



# Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 10:09 AM JST

PDB ID : 7BVP  
EMDB ID : EMD-30220  
Title : AdhE spirosome in extended conformation  
Authors : Kim, G.J.; Song, J.J.  
Deposited on : 2020-04-11  
Resolution : 3.45 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

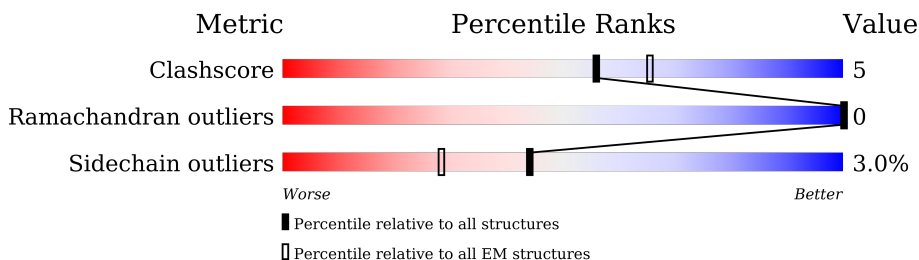
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.45 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  $\geq 3$ , 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	893	
1	B	893	
1	C	893	
1	D	893	
1	E	893	
1	F	893	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	F	902	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 40146 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 Aldehyde-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	869	6602	4193	1125	1254	30	0	0
1	B	869	6602	4193	1125	1254	30	0	0
1	C	869	6602	4193	1125	1254	30	0	0
1	D	869	6602	4193	1125	1254	30	0	0
1	E	869	6602	4193	1125	1254	30	0	0
1	F	869	6602	4193	1125	1254	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P0A9Q7
A	0	SER	-	expression tag	UNP P0A9Q7
B	-1	GLY	-	expression tag	UNP P0A9Q7
B	0	SER	-	expression tag	UNP P0A9Q7
C	-1	GLY	-	expression tag	UNP P0A9Q7
C	0	SER	-	expression tag	UNP P0A9Q7
D	-1	GLY	-	expression tag	UNP P0A9Q7
D	0	SER	-	expression tag	UNP P0A9Q7
E	-1	GLY	-	expression tag	UNP P0A9Q7
E	0	SER	-	expression tag	UNP P0A9Q7
F	-1	GLY	-	expression tag	UNP P0A9Q7
F	0	SER	-	expression tag	UNP P0A9Q7

- Molecule 2 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).



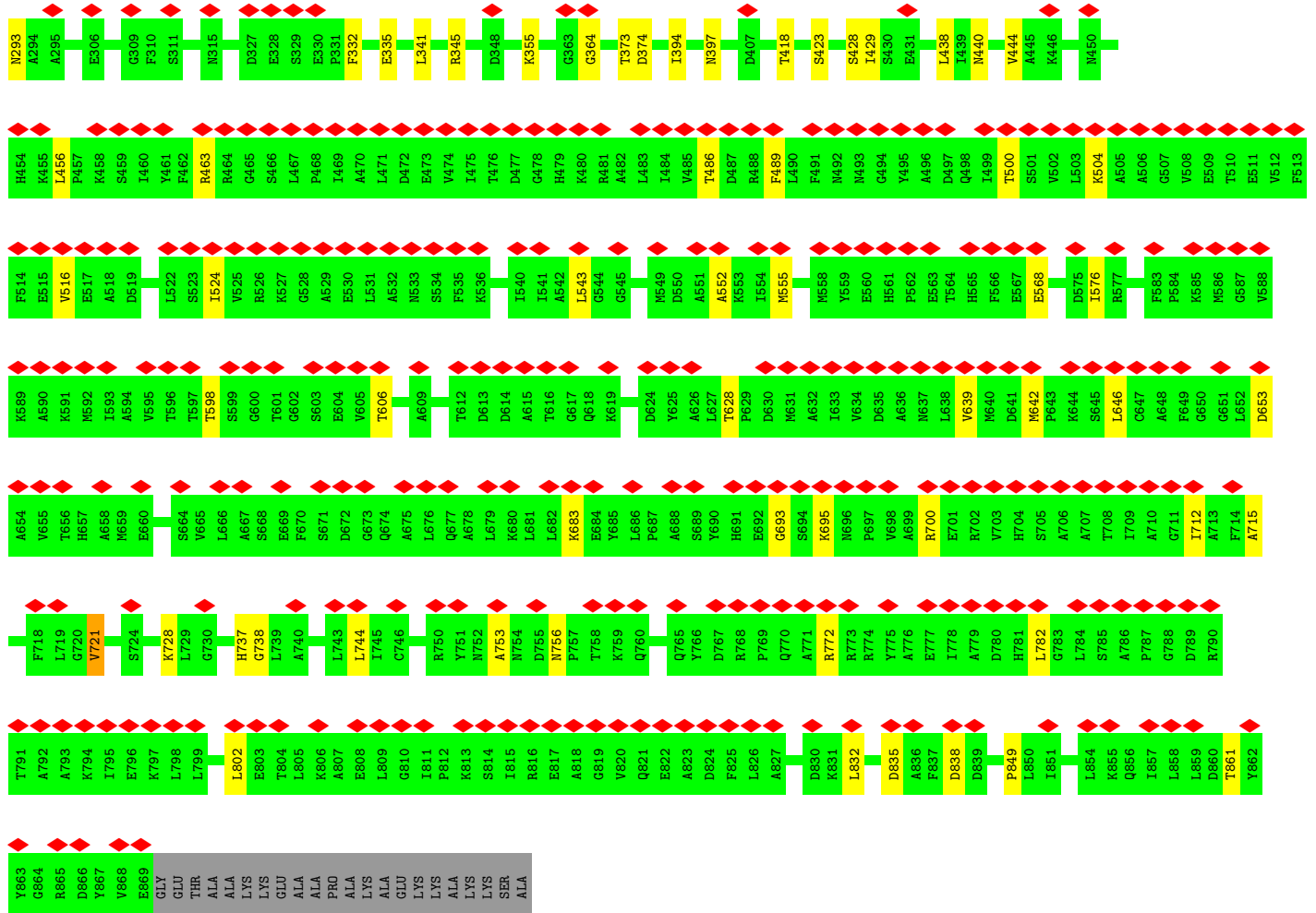
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0
3	E	1	Total 1	Zn 1	0
3	F	1	Total 1	Zn 1	0











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.76	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	350.06403, 350.06403, 350.06403	wwPDB
Map dimensions	306, 306, 306	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.144, 1.144, 1.144	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: ZN, 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	0.25	0/6730	0.45	0/9130
1	B	0.25	0/6730	0.45	0/9130
1	C	0.25	0/6730	0.45	0/9130
1	D	0.25	0/6730	0.45	0/9130
1	E	0.25	0/6730	0.45	0/9130
1	F	0.25	0/6730	0.44	0/9130
All	All	0.25	0/40380	0.45	0/54780

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	A	6602	0	6646	89	0
1	B	6602	0	6646	84	0
1	C	6602	0	6646	61	0
1	D	6602	0	6646	78	0
1	E	6602	0	6646	68	0
1	F	6602	0	6646	79	0
2	A	88	0	52	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	88	0	52	24	0
2	C	88	0	52	10	0
2	D	88	0	52	29	0
2	E	88	0	52	18	0
2	F	88	0	52	37	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	40146	0	40188	421	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 5.

