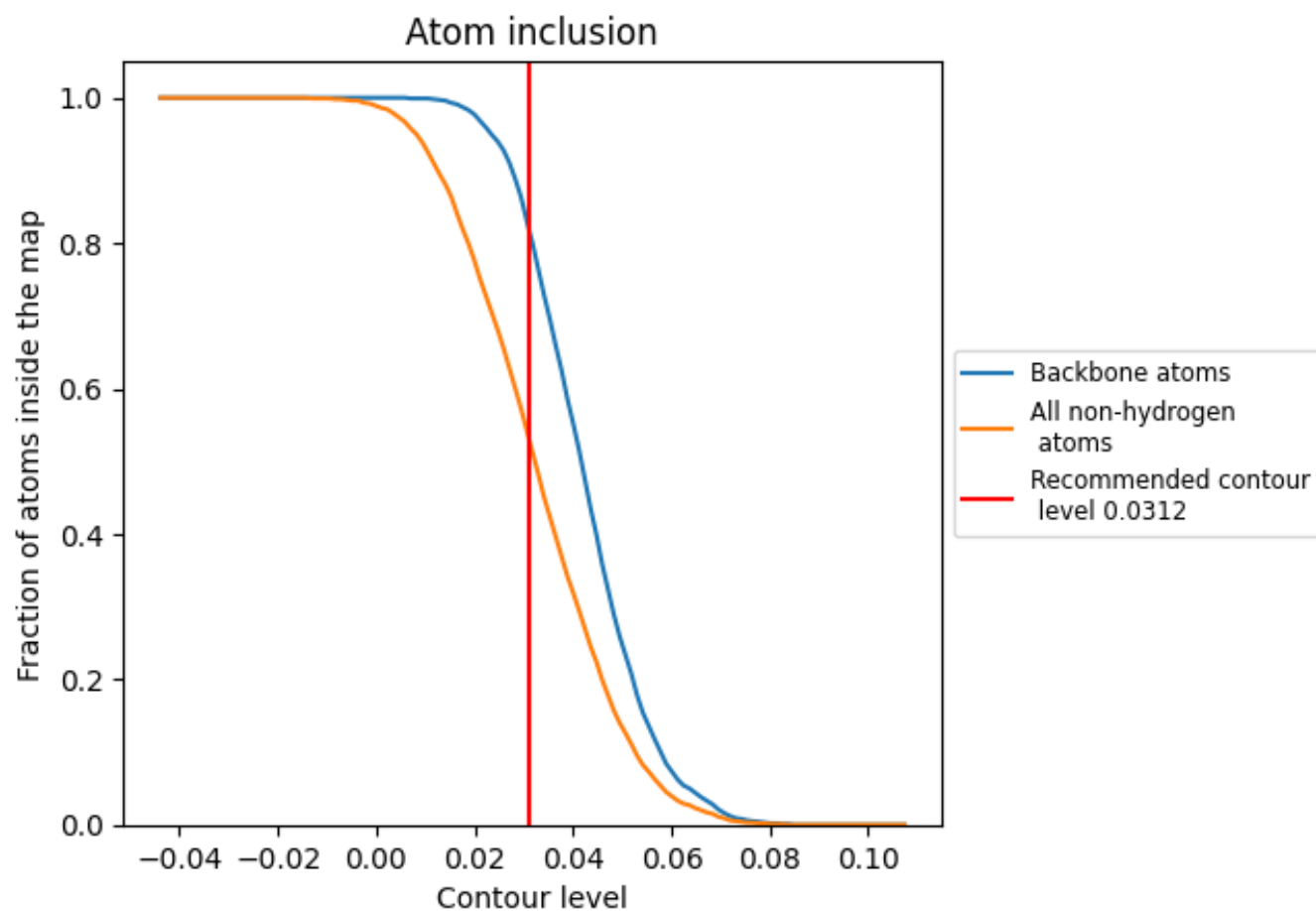


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 53% 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 (0.0312) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5260	0.2280
O	0.5260	0.2260
P	0.5290	0.2290
Q	0.5250	0.2270
R	0.5220	0.2290