All (421) 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:B:696:ASN:HD21	1:B:699:ALA:CB	1.42	1.30
1:F:598:THR:HG22	2:F:902:NAD:N7A	1.46	1.29
1:B:696:ASN:ND2	1:B:699:ALA:HB3	1.48	1.27
1:A:690:TYR:HE2	1:A:809:LEU:HA	1.07	1.13
1:E:546:GLY:CA	2:E:902:NAD:H52N	1.79	1.11
1:E:693:GLY:HA2	1:E:700:ARG:HH21	1.15	1.11
1:A:690:TYR:CE2	1:A:809:LEU:HA	1.86	1.08
1:E:546:GLY:HA3	2:E:902:NAD:C5D	1.85	1.07
1:A:696:ASN:HD21	1:A:699:ALA:HB2	1.23	1.04
1:D:214:ALA:CB	2:D:901:NAD:O2D	2.06	1.03
1:B:139:HIS:HA	2:B:901:NAD:O3B	1.61	1.00
1:E:489:PHE:HE2	2:E:902:NAD:C2A	1.75	0.99
1:A:696:ASN:ND2	1:A:699:ALA:CB	2.25	0.99
1:A:688:ALA:O	1:A:692:GLU:HG3	1.63	0.99
1:F:646:LEU:HD21	2:F:902:NAD:C8A	1.93	0.98
1:E:546:GLY:HA3	2:E:902:NAD:H52N	1.03	0.98
1:F:642:MET:HG3	2:F:902:NAD:C6A	1.92	0.98
1:B:696:ASN:HD21	1:B:699:ALA:HB3	0.84	0.97
1:B:693:GLY:HA2	1:B:700:ARG:HH21	1.30	0.97
1:F:737:HIS:NE2	2:F:902:NAD:H5N	1.83	0.92
1:C:214:ALA:CB	2:C:901:NAD:O2D	2.17	0.91
1:D:214:ALA:HB2	2:D:901:NAD:O2D	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ASN:ND2	1:A:699:ALA:HB3	1.85	0.90
1:B:139:HIS:HD2	2:B:901:NAD:H51A	1.37	0.89
1:F:598:THR:CG2	2:F:902:NAD:N7A	2.34	0.89
1:E:489:PHE:HE2	2:E:902:NAD:H2A	1.38	0.88
1:F:642:MET:SD	2:F:902:NAD:N6A	2.47	0.88
1:E:489:PHE:CE2	2:E:902:NAD:C2A	2.57	0.86
1:D:693:GLY:HA2	1:D:700:ARG:HH21	1.40	0.86
1:B:696:ASN:ND2	1:B:696:ASN:O	2.09	0.85
1:B:695:LYS:HB2	1:B:695:LYS:NZ	1.89	0.85
1:A:690:TYR:HE2	1:A:809:LEU:CA	1.90	0.85
1:A:696:ASN:HD21	1:A:699:ALA:CB	1.88	0.84
1:A:696:ASN:ND2	1:A:699:ALA:HB2	1.88	0.84
1:A:367:HIS:HE1	2:A:901:NAD:N7N	1.76	0.83
1:E:139:HIS:HA	2:E:901:NAD:O3B	1.79	0.82
1:D:139:HIS:HD2	2:D:901:NAD:H51A	1.43	0.82
1:F:598:THR:HG22	2:F:902:NAD:C8A	2.11	0.80
1:F:642:MET:CG	2:F:902:NAD:C6A	2.59	0.80
1:A:693:GLY:CA	1:A:700:ARG:HH21	1.95	0.79
1:C:214:ALA:HB2	2:C:901:NAD:O2D	1.82	0.79
1:B:693:GLY:CA	1:B:700:ARG:HH21	1.96	0.79
1:F:737:HIS:CD2	2:F:902:NAD:H5N	2.17	0.79
1:E:139:HIS:HD2	2:E:901:NAD:H51A	1.46	0.79
1:B:489:PHE:CE2	2:B:902:NAD:C2A	2.67	0.78
1:E:693:GLY:HA2	1:E:700:ARG:NH2	1.97	0.78
1:A:688:ALA:O	1:A:692:GLU:CG	2.30	0.77
1:E:489:PHE:CE2	2:E:902:NAD:H2A	2.17	0.77
1:B:139:HIS:CA	2:B:901:NAD:O3B	2.31	0.77
1:F:642:MET:HA	2:F:902:NAD:N1A	2.01	0.76
1:B:489:PHE:HE2	2:B:902:NAD:C2A	2.00	0.75
1:A:598:THR:HG22	2:A:902:NAD:N7A	2.00	0.75
1:D:214:ALA:CB	2:D:901:NAD:HO2N	1.99	0.74
1:A:598:THR:CG2	2:A:902:NAD:N7A	2.51	0.74
1:E:489:PHE:CE2	2:E:902:NAD:N3A	2.56	0.74
1:F:646:LEU:CD2	2:F:902:NAD:C8A	2.66	0.73
1:B:688:ALA:O	1:B:692:GLU:HG2	1.89	0.73
1:C:693:GLY:HA2	1:C:700:ARG:HH21	1.53	0.72
1:A:367:HIS:HE1	2:A:901:NAD:H72N	1.36	0.72
1:B:139:HIS:HD2	2:B:901:NAD:C5B	2.03	0.71
1:B:139:HIS:CD2	2:B:901:NAD:H51A	2.25	0.70
1:A:367:HIS:CE1	2:A:901:NAD:N7N	2.58	0.70
1:C:550:ASP:OD2	2:C:902:NAD:H2N	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:HIS:CD2	2:E:901:NAD:H51A	2.26	0.69
1:E:693:GLY:CA	1:E:700:ARG:HH21	2.00	0.69
1:B:696:ASN:ND2	1:B:699:ALA:CB	2.25	0.68
1:E:335:GLU:OE2	2:E:901:NAD:O2D	2.11	0.68
1:F:598:THR:CG2	2:F:902:NAD:C8A	2.72	0.67
1:D:112:PRO:CB	2:D:901:NAD:O2N	2.43	0.67
1:A:214:ALA:CB	2:A:901:NAD:O2D	2.43	0.67
1:D:214:ALA:HB1	2:D:901:NAD:HO2N	1.60	0.66
1:A:198:MET:HG3	2:A:901:NAD:C1B	2.25	0.66
1:B:198:MET:HG3	2:B:901:NAD:C8A	2.26	0.66
1:F:642:MET:HG3	2:F:902:NAD:N1A	2.12	0.65
1:D:367:HIS:HE1	2:D:901:NAD:N7N	1.93	0.65
1:D:112:PRO:HB2	2:D:901:NAD:O2N	1.97	0.65
1:D:214:ALA:CA	2:D:901:NAD:O2D	2.45	0.65
1:F:139:HIS:HD2	2:F:901:NAD:C5B	2.09	0.65
1:A:690:TYR:CD2	1:A:809:LEU:HG	2.30	0.64
1:A:693:GLY:HA3	1:A:700:ARG:HH21	1.61	0.64
1:B:696:ASN:HD21	1:B:699:ALA:HB2	1.56	0.64
1:E:550:ASP:OD2	2:E:902:NAD:H2N	1.97	0.64
1:F:139:HIS:HD2	2:F:901:NAD:H51A	1.63	0.63
1:F:642:MET:HA	2:F:902:NAD:C2A	2.28	0.63
1:D:139:HIS:CD2	2:D:901:NAD:H51A	2.30	0.63
1:A:696:ASN:HD22	1:A:699:ALA:HB3	1.64	0.62
1:C:214:ALA:HB1	2:C:901:NAD:O2D	2.00	0.61
1:D:214:ALA:HA	2:D:901:NAD:O2D	2.00	0.61
1:A:519:ASP:OD1	2:A:902:NAD:O3D	2.20	0.60
1:F:646:LEU:HD23	2:F:902:NAD:C5A	2.32	0.60
1:A:693:GLY:HA2	1:A:700:ARG:HH21	1.63	0.60
1:D:113:THR:HG22	2:D:901:NAD:O1N	2.02	0.60
1:D:737:HIS:HB3	2:D:902:NAD:H3D	1.83	0.60
1:D:139:HIS:HA	2:D:901:NAD:O3B	2.02	0.60
1:A:3:VAL:HG23	1:A:171:ASP:H	1.69	0.58
1:E:3:VAL:HG23	1:E:171:ASP:H	1.69	0.58
1:D:603:SER:OG	2:D:902:NAD:N7N	2.37	0.58
1:A:215:GLY:HA2	1:A:364:GLY:HA3	1.86	0.58
1:E:696:ASN:N	1:E:697:PRO:CD	2.66	0.58
1:F:213:GLY:O	2:F:901:NAD:H2N	2.02	0.58
1:F:3:VAL:HG23	1:F:171:ASP:H	1.69	0.58
1:A:601:THR:HG23	2:A:902:NAD:C4N	2.34	0.57
1:A:690:TYR:CE2	1:A:809:LEU:CA	2.75	0.57
1:C:215:GLY:HA2	1:C:364:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HG3	2:A:901:NAD:O4B	2.03	0.57
1:D:215:GLY:HA2	1:D:364:GLY:HA3	1.86	0.57
1:C:3:VAL:HG23	1:C:171:ASP:H	1.69	0.57
1:D:3:VAL:HG23	1:D:171:ASP:H	1.69	0.57
1:A:644:LYS:HE2	1:A:690:TYR:HE1	1.70	0.57
1:B:3:VAL:HG23	1:B:171:ASP:H	1.69	0.57
1:B:215:GLY:HA2	1:B:364:GLY:HA3	1.86	0.57
1:F:215:GLY:HA2	1:F:364:GLY:HA3	1.86	0.57
1:A:644:LYS:HE2	1:A:690:TYR:CE1	2.40	0.57
1:B:692:GLU:N	1:B:692:GLU:OE2	2.38	0.56
1:F:642:MET:CG	2:F:902:NAD:N6A	2.68	0.56
1:E:215:GLY:HA2	1:E:364:GLY:HA3	1.86	0.56
1:B:214:ALA:CB	2:B:901:NAD:O2D	2.54	0.56
1:D:603:SER:CB	2:D:902:NAD:N7N	2.69	0.55
1:C:608:PHE:HB2	2:C:902:NAD:O7N	2.07	0.55
1:D:139:HIS:HD2	2:D:901:NAD:C5B	2.17	0.55
1:B:695:LYS:HB2	1:B:695:LYS:HZ1	1.70	0.55
1:F:646:LEU:CD2	2:F:902:NAD:N9A	2.71	0.54
1:E:423:SER:OG	1:F:440:ASN:ND2	2.39	0.54
1:C:693:GLY:CA	1:C:700:ARG:HH21	2.20	0.54
1:E:139:HIS:CA	2:E:901:NAD:O3B	2.53	0.54
1:A:374:ASP:OD1	1:A:374:ASP:N	2.40	0.54
1:D:765:GLN:OE1	1:E:463:ARG:NH2	2.42	0.54
1:E:337:LEU:HD11	2:E:901:NAD:O3D	2.08	0.54
1:F:642:MET:CA	2:F:902:NAD:N1A	2.69	0.53
1:D:688:ALA:O	1:D:692:GLU:HB2	2.08	0.53
1:D:753:ALA:HB1	1:D:772:ARG:HG3	1.91	0.53
1:F:139:HIS:HA	2:F:901:NAD:O3B	2.07	0.53
2:A:902:NAD:H52N	2:A:902:NAD:H6N	1.90	0.53
1:C:753:ALA:HB1	1:C:772:ARG:HG3	1.91	0.53
1:F:335:GLU:OE2	2:F:901:NAD:O2D	2.27	0.53
1:A:568:GLU:HG2	1:B:40:LEU:HD21	1.90	0.53
1:B:195:GLY:N	2:B:901:NAD:O2A	2.30	0.53
1:A:440:ASN:ND2	1:B:423:SER:OG	2.40	0.53
1:B:212:VAL:CG2	2:B:901:NAD:N7N	2.72	0.53
1:B:653:ASP:HB2	1:B:738:GLY:HA2	1.91	0.52
1:C:653:ASP:HB2	1:C:738:GLY:HA2	1.91	0.52
1:B:198:MET:CG	2:B:901:NAD:C8A	2.87	0.52
1:C:423:SER:OG	1:D:440:ASN:ND2	2.41	0.52
1:E:394:ILE:HB	1:F:444:VAL:HA	1.91	0.52
1:A:40:LEU:HD21	1:B:568:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ASP:HB2	1:D:738:GLY:HA2	1.91	0.52
1:A:653:ASP:HB2	1:A:738:GLY:HA2	1.91	0.52
1:E:653:ASP:HB2	1:E:738:GLY:HA2	1.91	0.52
1:D:737:HIS:CB	2:D:902:NAD:H3D	2.40	0.52
1:A:753:ALA:HB1	1:A:772:ARG:HG3	1.91	0.52
1:F:646:LEU:HD21	2:F:902:NAD:N7A	2.25	0.52
1:F:753:ALA:HB1	1:F:772:ARG:HG3	1.91	0.52
1:C:440:ASN:ND2	1:D:423:SER:OG	2.42	0.51
1:E:753:ALA:HB1	1:E:772:ARG:HG3	1.91	0.51
1:F:646:LEU:CD2	2:F:902:NAD:C4A	2.88	0.51
1:C:40:LEU:HD21	1:D:568:GLU:HG2	1.92	0.51
1:C:288:LYS:HB2	1:C:293:ASN:HB3	1.92	0.51
1:B:288:LYS:HB2	1:B:293:ASN:HB3	1.92	0.51
1:F:653:ASP:HB2	1:F:738:GLY:HA2	1.91	0.51
1:B:753:ALA:HB1	1:B:772:ARG:HG3	1.91	0.51
1:D:288:LYS:HB2	1:D:293:ASN:HB3	1.92	0.51
1:E:288:LYS:HB2	1:E:293:ASN:HB3	1.92	0.51
1:F:288:LYS:HB2	1:F:293:ASN:HB3	1.92	0.51
1:C:214:ALA:HB1	2:C:901:NAD:HO2N	1.74	0.51
1:F:728:LYS:HE3	1:F:835:ASP:HB3	1.93	0.51
1:D:546:GLY:HA3	2:D:902:NAD:O5D	2.11	0.50
1:A:288:LYS:HB2	1:A:293:ASN:HB3	1.92	0.50
1:D:82:ASP:OD1	1:D:82:ASP:N	2.43	0.50
1:D:728:LYS:HE3	1:D:835:ASP:HB3	1.93	0.50
1:B:463:ARG:NH2	1:C:765:GLN:OE1	2.44	0.50
1:F:82:ASP:OD1	1:F:82:ASP:N	2.43	0.50
1:D:212:VAL:HG21	2:D:901:NAD:O7N	2.12	0.50
1:E:40:LEU:HD21	1:F:568:GLU:HG2	1.92	0.50
1:E:374:ASP:OD1	1:E:374:ASP:N	2.40	0.50
1:B:82:ASP:OD1	1:B:82:ASP:N	2.43	0.50
1:C:728:LYS:HE3	1:C:835:ASP:HB3	1.93	0.50
1:D:463:ARG:NH2	1:E:765:GLN:OE1	2.41	0.50
1:D:597:THR:HB	2:D:902:NAD:H61A	1.76	0.50
1:B:139:HIS:CD2	2:B:901:NAD:H3B	2.47	0.50
1:A:423:SER:OG	1:B:440:ASN:ND2	2.45	0.50
1:B:765:GLN:OE1	1:C:463:ARG:NH2	2.44	0.50
1:C:82:ASP:OD1	1:C:82:ASP:N	2.43	0.49
1:E:568:GLU:HG2	1:F:40:LEU:HD21	1.94	0.49
1:B:728:LYS:HE3	1:B:835:ASP:HB3	1.93	0.49
1:E:728:LYS:HE3	1:E:835:ASP:HB3	1.93	0.49
1:B:744:LEU:HD12	1:B:861:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:744:LEU:HD12	1:E:861:THR:HG21	1.95	0.49
1:C:444:VAL:HA	1:D:394:ILE:HB	1.95	0.49
1:D:693:GLY:CA	1:D:700:ARG:HH21	2.18	0.49
1:A:28:GLN:NE2	1:A:32:ASP:OD1	2.46	0.49
1:B:374:ASP:OD1	1:B:374:ASP:N	2.40	0.49
1:A:728:LYS:HE3	1:A:835:ASP:HB3	1.93	0.49
1:C:568:GLU:HG2	1:D:40:LEU:HD21	1.95	0.49
1:A:756:ASN:N	1:A:756:ASN:OD1	2.46	0.49
1:C:374:ASP:OD1	1:C:374:ASP:N	2.40	0.49
1:E:28:GLN:NE2	1:E:32:ASP:OD1	2.46	0.49
1:E:440:ASN:ND2	1:F:423:SER:OG	2.46	0.49
1:D:28:GLN:NE2	1:D:32:ASP:OD1	2.46	0.49
1:D:756:ASN:OD1	1:D:756:ASN:N	2.46	0.49
1:A:744:LEU:HD12	1:A:861:THR:HG21	1.94	0.49
1:C:756:ASN:N	1:C:756:ASN:OD1	2.46	0.49
1:D:603:SER:HB2	2:D:902:NAD:N7N	2.28	0.49
1:C:394:ILE:HB	1:D:444:VAL:HA	1.95	0.49
1:D:486:THR:HG22	1:D:543:LEU:HB3	1.95	0.49
1:D:744:LEU:HD12	1:D:861:THR:HG21	1.95	0.49
1:C:744:LEU:HD12	1:C:861:THR:HG21	1.95	0.48
1:A:82:ASP:OD1	1:A:82:ASP:N	2.43	0.48
1:C:683:LYS:HD2	1:C:782:LEU:HB3	1.95	0.48
1:E:683:LYS:HD2	1:E:782:LEU:HB3	1.95	0.48
1:E:756:ASN:OD1	1:E:756:ASN:N	2.46	0.48
1:B:28:GLN:NE2	1:B:32:ASP:OD1	2.46	0.48
1:F:744:LEU:HD12	1:F:861:THR:HG21	1.94	0.48
2:A:901:NAD:H52A	2:A:901:NAD:O2N	2.12	0.48
1:B:486:THR:HG22	1:B:543:LEU:HB3	1.95	0.48
1:C:373:THR:O	1:C:397:ASN:ND2	2.45	0.48
1:C:486:THR:HG22	1:C:543:LEU:HB3	1.95	0.48
1:F:212:VAL:HB	2:F:901:NAD:N7N	2.29	0.48
1:D:728:LYS:HB3	1:D:832:LEU:HD22	1.96	0.48
1:D:367:HIS:CE1	2:D:901:NAD:N7N	2.78	0.48
1:A:486:THR:HG22	1:A:543:LEU:HB3	1.95	0.48
2:E:902:NAD:H2D	2:E:902:NAD:H6N	1.43	0.48
1:B:683:LYS:HD2	1:B:782:LEU:HB3	1.95	0.48
1:C:28:GLN:NE2	1:C:32:ASP:OD1	2.46	0.48
1:F:486:THR:HG22	1:F:543:LEU:HB3	1.95	0.48
1:F:683:LYS:HD2	1:F:782:LEU:HB3	1.95	0.48
1:A:463:ARG:HA	1:A:463:ARG:HD3	1.57	0.47
1:F:28:GLN:NE2	1:F:32:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:THR:HG22	1:E:543:LEU:HB3	1.95	0.47
1:E:728:LYS:HB3	1:E:832:LEU:HD22	1.96	0.47
1:D:683:LYS:HD2	1:D:782:LEU:HB3	1.95	0.47
1:F:728:LYS:HB3	1:F:832:LEU:HD22	1.96	0.47
1:F:756:ASN:N	1:F:756:ASN:OD1	2.46	0.47
1:A:683:LYS:HD2	1:A:782:LEU:HB3	1.95	0.47
1:A:728:LYS:HB3	1:A:832:LEU:HD22	1.96	0.47
1:B:16:VAL:HG21	1:B:135:ILE:HD11	1.97	0.47
1:C:16:VAL:HG21	1:C:135:ILE:HD11	1.96	0.47
1:C:737:HIS:HB3	2:C:902:NAD:H3D	1.96	0.47
1:E:82:ASP:OD1	1:E:82:ASP:N	2.43	0.47
1:E:423:SER:H	1:F:440:ASN:HD21	1.62	0.47
1:B:756:ASN:OD1	1:B:756:ASN:N	2.46	0.47
1:C:213:GLY:O	2:C:901:NAD:H2N	2.14	0.47
1:C:463:ARG:HA	1:C:463:ARG:HD3	1.57	0.47
1:D:16:VAL:HG21	1:D:135:ILE:HD11	1.97	0.47
1:A:373:THR:O	1:A:397:ASN:ND2	2.45	0.47
1:B:456:LEU:HD12	1:C:456:LEU:HD12	1.96	0.47
1:C:423:SER:H	1:D:440:ASN:HD21	1.61	0.47
1:D:456:LEU:HD12	1:E:456:LEU:HD12	1.95	0.47
1:E:195:GLY:N	2:E:901:NAD:O2A	2.44	0.47
1:F:16:VAL:HG21	1:F:135:ILE:HD11	1.97	0.47
1:A:16:VAL:HG21	1:A:135:ILE:HD11	1.96	0.47
1:A:692:GLU:H	1:A:692:GLU:HG2	1.39	0.47
1:A:693:GLY:CA	1:A:700:ARG:NH2	2.74	0.47
1:B:728:LYS:HB3	1:B:832:LEU:HD22	1.96	0.47
1:D:111:VAL:HG22	1:D:138:PRO:HA	1.97	0.47
1:E:444:VAL:HA	1:F:394:ILE:HB	1.96	0.47
1:F:646:LEU:HD23	2:F:902:NAD:C4A	2.45	0.47
1:B:489:PHE:CE2	2:B:902:NAD:H2A	2.47	0.46
1:A:111:VAL:HG22	1:A:138:PRO:HA	1.97	0.46
1:E:373:THR:O	1:E:397:ASN:ND2	2.45	0.46
1:D:130:THR:OG1	1:D:132:ASN:ND2	2.48	0.46
1:D:139:HIS:CA	2:D:901:NAD:O3B	2.63	0.46
1:E:130:THR:OG1	1:E:132:ASN:ND2	2.48	0.46
1:E:16:VAL:HG21	1:E:135:ILE:HD11	1.96	0.46
1:B:111:VAL:HG22	1:B:138:PRO:HA	1.97	0.46
1:C:728:LYS:HB3	1:C:832:LEU:HD22	1.96	0.46
1:E:463:ARG:HD3	1:E:463:ARG:HA	1.57	0.46
1:A:644:LYS:HB3	1:A:690:TYR:HE1	1.81	0.46
1:B:693:GLY:CA	1:B:700:ARG:NH2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HG22	1:C:138:PRO:HA	1.97	0.46
1:C:440:ASN:HD21	1:D:423:SER:H	1.63	0.46
1:E:208:PRO:HB3	1:F:428:SER:HB3	1.97	0.46
1:E:440:ASN:HD21	1:F:423:SER:H	1.64	0.46
1:C:552:ALA:HA	1:C:555:MET:HG2	1.98	0.46
1:E:489:PHE:CD2	2:E:902:NAD:N3A	2.83	0.46
1:E:552:ALA:HA	1:E:555:MET:HG2	1.98	0.46
1:B:130:THR:OG1	1:B:132:ASN:ND2	2.48	0.45
1:C:208:PRO:HB3	1:D:428:SER:HB3	1.98	0.45
1:E:456:LEU:HD21	1:E:712:ILE:HG23	1.98	0.45
1:D:552:ALA:HA	1:D:555:MET:HG2	1.98	0.45
1:A:428:SER:HB3	1:B:208:PRO:HB3	1.97	0.45
1:B:373:THR:O	1:B:397:ASN:ND2	2.45	0.45
1:F:737:HIS:CD2	2:F:902:NAD:C5N	2.96	0.45
1:D:373:THR:O	1:D:397:ASN:ND2	2.45	0.45
1:E:111:VAL:HG22	1:E:138:PRO:HA	1.97	0.45
1:F:111:VAL:HG22	1:F:138:PRO:HA	1.97	0.45
1:A:601:THR:CG2	2:A:902:NAD:C4N	2.94	0.45
1:F:130:THR:OG1	1:F:132:ASN:ND2	2.48	0.45
1:A:440:ASN:HD21	1:B:423:SER:H	1.65	0.45
1:A:456:LEU:HD21	1:A:712:ILE:HG23	1.99	0.45
1:B:139:HIS:CD2	2:B:901:NAD:C5B	2.93	0.45
1:C:377:ASN:HD21	1:E:695:LYS:HA	1.80	0.45
1:A:130:THR:OG1	1:A:132:ASN:ND2	2.48	0.45
1:D:367:HIS:HE1	2:D:901:NAD:H72N	1.63	0.45
1:F:642:MET:HB2	2:F:902:NAD:H62A	1.82	0.45
1:A:213:GLY:O	2:A:901:NAD:H2N	2.16	0.45
1:A:444:VAL:HA	1:B:394:ILE:HB	1.98	0.45
1:B:112:PRO:CB	2:B:901:NAD:O2N	2.65	0.45
1:D:516:VAL:HA	1:D:524:ILE:HD12	1.99	0.45
1:E:724:SER:OG	1:E:836:ALA:O	2.32	0.45
1:F:456:LEU:HD21	1:F:712:ILE:HG23	1.98	0.45
1:B:463:ARG:HA	1:B:463:ARG:HD3	1.57	0.44
1:B:552:ALA:HA	1:B:555:MET:HG2	1.98	0.44
1:C:516:VAL:HA	1:C:524:ILE:HD12	1.99	0.44
1:B:114:THR:CG2	2:B:901:NAD:H51N	2.47	0.44
1:C:456:LEU:HD21	1:C:712:ILE:HG23	1.98	0.44
1:F:646:LEU:CD2	2:F:902:NAD:C5A	2.95	0.44
1:B:6:VAL:O	1:B:10:ASN:ND2	2.50	0.44
1:D:456:LEU:HD21	1:D:712:ILE:HG23	1.98	0.44
1:F:6:VAL:O	1:F:10:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:SER:H	1:B:440:ASN:HD21	1.65	0.44
1:A:838:ASP:OD1	1:A:838:ASP:N	2.51	0.44
1:B:456:LEU:HD21	1:B:712:ILE:HG23	1.99	0.44
1:A:214:ALA:HB1	2:A:901:NAD:O2D	2.17	0.44
1:B:838:ASP:OD1	1:B:838:ASP:N	2.51	0.44
1:C:428:SER:HB3	1:D:208:PRO:HB3	1.99	0.44
1:C:866:ASP:OD1	1:C:866:ASP:N	2.51	0.44
1:F:139:HIS:CA	2:F:901:NAD:O3B	2.65	0.44
1:A:214:ALA:HB2	2:A:901:NAD:O2D	2.18	0.44
1:A:229:ARG:NH2	1:B:767:ASP:OD1	2.51	0.44
1:B:606:THR:HG22	1:B:715:ALA:HB2	2.00	0.44
1:C:130:THR:OG1	1:C:132:ASN:ND2	2.48	0.44
1:C:838:ASP:N	1:C:838:ASP:OD1	2.51	0.44
1:E:6:VAL:O	1:E:10:ASN:ND2	2.50	0.44
1:A:367:HIS:CE1	2:A:901:NAD:H72N	2.26	0.44
1:A:688:ALA:O	1:A:692:GLU:HG2	2.17	0.44
1:E:606:THR:HG22	1:E:715:ALA:HB2	2.00	0.43
1:F:374:ASP:OD1	1:F:374:ASP:N	2.40	0.43
1:B:489:PHE:CE2	2:B:902:NAD:N3A	2.86	0.43
1:D:374:ASP:OD1	1:D:374:ASP:N	2.40	0.43
1:F:516:VAL:HA	1:F:524:ILE:HD12	1.99	0.43
1:D:6:VAL:O	1:D:10:ASN:ND2	2.50	0.43
1:D:838:ASP:OD1	1:D:838:ASP:N	2.51	0.43
1:F:552:ALA:HA	1:F:555:MET:HG2	1.99	0.43
1:A:552:ALA:HA	1:A:555:MET:HG2	1.98	0.43
1:C:6:VAL:O	1:C:10:ASN:ND2	2.50	0.43
1:E:516:VAL:HA	1:E:524:ILE:HD12	1.99	0.43
1:E:838:ASP:N	1:E:838:ASP:OD1	2.51	0.43
1:F:373:THR:O	1:F:397:ASN:ND2	2.45	0.43
1:F:642:MET:CB	2:F:902:NAD:N1A	2.81	0.43
1:A:6:VAL:O	1:A:10:ASN:ND2	2.50	0.43
1:A:516:VAL:HA	1:A:524:ILE:HD12	1.99	0.43
1:B:516:VAL:HA	1:B:524:ILE:HD12	1.99	0.43
1:C:377:ASN:ND2	1:E:695:LYS:HA	2.33	0.43
1:A:63:GLU:HG2	1:B:850:LEU:HA	2.01	0.43
1:C:606:THR:HG22	1:C:715:ALA:HB2	2.00	0.43
1:D:463:ARG:HA	1:D:463:ARG:HD3	1.57	0.43
1:D:550:ASP:OD2	2:D:902:NAD:H2N	2.19	0.43
1:D:606:THR:HG22	1:D:715:ALA:HB2	2.00	0.43
1:A:418:THR:O	1:A:418:THR:OG1	2.36	0.42
1:E:332:PHE:HD1	1:E:332:PHE:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HG3	2:A:901:NAD:N9A	2.34	0.42
1:C:214:ALA:CA	2:C:901:NAD:O2D	2.67	0.42
1:F:598:THR:CG2	2:F:902:NAD:H8A	2.48	0.42
1:F:606:THR:HG22	1:F:715:ALA:HB2	2.00	0.42
1:A:606:THR:HG22	1:A:715:ALA:HB2	2.00	0.42
1:E:439:ILE:HD13	1:E:439:ILE:HA	1.90	0.42
1:A:690:TYR:CD2	1:A:809:LEU:HA	2.46	0.42
1:B:696:ASN:ND2	1:B:696:ASN:C	2.73	0.42
1:C:737:HIS:CB	2:C:902:NAD:H3D	2.50	0.42
1:C:439:ILE:HD13	1:C:439:ILE:HA	1.91	0.42
1:D:439:ILE:HD13	1:D:439:ILE:HA	1.91	0.42
1:D:608:PHE:HB2	2:D:902:NAD:O7N	2.19	0.42
1:A:198:MET:HG2	2:A:901:NAD:C4A	2.50	0.42
1:F:345:ARG:O	1:F:355:LYS:NZ	2.46	0.42
1:A:696:ASN:HD22	1:A:699:ALA:CB	2.22	0.42
1:B:34:ILE:HG22	1:B:128:LEU:HD13	2.02	0.42
1:C:34:ILE:HG22	1:C:128:LEU:HD13	2.02	0.42
1:F:642:MET:SD	2:F:902:NAD:C6A	3.05	0.42
1:B:737:HIS:HB3	2:B:902:NAD:H3D	2.01	0.41
1:A:208:PRO:HB3	1:B:428:SER:HB3	2.01	0.41
1:A:767:ASP:OD1	1:B:229:ARG:NH2	2.53	0.41
1:C:724:SER:OG	1:C:836:ALA:O	2.32	0.41
1:D:367:HIS:CE1	2:D:901:NAD:H71N	2.38	0.41
1:F:34:ILE:HG22	1:F:128:LEU:HD13	2.02	0.41
1:A:550:ASP:OD2	2:A:902:NAD:H2N	2.20	0.41
1:A:367:HIS:CE1	2:A:901:NAD:H71N	2.37	0.41
1:B:212:VAL:HB	2:B:901:NAD:N7N	2.35	0.41
1:C:820:VAL:O	1:C:862:TYR:OH	2.35	0.41
1:E:34:ILE:HG22	1:E:128:LEU:HD13	2.02	0.41
1:A:34:ILE:HG22	1:A:128:LEU:HD13	2.02	0.41
1:A:394:ILE:HB	1:B:444:VAL:HA	2.02	0.41
1:B:212:VAL:HG23	2:B:901:NAD:H71N	1.85	0.41
1:F:418:THR:O	1:F:418:THR:OG1	2.36	0.41
1:F:693:GLY:HA3	1:F:700:ARG:HH21	1.85	0.41
1:B:724:SER:OG	1:B:836:ALA:O	2.32	0.41
1:E:345:ARG:O	1:E:355:LYS:NZ	2.46	0.41
1:F:646:LEU:CD2	2:F:902:NAD:N7A	2.83	0.41
1:C:687:PRO:O	1:C:691:HIS:HD2	2.03	0.41
1:D:114:THR:HG21	2:D:901:NAD:H51N	2.02	0.41
1:E:857:ILE:O	1:E:861:THR:OG1	2.34	0.41
1:A:690:TYR:HD2	1:A:809:LEU:CD1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:NAD:C5B	2:A:901:NAD:PN	3.09	0.41
1:B:375:GLN:OE1	1:B:397:ASN:ND2	2.47	0.41
1:D:345:ARG:O	1:D:355:LYS:NZ	2.46	0.41
1:D:500:THR:HB	1:D:504:LYS:HE2	2.03	0.41
1:F:489:PHE:CD2	2:F:902:NAD:O2B	2.73	0.41
1:C:63:GLU:HG2	1:D:850:LEU:HA	2.03	0.41
1:A:639:VAL:HG13	1:A:700:ARG:HG3	2.03	0.40
1:C:500:THR:HB	1:C:504:LYS:HE2	2.03	0.40
1:D:721:VAL:HG21	1:D:849:PRO:HG3	2.04	0.40
1:A:500:THR:HB	1:A:504:LYS:HE2	2.03	0.40
1:A:721:VAL:HG21	1:A:849:PRO:HG3	2.04	0.40
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.98	0.40
1:D:23:TYR:HB2	1:D:163:PRO:HG2	2.03	0.40
1:F:639:VAL:HG13	1:F:700:ARG:HG3	2.03	0.40
1:F:642:MET:CG	2:F:902:NAD:N1A	2.81	0.40
1:B:139:HIS:CD2	2:B:901:NAD:C3B	3.05	0.40
1:B:139:HIS:CB	2:B:901:NAD:O3B	2.69	0.40
1:B:213:GLY:O	2:B:901:NAD:H2N	2.21	0.40
1:C:375:GLN:OE1	1:C:397:ASN:ND2	2.47	0.40
1:D:54:VAL:HG21	1:D:62:VAL:HG22	2.03	0.40
1:F:721:VAL:HG21	1:F:849:PRO:HG3	2.04	0.40
1:F:838:ASP:OD1	1:F:838:ASP:N	2.51	0.40
1:B:23:TYR:HB2	1:B:163:PRO:HG2	2.04	0.40
1:F:500:THR:HB	1:F:504:LYS:HE2	2.03	0.40
1:A:54:VAL:HG21	1:A:62:VAL:HG22	2.03	0.40
1:A:690:TYR:C	1:A:690:TYR:CD1	2.92	0.40
1:D:34:ILE:HG22	1:D:128:LEU:HD13	2.02	0.40
1:E:375:GLN:OE1	1:E:397:ASN:ND2	2.47	0.40
1:E:428:SER:HB3	1:F:208:PRO:HB3	2.03	0.40
1:F:54:VAL:HG21	1:F:62:VAL:HG22	2.04	0.40

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	867/893 (97%)	829 (96%)	38 (4%)	0	100	100
1	B	867/893 (97%)	829 (96%)	38 (4%)	0	100	100
1	C	867/893 (97%)	830 (96%)	37 (4%)	0	100	100
1	D	867/893 (97%)	831 (96%)	36 (4%)	0	100	100
1	E	867/893 (97%)	829 (96%)	38 (4%)	0	100	100
1	F	867/893 (97%)	828 (96%)	39 (4%)	0	100	100
All	All	5202/5358 (97%)	4976 (96%)	226 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	694/709 (98%)	673 (97%)	21 (3%)	41	70
1	B	694/709 (98%)	670 (96%)	24 (4%)	36	67
1	C	694/709 (98%)	674 (97%)	20 (3%)	42	71
1	D	694/709 (98%)	674 (97%)	20 (3%)	42	71
1	E	694/709 (98%)	672 (97%)	22 (3%)	39	69
1	F	694/709 (98%)	674 (97%)	20 (3%)	42	71
All	All	4164/4254 (98%)	4037 (97%)	127 (3%)	44	70

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	6	VAL
1	A	21	ARG
1	A	32	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	70	HIS
1	A	74	GLU
1	A	207	LYS
1	A	241	ASP
1	A	288	LYS
1	A	332	PHE
1	A	341	LEU
1	A	429	ILE
1	A	438	LEU
1	A	463	ARG
1	A	576	ILE
1	A	628	THR
1	A	692	GLU
1	A	694	SER
1	A	695	LYS
1	A	721	VAL
1	A	802	LEU
1	B	3	VAL
1	B	6	VAL
1	B	21	ARG
1	B	32	ASP
1	B	70	HIS
1	B	74	GLU
1	B	207	LYS
1	B	241	ASP
1	B	285	VAL
1	B	288	LYS
1	B	332	PHE
1	B	341	LEU
1	B	429	ILE
1	B	438	LEU
1	B	463	ARG
1	B	576	ILE
1	B	628	THR
1	B	691	HIS
1	B	692	GLU
1	B	695	LYS
1	B	696	ASN
1	B	698	VAL
1	B	721	VAL
1	B	802	LEU
1	C	3	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	6	VAL
1	C	21	ARG
1	C	32	ASP
1	C	70	HIS
1	C	74	GLU
1	C	207	LYS
1	C	241	ASP
1	C	285	VAL
1	C	288	LYS
1	C	332	PHE
1	C	341	LEU
1	C	429	ILE
1	C	438	LEU
1	C	463	ARG
1	C	576	ILE
1	C	628	THR
1	C	695	LYS
1	C	721	VAL
1	C	802	LEU
1	D	3	VAL
1	D	6	VAL
1	D	21	ARG
1	D	32	ASP
1	D	70	HIS
1	D	74	GLU
1	D	207	LYS
1	D	241	ASP
1	D	285	VAL
1	D	288	LYS
1	D	332	PHE
1	D	341	LEU
1	D	429	ILE
1	D	438	LEU
1	D	463	ARG
1	D	576	ILE
1	D	628	THR
1	D	694	SER
1	D	721	VAL
1	D	802	LEU
1	E	3	VAL
1	E	6	VAL
1	E	21	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	32	ASP
1	E	70	HIS
1	E	74	GLU
1	E	207	LYS
1	E	241	ASP
1	E	285	VAL
1	E	288	LYS
1	E	332	PHE
1	E	341	LEU
1	E	429	ILE
1	E	438	LEU
1	E	463	ARG
1	E	576	ILE
1	E	628	THR
1	E	692	GLU
1	E	694	SER
1	E	695	LYS
1	E	721	VAL
1	E	802	LEU
1	F	3	VAL
1	F	6	VAL
1	F	21	ARG
1	F	32	ASP
1	F	70	HIS
1	F	74	GLU
1	F	207	LYS
1	F	241	ASP
1	F	285	VAL
1	F	288	LYS
1	F	332	PHE
1	F	341	LEU
1	F	429	ILE
1	F	438	LEU
1	F	463	ARG
1	F	576	ILE
1	F	628	THR
1	F	695	LYS
1	F	721	VAL
1	F	802	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	147	ASN
1	A	440	ASN
1	A	618	GLN
1	A	696	ASN
1	A	765	GLN
1	B	132	ASN
1	B	139	HIS
1	B	147	ASN
1	B	440	ASN
1	B	618	GLN
1	B	696	ASN
1	C	132	ASN
1	C	147	ASN
1	C	377	ASN
1	C	440	ASN
1	C	618	GLN
1	C	691	HIS
1	D	132	ASN
1	D	147	ASN
1	D	440	ASN
1	D	618	GLN
1	E	132	ASN
1	E	147	ASN
1	E	440	ASN
1	E	618	GLN
1	F	132	ASN
1	F	139	HIS
1	F	147	ASN
1	F	440	ASN
1	F	618	GLN
1	F	691	HIS
1	F	765	GLN

### 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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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
2	NAD	D	902	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	A	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	C	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.31	5 (10%)
2	NAD	E	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	D	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	B	902	-	42,48,48	0.82	1 (2%)	50,73,73	1.31	5 (10%)
2	NAD	A	902	-	42,48,48	0.82	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	F	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.31	5 (10%)
2	NAD	F	902	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	E	902	-	42,48,48	0.82	1 (2%)	50,73,73	1.31	5 (10%)
2	NAD	B	901	-	42,48,48	0.81	1 (2%)	50,73,73	1.31	5 (10%)
2	NAD	C	902	-	42,48,48	0.81	1 (2%)	50,73,73	1.30	5 (10%)

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
2	NAD	D	902	-	-	12/26/62/62	0/5/5/5
2	NAD	A	901	-	-	6/26/62/62	0/5/5/5
2	NAD	C	901	-	-	8/26/62/62	0/5/5/5
2	NAD	E	901	-	-	6/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	901	-	-	10/26/62/62	0/5/5/5
2	NAD	B	902	-	-	12/26/62/62	0/5/5/5
2	NAD	A	902	-	-	9/26/62/62	0/5/5/5
2	NAD	F	901	-	-	9/26/62/62	0/5/5/5
2	NAD	F	902	-	-	14/26/62/62	0/5/5/5
2	NAD	E	902	-	-	15/26/62/62	0/5/5/5
2	NAD	B	901	-	-	12/26/62/62	0/5/5/5
2	NAD	C	902	-	-	11/26/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	NAD	C5A-C4A	2.52	1.47	1.40
2	F	902	NAD	C5A-C4A	2.51	1.47	1.40
2	A	902	NAD	C5A-C4A	2.51	1.47	1.40
2	E	902	NAD	C5A-C4A	2.51	1.47	1.40
2	F	901	NAD	C5A-C4A	2.50	1.47	1.40
2	C	902	NAD	C5A-C4A	2.49	1.47	1.40
2	C	901	NAD	C5A-C4A	2.49	1.47	1.40
2	B	902	NAD	C5A-C4A	2.49	1.47	1.40
2	D	901	NAD	C5A-C4A	2.48	1.47	1.40
2	B	901	NAD	C5A-C4A	2.48	1.47	1.40
2	A	901	NAD	C5A-C4A	2.48	1.47	1.40
2	D	902	NAD	C5A-C4A	2.48	1.47	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	NAD	PN-O3-PA	-3.61	120.43	132.83
2	C	901	NAD	PN-O3-PA	-3.61	120.44	132.83
2	B	901	NAD	PN-O3-PA	-3.60	120.47	132.83
2	B	902	NAD	PN-O3-PA	-3.59	120.51	132.83
2	E	901	NAD	PN-O3-PA	-3.58	120.53	132.83
2	D	901	NAD	PN-O3-PA	-3.58	120.53	132.83
2	F	902	NAD	PN-O3-PA	-3.57	120.57	132.83
2	F	901	NAD	PN-O3-PA	-3.57	120.59	132.83
2	C	902	NAD	PN-O3-PA	-3.56	120.59	132.83
2	A	901	NAD	PN-O3-PA	-3.55	120.63	132.83
2	E	902	NAD	PN-O3-PA	-3.55	120.63	132.83
2	D	902	NAD	PN-O3-PA	-3.55	120.64	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	902	NAD	C3D-C2D-C1D	3.47	106.21	100.98
2	B	902	NAD	C3D-C2D-C1D	3.45	106.17	100.98
2	E	902	NAD	C3B-C2B-C1B	3.45	106.17	100.98
2	F	901	NAD	C3B-C2B-C1B	3.44	106.16	100.98
2	D	902	NAD	C3D-C2D-C1D	3.44	106.15	100.98
2	B	901	NAD	C3D-C2D-C1D	3.44	106.15	100.98
2	C	901	NAD	C3D-C2D-C1D	3.43	106.14	100.98
2	C	902	NAD	C3D-C2D-C1D	3.43	106.14	100.98
2	F	902	NAD	C3D-C2D-C1D	3.43	106.14	100.98
2	A	902	NAD	C3B-C2B-C1B	3.42	106.13	100.98
2	F	901	NAD	C3D-C2D-C1D	3.42	106.13	100.98
2	E	901	NAD	C3D-C2D-C1D	3.42	106.12	100.98
2	D	901	NAD	C3D-C2D-C1D	3.41	106.11	100.98
2	C	902	NAD	C3B-C2B-C1B	3.41	106.11	100.98
2	B	901	NAD	C3B-C2B-C1B	3.41	106.11	100.98
2	A	901	NAD	C3B-C2B-C1B	3.40	106.10	100.98
2	D	902	NAD	C3B-C2B-C1B	3.40	106.10	100.98
2	D	901	NAD	C3B-C2B-C1B	3.39	106.08	100.98
2	F	902	NAD	C3B-C2B-C1B	3.39	106.08	100.98
2	A	901	NAD	C3D-C2D-C1D	3.38	106.07	100.98
2	B	902	NAD	C3B-C2B-C1B	3.38	106.07	100.98
2	C	901	NAD	C3B-C2B-C1B	3.38	106.06	100.98
2	A	902	NAD	C3D-C2D-C1D	3.37	106.05	100.98
2	E	901	NAD	C3B-C2B-C1B	3.33	106.00	100.98
2	A	901	NAD	N3A-C2A-N1A	-3.20	123.68	128.68
2	F	901	NAD	N3A-C2A-N1A	-3.19	123.69	128.68
2	B	901	NAD	N3A-C2A-N1A	-3.18	123.70	128.68
2	B	902	NAD	N3A-C2A-N1A	-3.18	123.71	128.68
2	E	902	NAD	N3A-C2A-N1A	-3.18	123.71	128.68
2	C	901	NAD	N3A-C2A-N1A	-3.18	123.71	128.68
2	D	902	NAD	N3A-C2A-N1A	-3.15	123.75	128.68
2	E	901	NAD	N3A-C2A-N1A	-3.15	123.75	128.68
2	F	902	NAD	N3A-C2A-N1A	-3.15	123.76	128.68
2	C	902	NAD	N3A-C2A-N1A	-3.14	123.76	128.68
2	A	902	NAD	N3A-C2A-N1A	-3.14	123.77	128.68
2	D	901	NAD	N3A-C2A-N1A	-3.13	123.78	128.68
2	E	902	NAD	C4A-C5A-N7A	-2.73	106.55	109.40
2	C	901	NAD	C4A-C5A-N7A	-2.73	106.56	109.40
2	F	901	NAD	C4A-C5A-N7A	-2.72	106.57	109.40
2	A	901	NAD	C4A-C5A-N7A	-2.71	106.57	109.40
2	F	902	NAD	C4A-C5A-N7A	-2.71	106.57	109.40
2	D	902	NAD	C4A-C5A-N7A	-2.71	106.57	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	NAD	C4A-C5A-N7A	-2.71	106.58	109.40
2	D	901	NAD	C4A-C5A-N7A	-2.70	106.59	109.40
2	B	901	NAD	C4A-C5A-N7A	-2.68	106.60	109.40
2	B	902	NAD	C4A-C5A-N7A	-2.68	106.60	109.40
2	E	901	NAD	C4A-C5A-N7A	-2.68	106.61	109.40
2	A	902	NAD	C4A-C5A-N7A	-2.67	106.62	109.40

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAD	C5B-O5B-PA-O1A
2	A	901	NAD	C5B-O5B-PA-O2A
2	A	901	NAD	C5B-O5B-PA-O3
2	A	902	NAD	C5D-O5D-PN-O3
2	A	902	NAD	C5D-O5D-PN-O2N
2	B	901	NAD	C5B-O5B-PA-O1A
2	B	901	NAD	PN-O3-PA-O5B
2	B	901	NAD	C3D-C4D-C5D-O5D
2	B	902	NAD	C5D-O5D-PN-O3
2	B	902	NAD	C5D-O5D-PN-O2N
2	B	902	NAD	O4D-C1D-N1N-C2N
2	B	902	NAD	O4D-C1D-N1N-C6N
2	B	902	NAD	C2D-C1D-N1N-C2N
2	C	901	NAD	C5B-O5B-PA-O1A
2	C	902	NAD	C5B-O5B-PA-O2A
2	C	902	NAD	C5D-O5D-PN-O3
2	C	902	NAD	C5D-O5D-PN-O2N
2	C	902	NAD	O4D-C1D-N1N-C2N
2	C	902	NAD	O4D-C1D-N1N-C6N
2	C	902	NAD	C2D-C1D-N1N-C2N
2	C	902	NAD	C2D-C1D-N1N-C6N
2	D	901	NAD	C5B-O5B-PA-O1A
2	D	901	NAD	C5B-O5B-PA-O2A
2	D	901	NAD	C3D-C4D-C5D-O5D
2	D	901	NAD	C2N-C3N-C7N-N7N
2	D	902	NAD	C5B-O5B-PA-O1A
2	D	902	NAD	C5B-O5B-PA-O2A
2	D	902	NAD	C5D-O5D-PN-O3
2	D	902	NAD	O4D-C1D-N1N-C2N
2	D	902	NAD	O4D-C1D-N1N-C6N
2	D	902	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	902	NAD	C2D-C1D-N1N-C6N
2	E	901	NAD	O4D-C1D-N1N-C2N
2	E	901	NAD	O4D-C1D-N1N-C6N
2	E	901	NAD	C2D-C1D-N1N-C2N
2	E	901	NAD	C2D-C1D-N1N-C6N
2	E	902	NAD	C5B-O5B-PA-O1A
2	E	902	NAD	C5B-O5B-PA-O2A
2	E	902	NAD	PA-O3-PN-O5D
2	E	902	NAD	C5D-O5D-PN-O1N
2	E	902	NAD	C5D-O5D-PN-O2N
2	E	902	NAD	O4D-C1D-N1N-C2N
2	E	902	NAD	C2D-C1D-N1N-C2N
2	F	901	NAD	C5B-O5B-PA-O1A
2	F	901	NAD	PN-O3-PA-O5B
2	F	901	NAD	O4D-C1D-N1N-C6N
2	F	902	NAD	C5B-O5B-PA-O2A
2	F	902	NAD	C3D-C4D-C5D-O5D
2	F	902	NAD	O4D-C1D-N1N-C2N
2	F	902	NAD	O4D-C1D-N1N-C6N
2	F	902	NAD	C2D-C1D-N1N-C2N
2	F	902	NAD	C2D-C1D-N1N-C6N
2	D	901	NAD	C4N-C3N-C7N-N7N
2	D	901	NAD	C2N-C3N-C7N-O7N
2	D	901	NAD	C4N-C3N-C7N-O7N
2	A	901	NAD	O4D-C4D-C5D-O5D
2	A	901	NAD	C3D-C4D-C5D-O5D
2	B	901	NAD	O4D-C4D-C5D-O5D
2	C	901	NAD	O4D-C4D-C5D-O5D
2	C	901	NAD	C3D-C4D-C5D-O5D
2	F	901	NAD	O4D-C4D-C5D-O5D
2	E	901	NAD	C4D-C5D-O5D-PN
2	D	901	NAD	O4D-C4D-C5D-O5D
2	F	902	NAD	O4D-C4D-C5D-O5D
2	F	901	NAD	C3D-C4D-C5D-O5D
2	D	901	NAD	C4D-C5D-O5D-PN
2	C	902	NAD	O4B-C4B-C5B-O5B
2	C	902	NAD	C3B-C4B-C5B-O5B
2	A	902	NAD	O4B-C4B-C5B-O5B
2	B	902	NAD	O4B-C4B-C5B-O5B
2	E	902	NAD	O4B-C4B-C5B-O5B
2	F	902	NAD	O4B-C4B-C5B-O5B
2	A	902	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	902	NAD	C3B-C4B-C5B-O5B
2	E	902	NAD	C3B-C4B-C5B-O5B
2	F	902	NAD	C3B-C4B-C5B-O5B
2	C	901	NAD	C4D-C5D-O5D-PN
2	B	901	NAD	C4D-C5D-O5D-PN
2	A	902	NAD	PA-O3-PN-O5D
2	F	902	NAD	PA-O3-PN-O5D
2	B	901	NAD	C5B-O5B-PA-O3
2	B	902	NAD	C5B-O5B-PA-O3
2	C	901	NAD	C5B-O5B-PA-O3
2	C	902	NAD	C5B-O5B-PA-O3
2	F	901	NAD	C5B-O5B-PA-O3
2	F	902	NAD	C5B-O5B-PA-O3
2	F	901	NAD	C3B-C4B-C5B-O5B
2	A	901	NAD	C4D-C5D-O5D-PN
2	B	901	NAD	C5B-O5B-PA-O2A
2	B	902	NAD	C5B-O5B-PA-O2A
2	C	901	NAD	C5B-O5B-PA-O2A
2	D	902	NAD	C5D-O5D-PN-O2N
2	F	901	NAD	C5B-O5B-PA-O2A
2	F	902	NAD	C5B-O5B-PA-O1A
2	A	902	NAD	C4N-C3N-C7N-N7N
2	C	901	NAD	C3B-C4B-C5B-O5B
2	A	902	NAD	C4N-C3N-C7N-O7N
2	B	901	NAD	C4N-C3N-C7N-O7N
2	F	901	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	C4N-C3N-C7N-N7N
2	C	901	NAD	O4B-C4B-C5B-O5B
2	B	902	NAD	PN-O3-PA-O2A
2	D	902	NAD	PN-O3-PA-O2A
2	A	902	NAD	C2N-C3N-C7N-N7N
2	A	902	NAD	C2N-C3N-C7N-O7N
2	D	902	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	C2N-C3N-C7N-O7N
2	B	901	NAD	C2N-C3N-C7N-N7N
2	B	902	NAD	C2D-C1D-N1N-C6N
2	D	901	NAD	C5B-O5B-PA-O3
2	D	902	NAD	C5B-O5B-PA-O3
2	E	902	NAD	C5B-O5B-PA-O3
2	E	902	NAD	C5D-O5D-PN-O3
2	E	902	NAD	C2D-C1D-N1N-C6N
2	B	901	NAD	C3B-C4B-C5B-O5B

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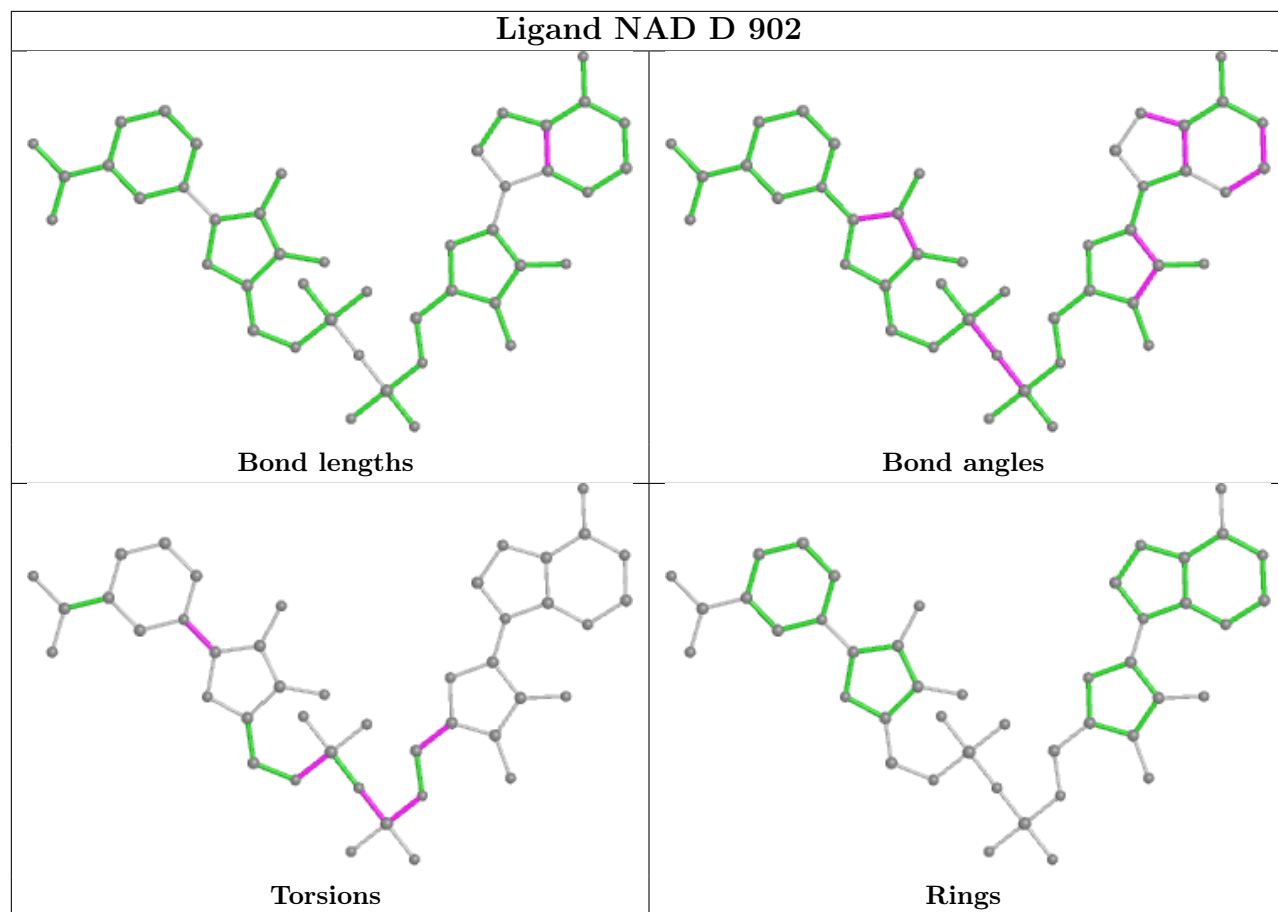
Mol	Chain	Res	Type	Atoms
2	D	902	NAD	PN-O3-PA-O1A
2	E	902	NAD	PN-O3-PA-O1A
2	E	902	NAD	PN-O3-PA-O2A
2	F	902	NAD	PN-O3-PA-O1A
2	B	902	NAD	C5B-O5B-PA-O1A
2	C	902	NAD	C5B-O5B-PA-O1A
2	F	902	NAD	C5D-O5D-PN-O1N
2	E	901	NAD	O4D-C4D-C5D-O5D
2	E	902	NAD	O4D-C4D-C5D-O5D

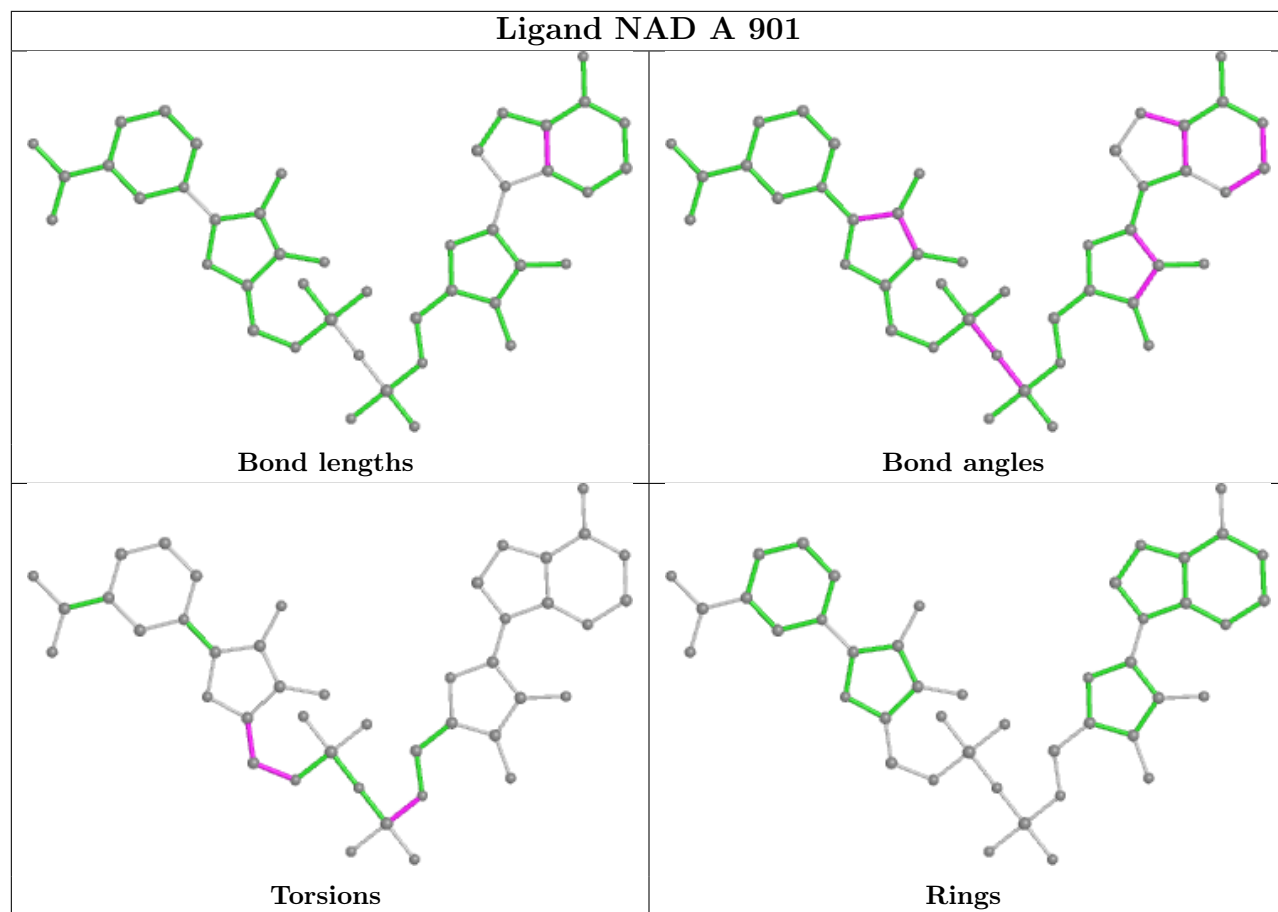
There are no ring outliers.

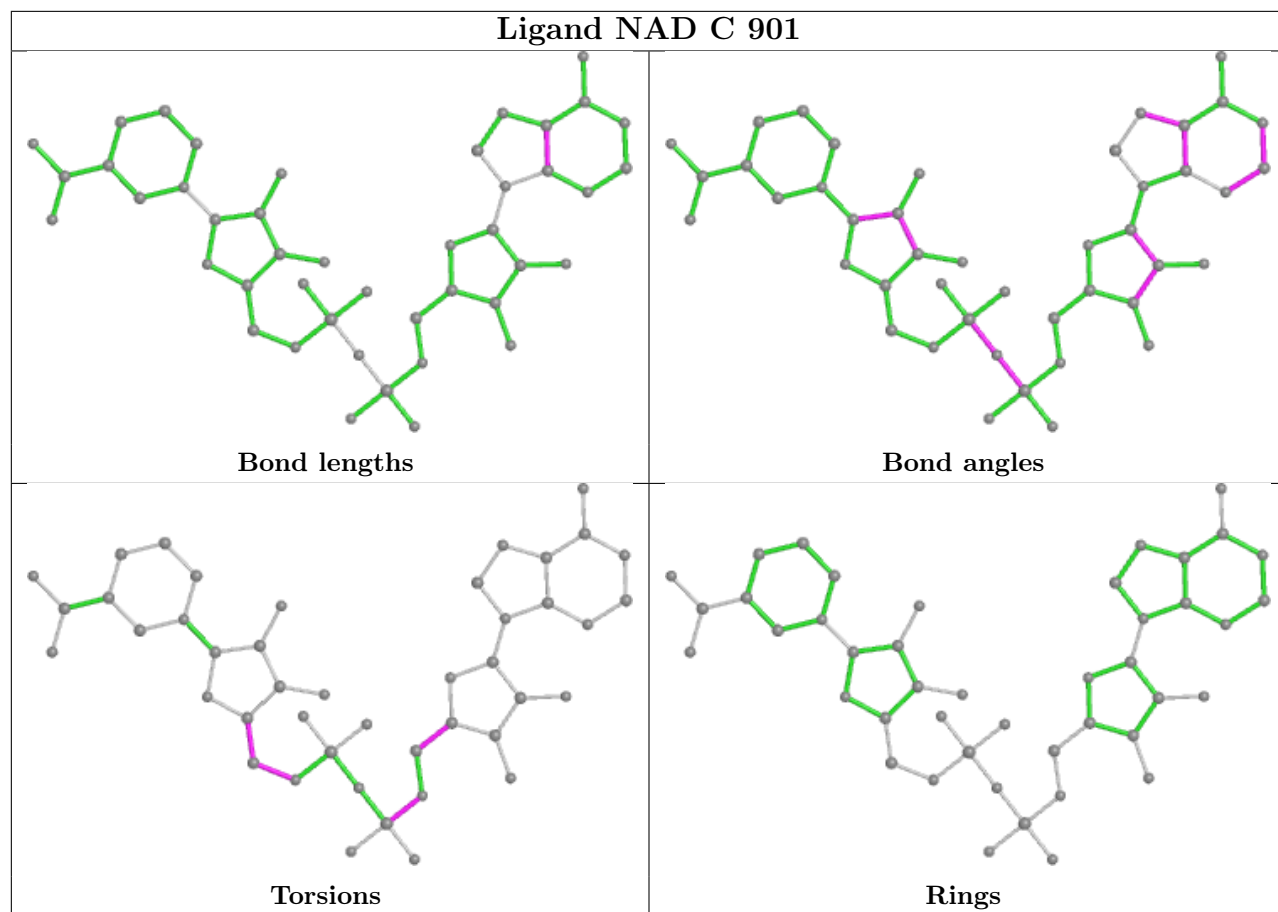
12 monomers are involved in 140 short contacts:

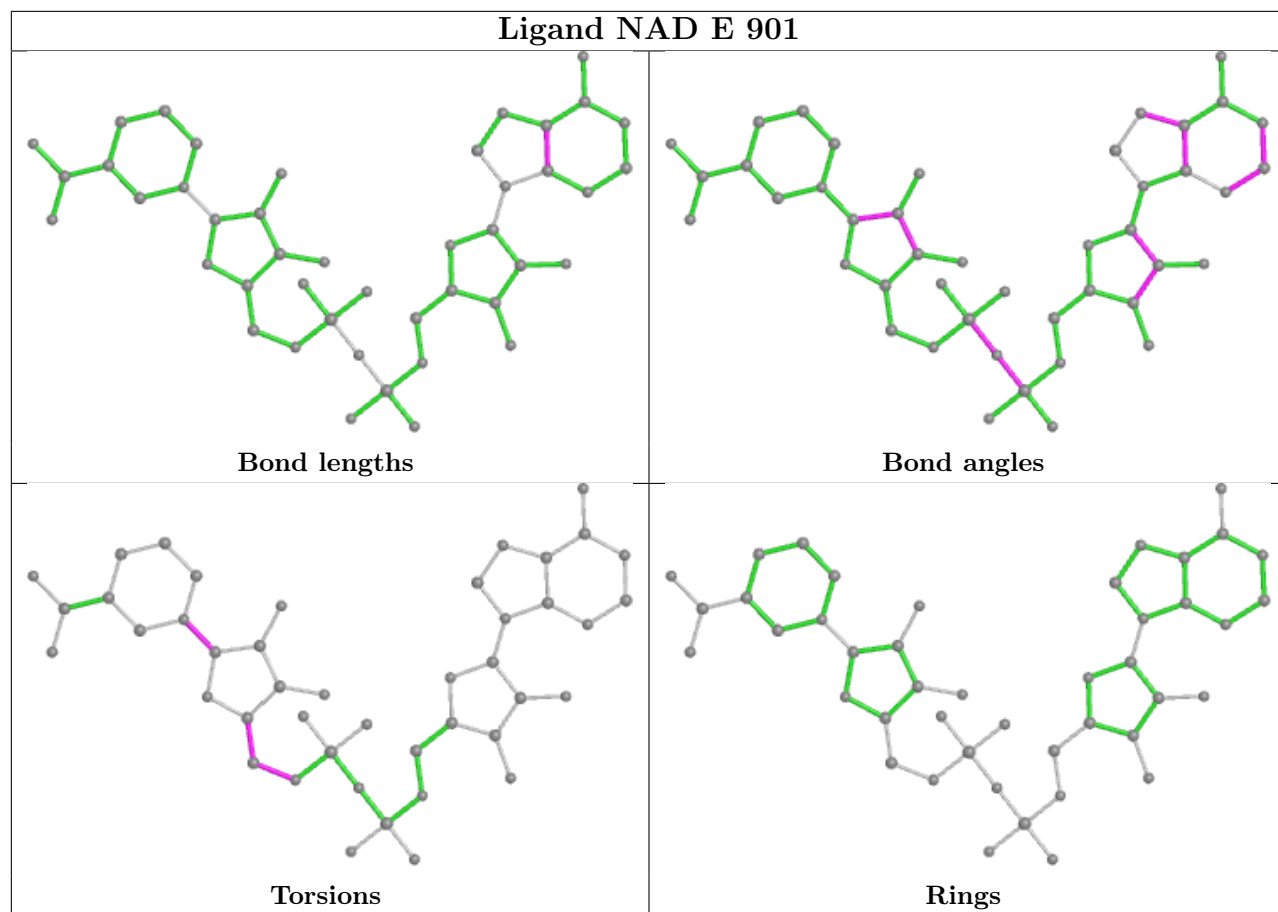
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	NAD	9	0
2	A	901	NAD	15	0
2	C	901	NAD	6	0
2	E	901	NAD	7	0
2	D	901	NAD	20	0
2	B	902	NAD	5	0
2	A	902	NAD	7	0
2	F	901	NAD	7	0
2	F	902	NAD	30	0
2	E	902	NAD	11	0
2	B	901	NAD	19	0
2	C	902	NAD	4	0

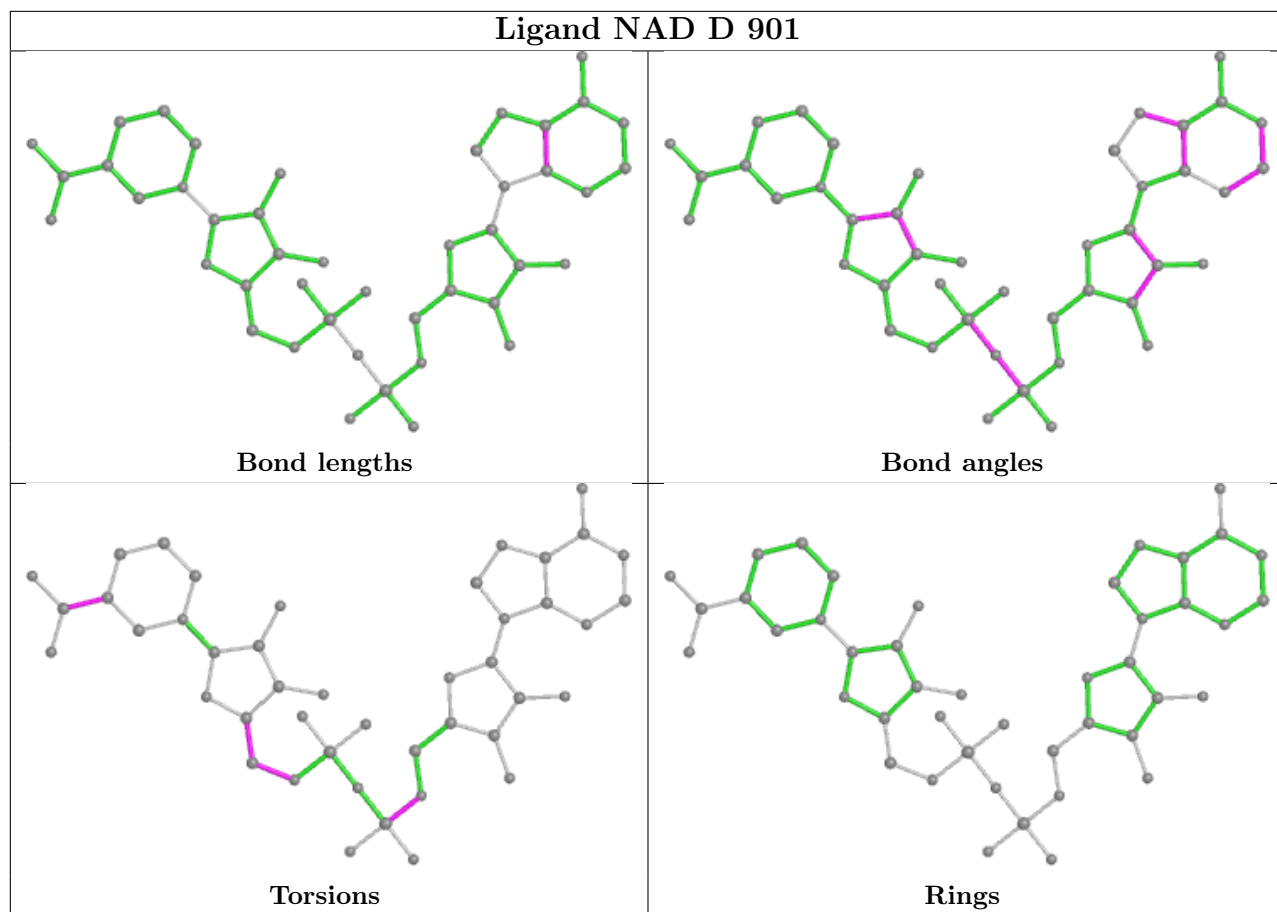
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



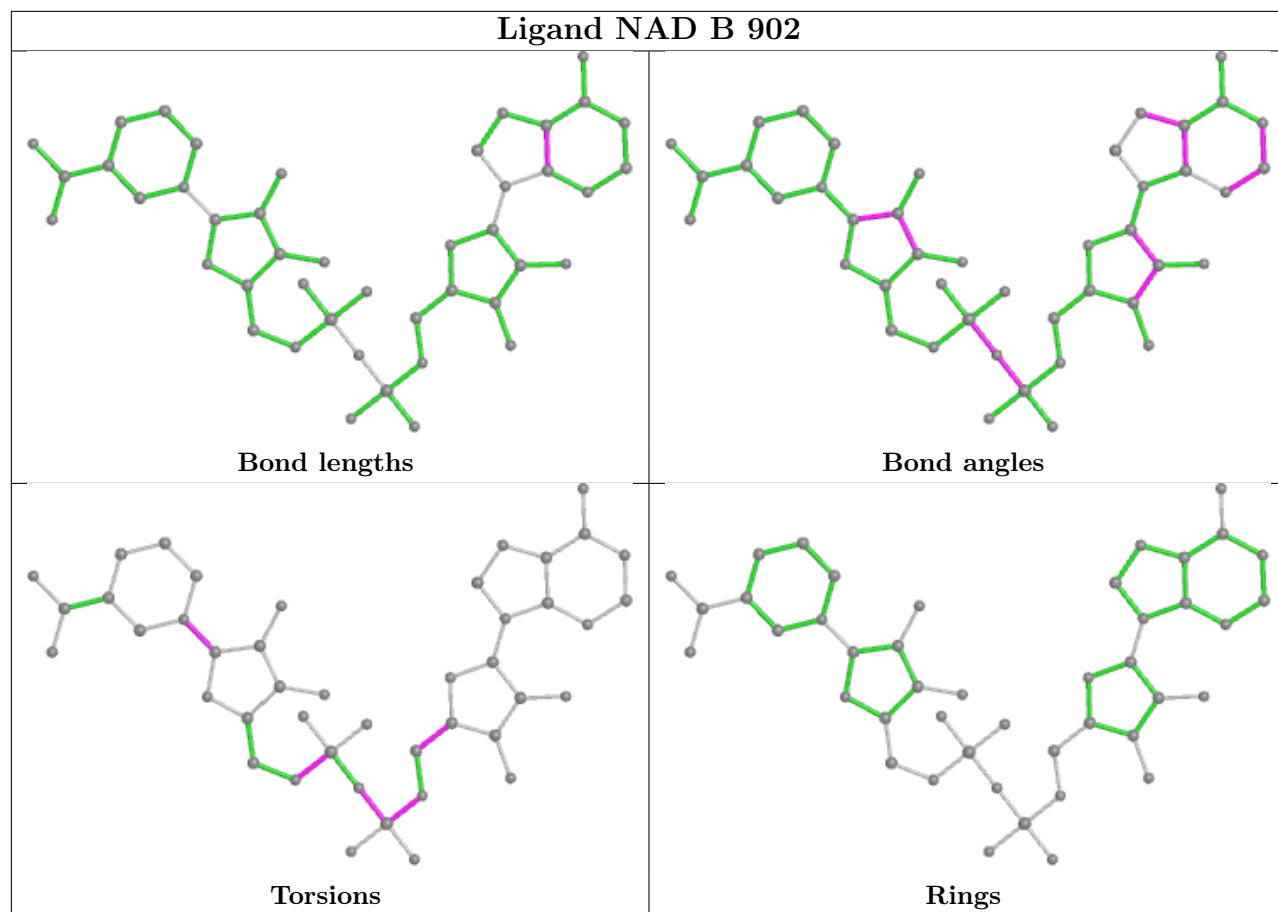


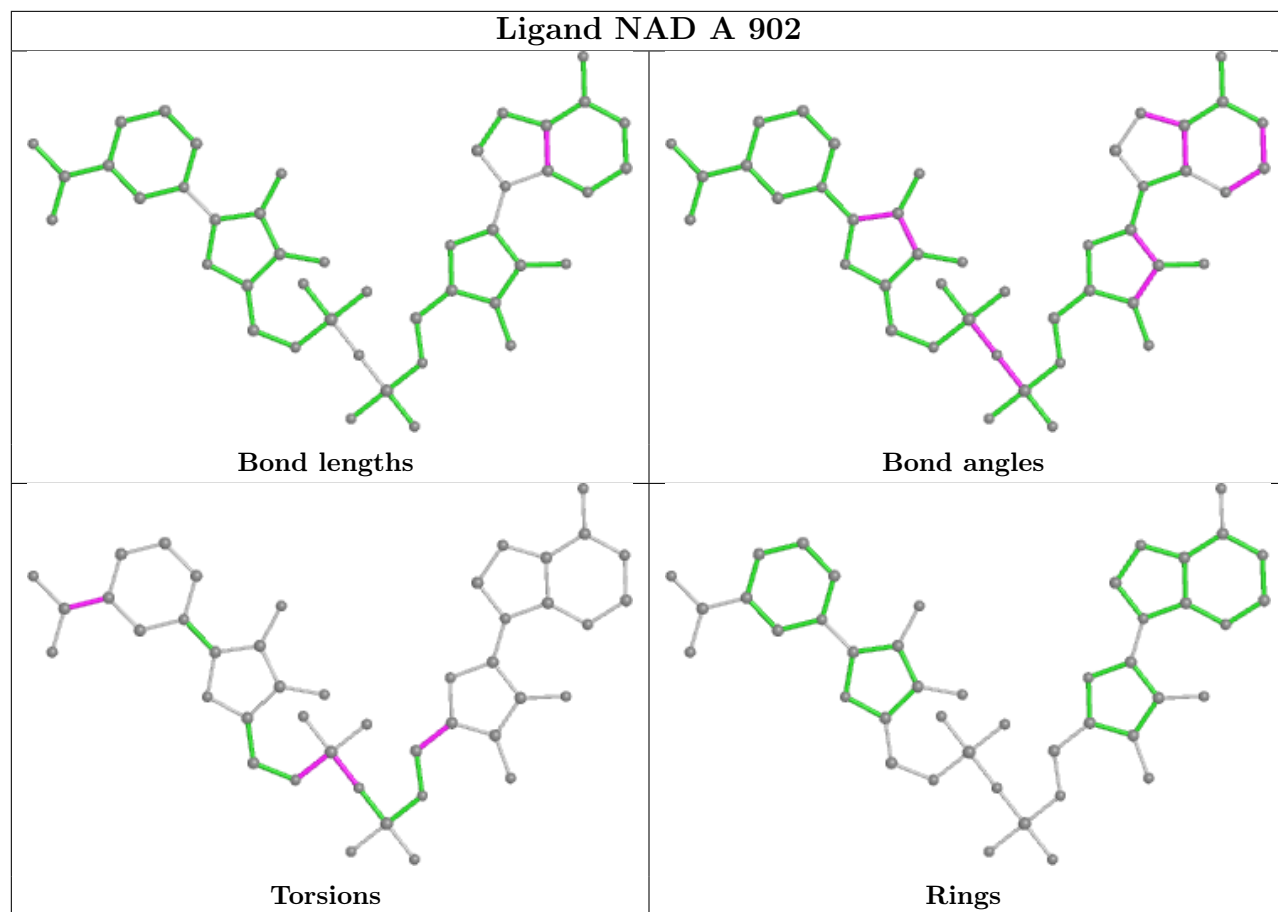


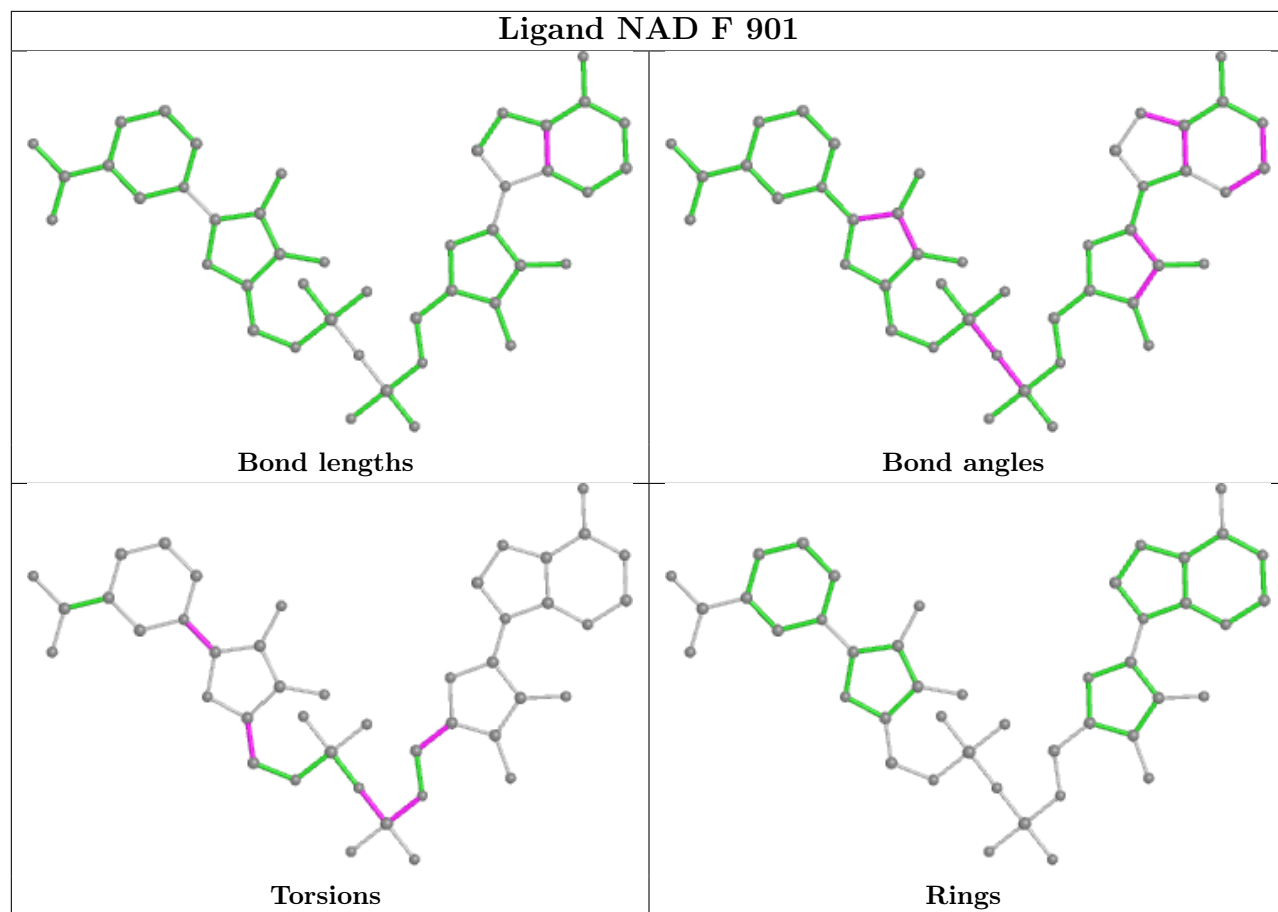


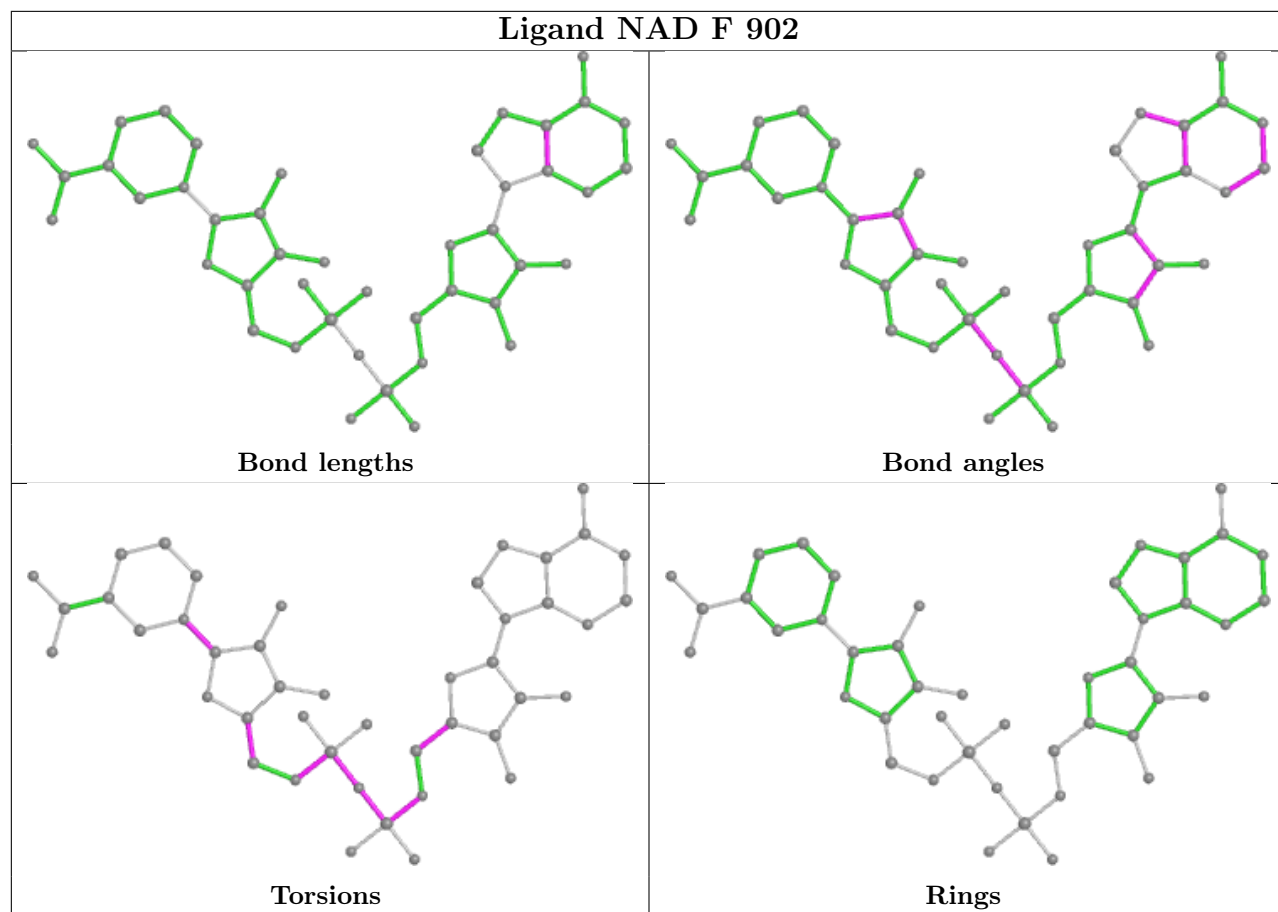


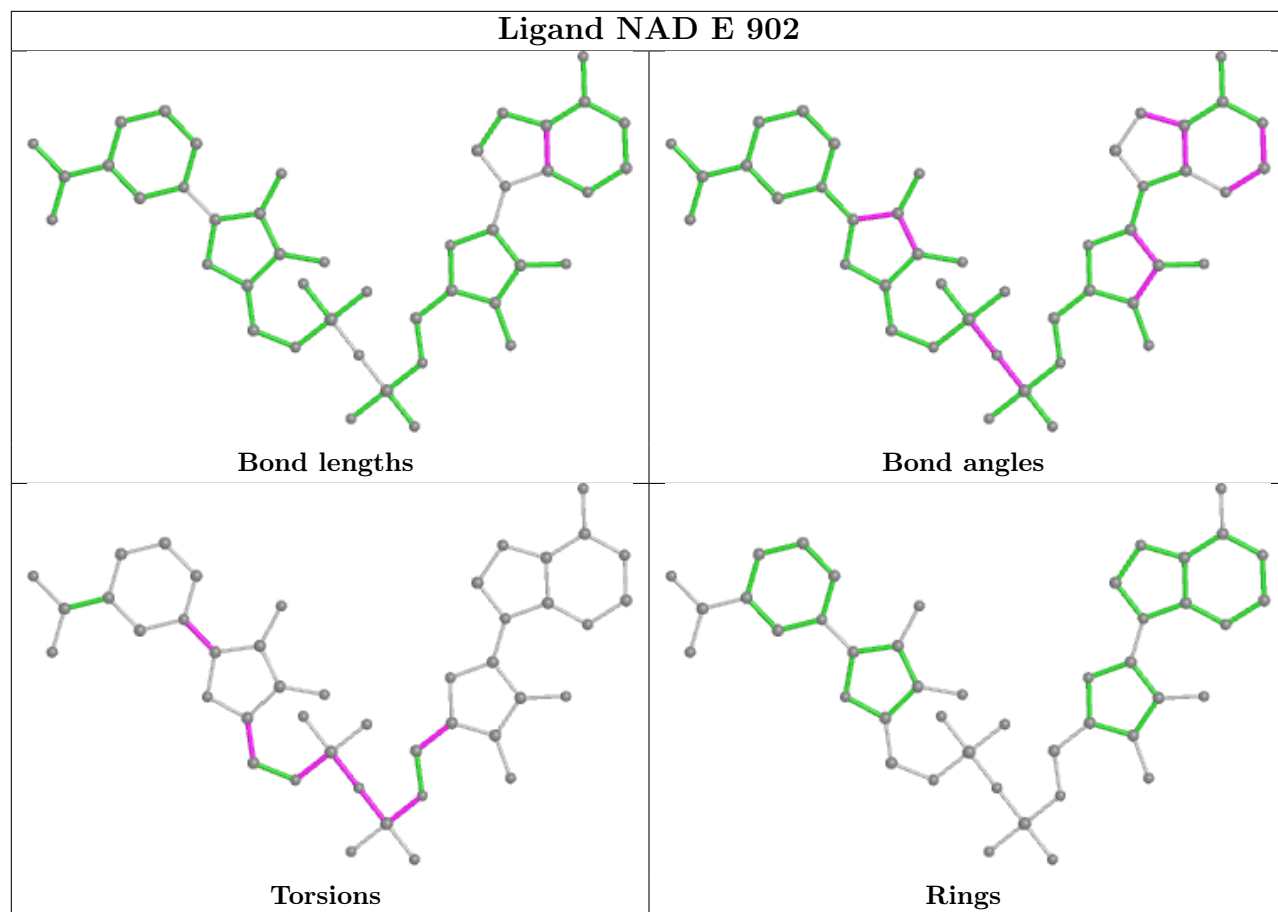


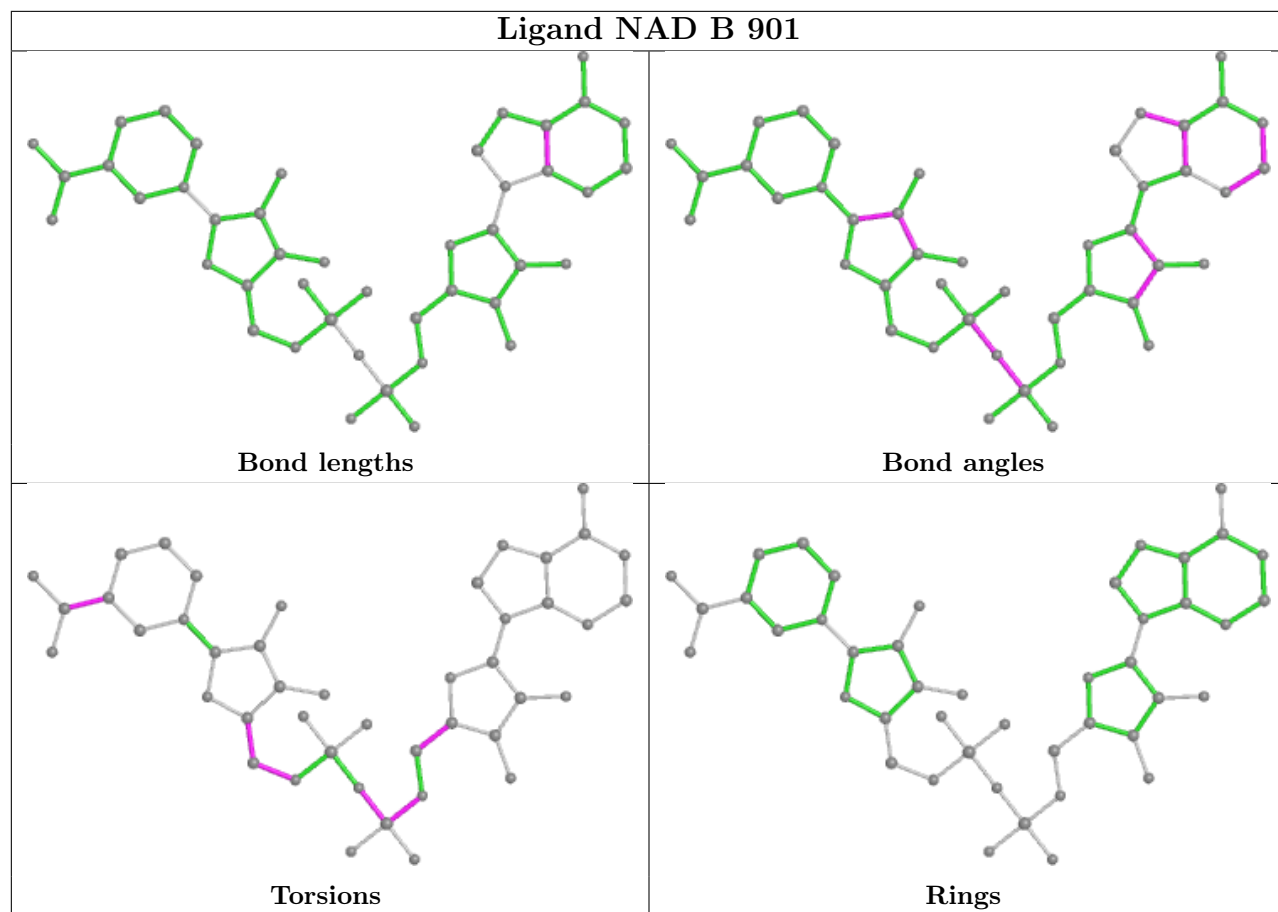


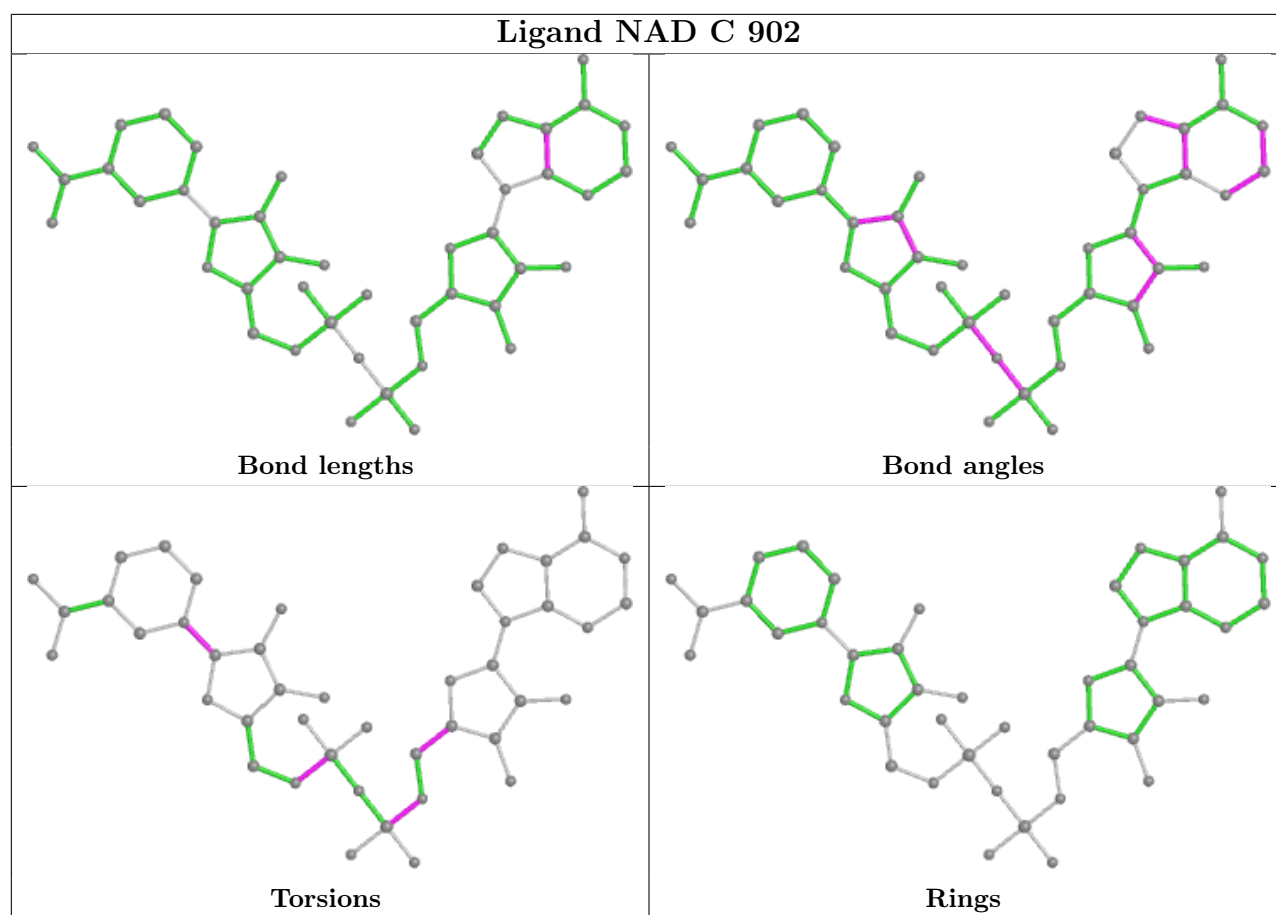












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

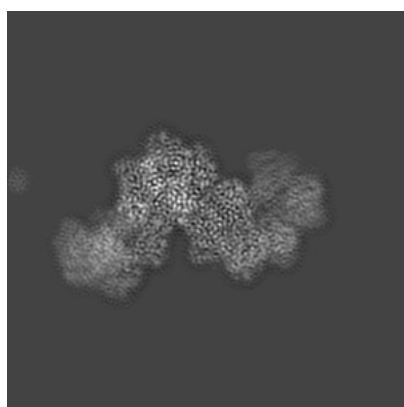
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30220. These allow visual inspection of the internal detail of the map and identification of artifacts.

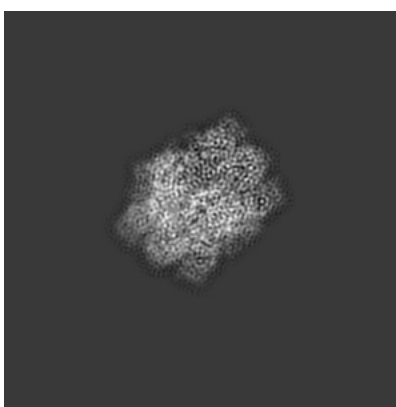
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

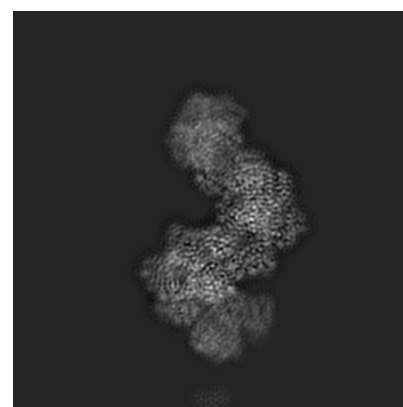
#### 6.1.1 Primary map



X



Y

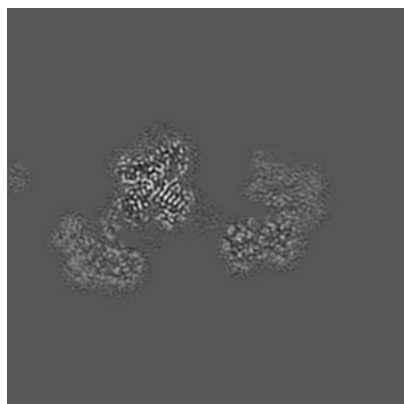


Z

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

### 6.2 Central slices [i](#)

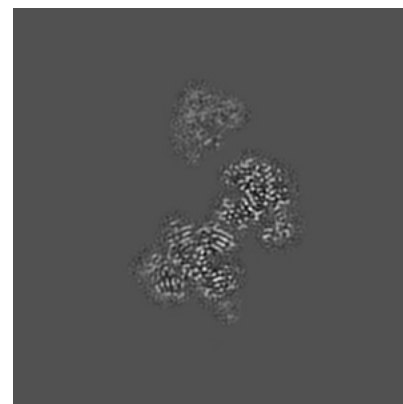
#### 6.2.1 Primary map



X Index: 153



Y Index: 153



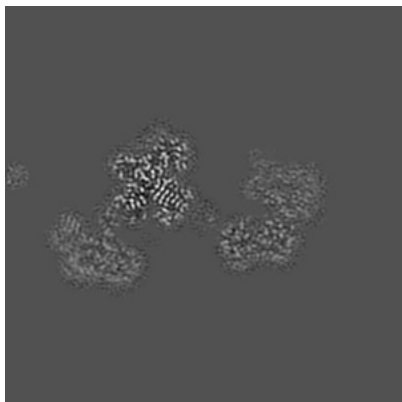
Z Index: 153



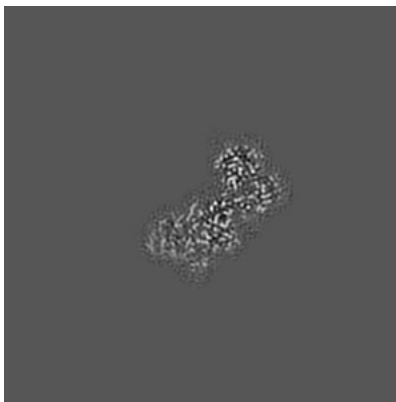
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

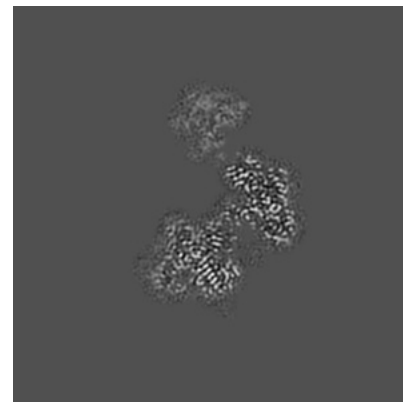
### 6.3.1 Primary map



X Index: 154



Y Index: 116

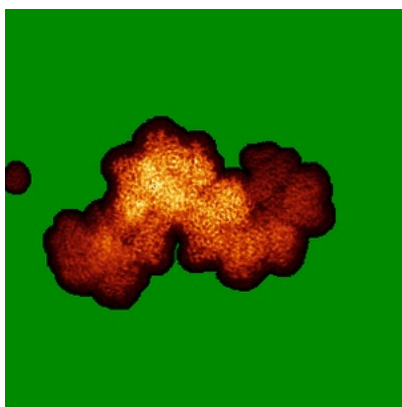


Z Index: 157

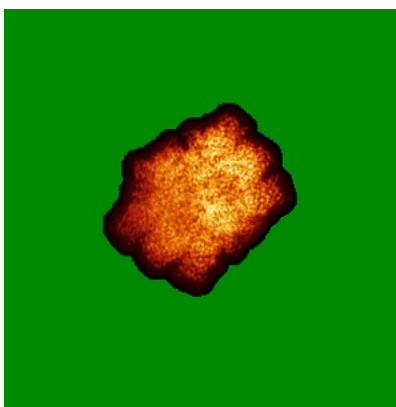
The images above show the largest variance slices of the map in three orthogonal directions.

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

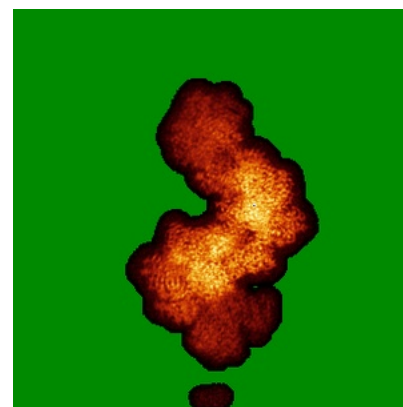
### 6.4.1 Primary map



X



Y

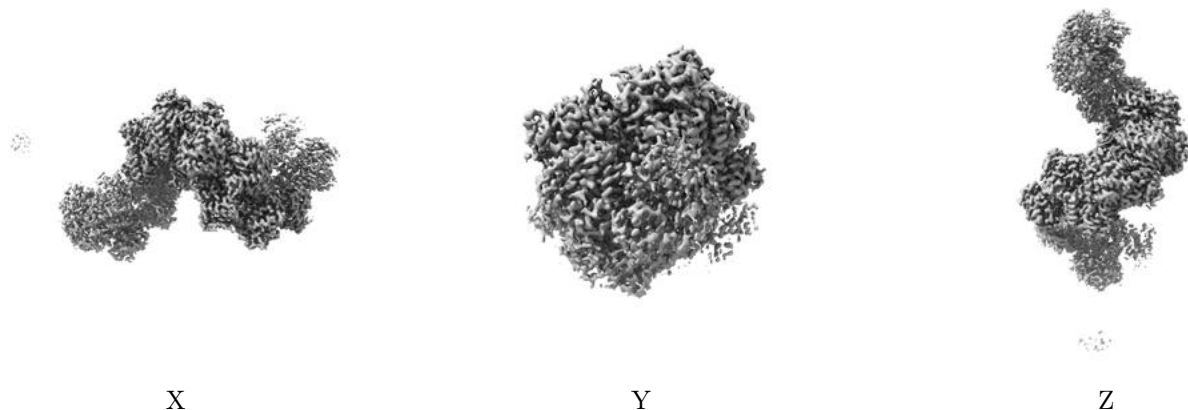


Z

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 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

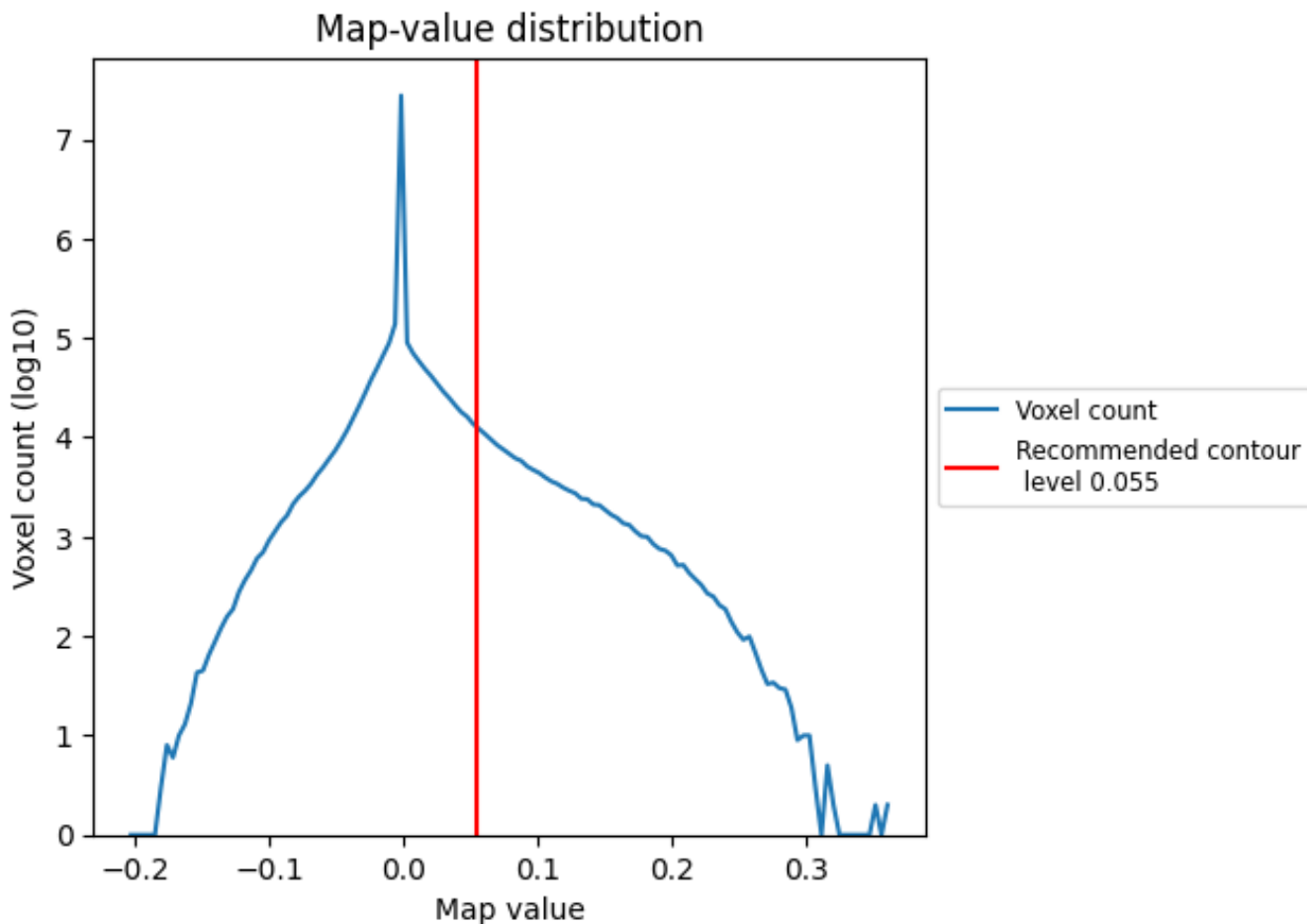
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

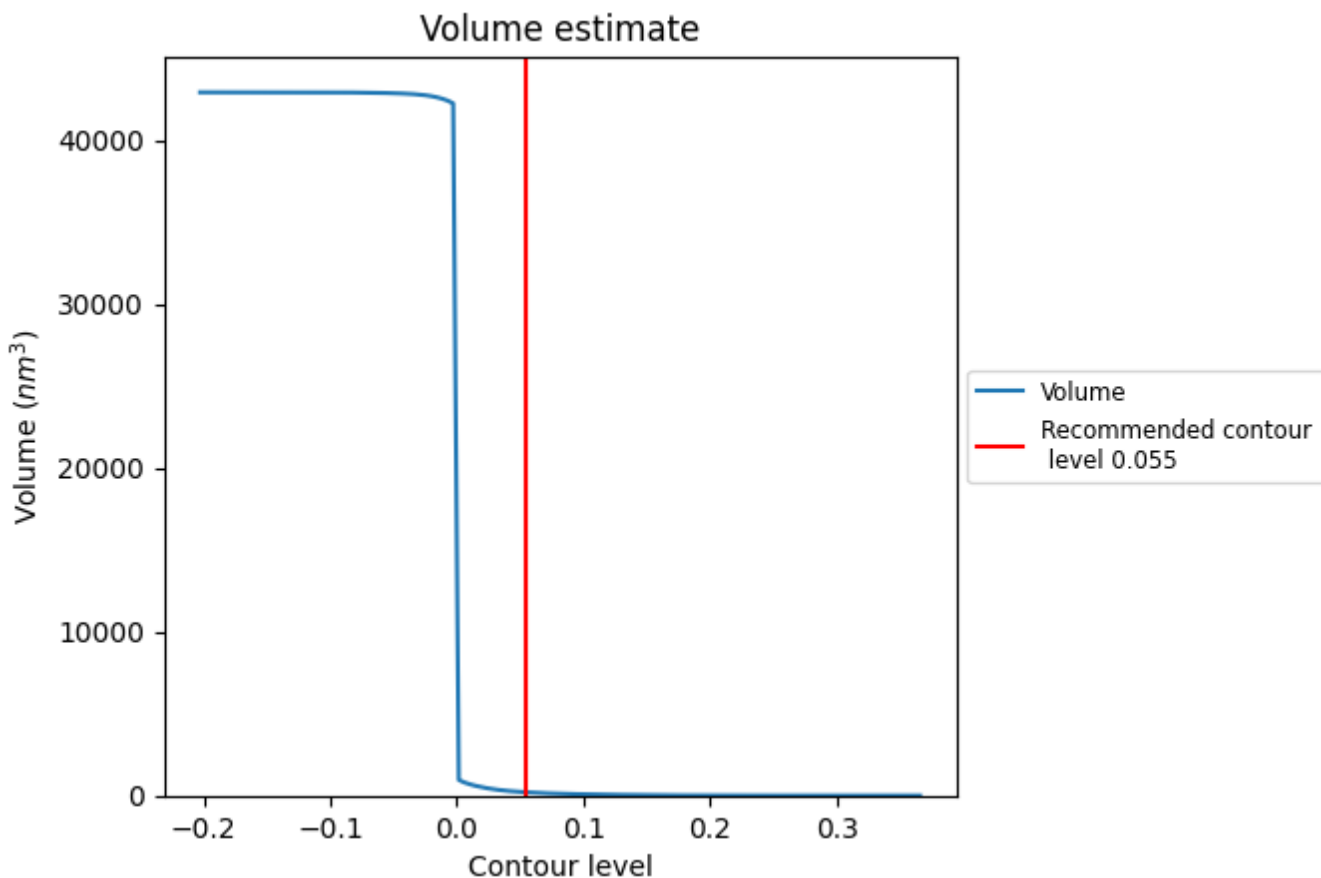
This section contains the results of statistical analysis of the map.

### 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.

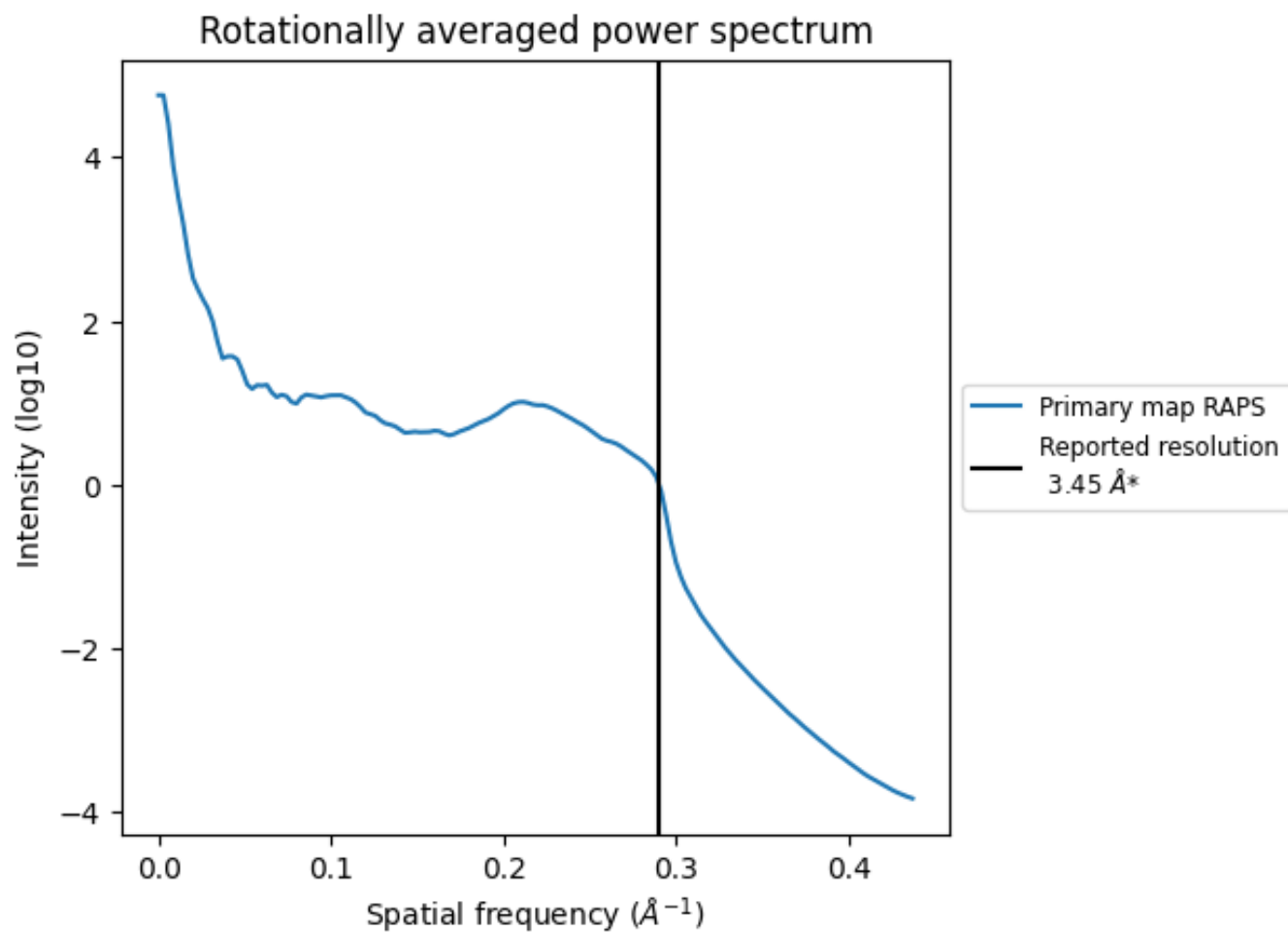
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm<sup>3</sup>; this corresponds to an approximate mass of 180 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  $0.290 \text{\AA}^{-1}$

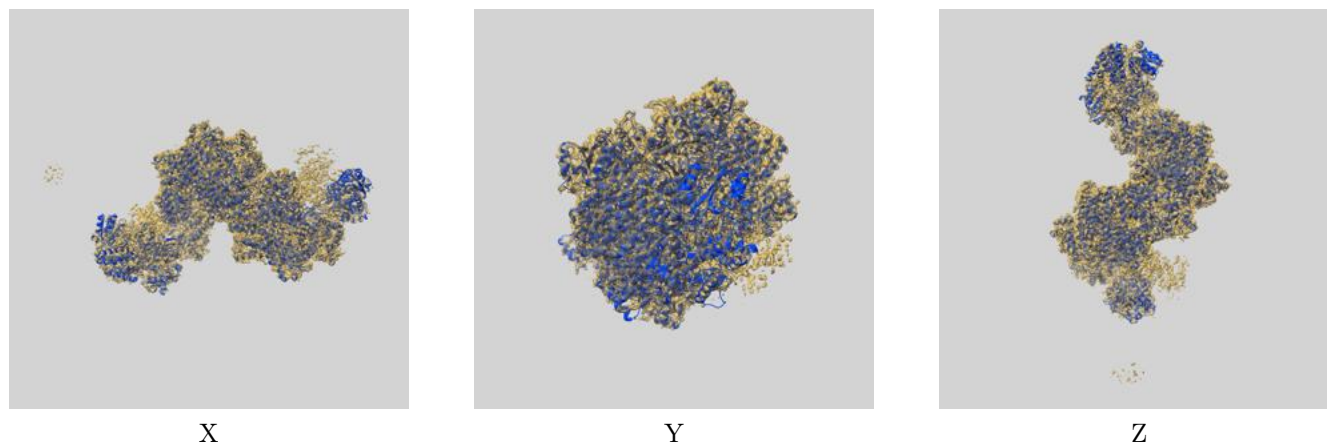
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

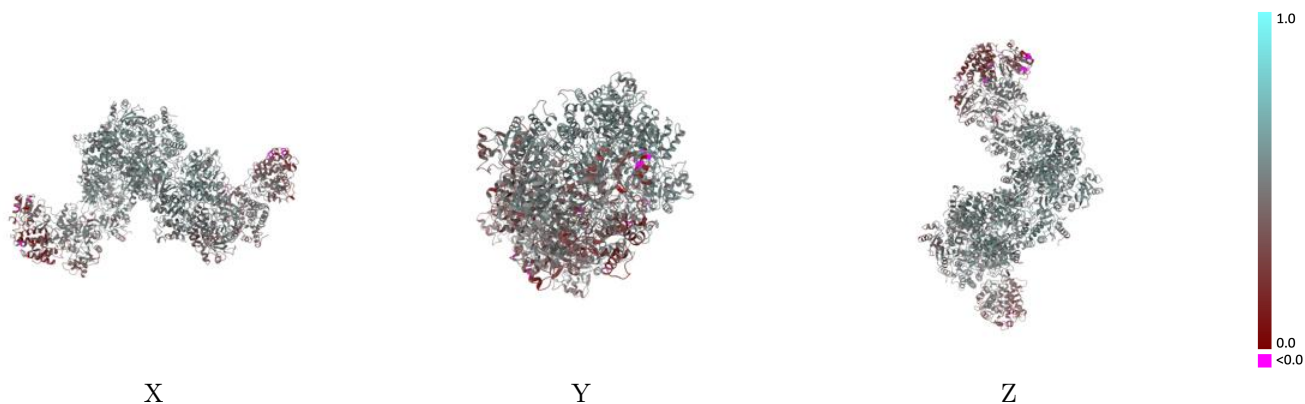
This section contains information regarding the fit between EMDB map EMD-30220 and PDB model 7BVP. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



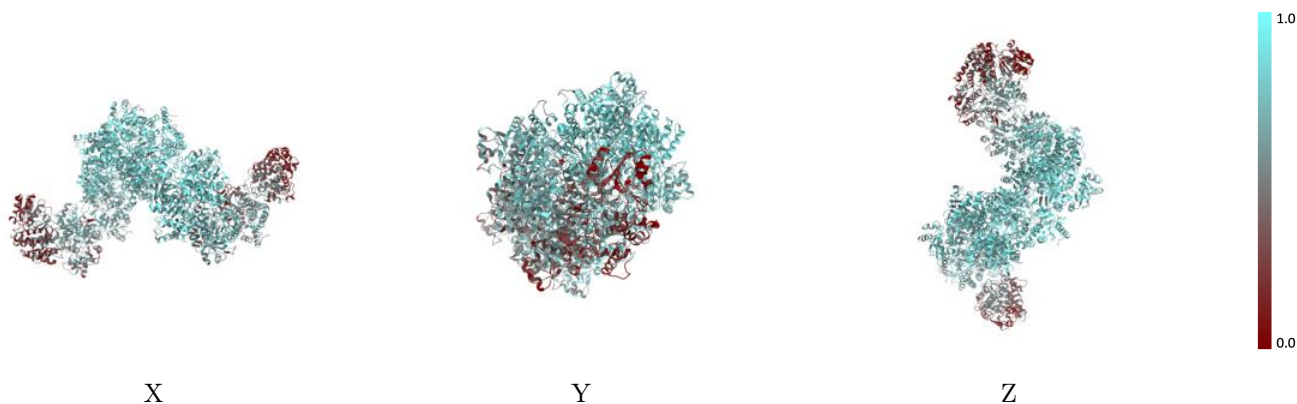
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

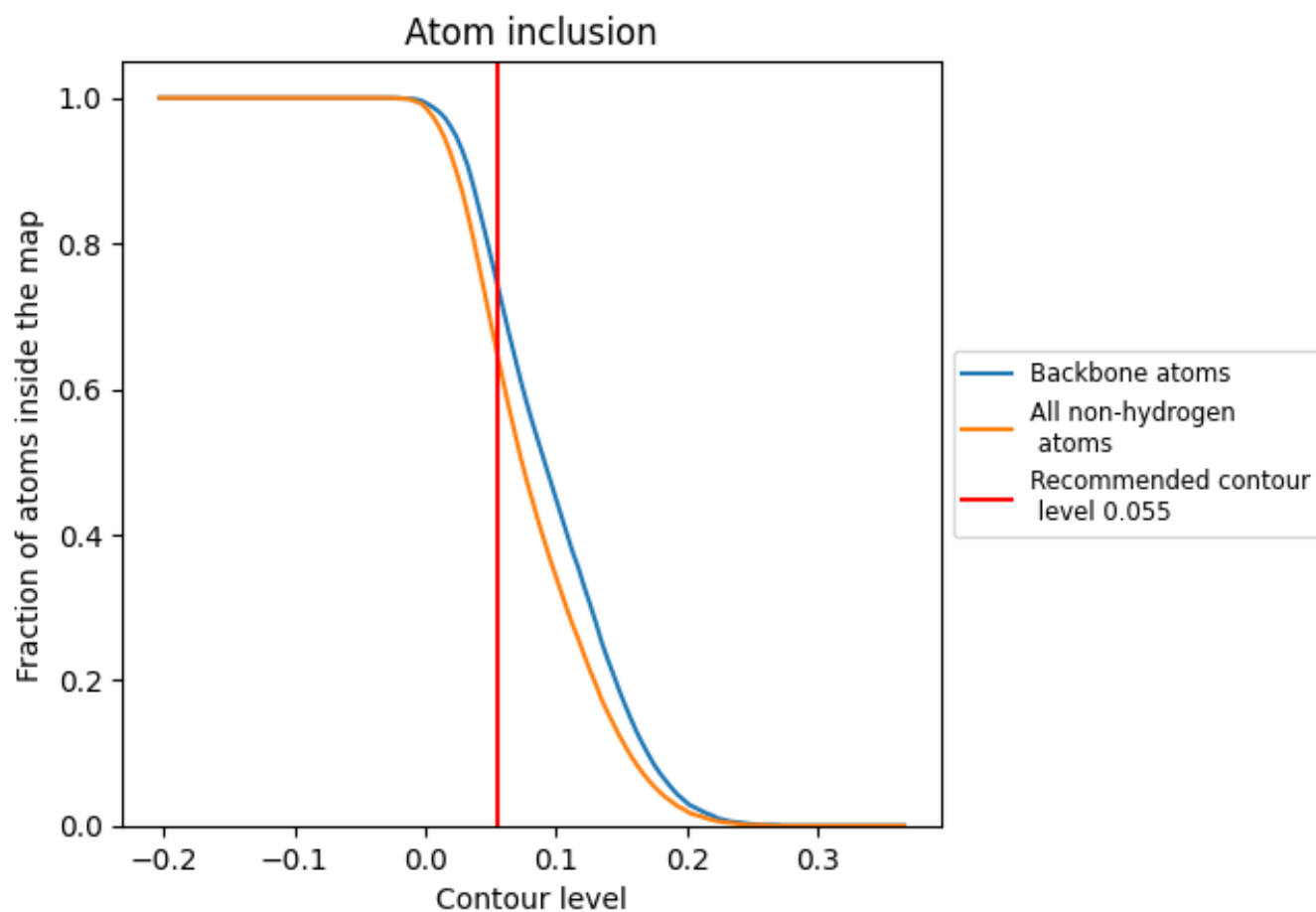
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.055).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6480	 0.4690
A	 0.5270	 0.4080
B	 0.6780	 0.4800
C	 0.7990	 0.5310
D	 0.7900	 0.5330
E	 0.6250	 0.4640
F	 0.4690	 0.3990

