



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:32 AM UTC

PDB ID : 9I07 / pdb\_00009i07  
EMDB ID : EMD-52553  
Title : Photosynthetic A8B8 glycerldeyde-3-phosphate dehydrogenase hexadecamer  
(major conformer) from Spinacia oleracea.  
Authors : Marotta, R.; Fermani, S.; Sparla, F.  
Deposited on : 2025-01-14  
Resolution : 3.10 Å(reported)  
Based on initial model : 2PKQ

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:

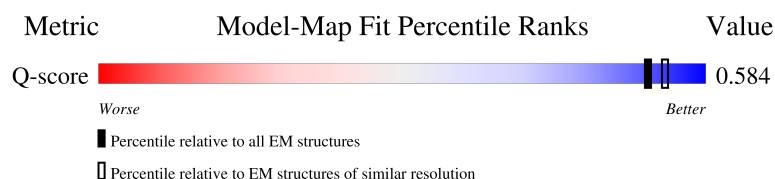
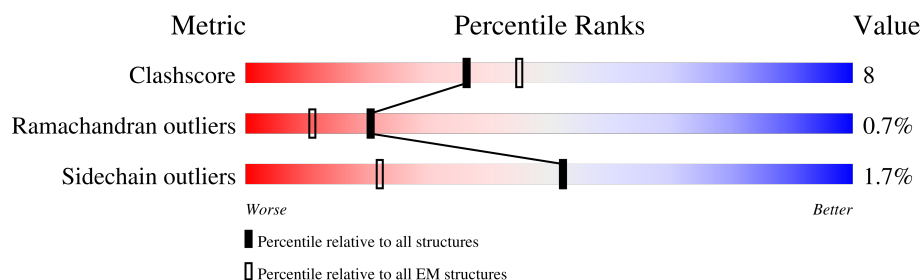
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.10 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.




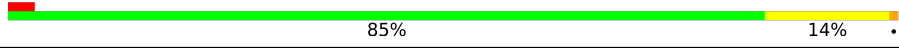

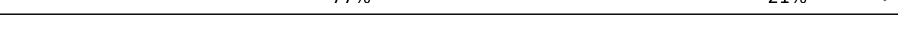
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 ( 2.60 - 3.60 )

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	368	 85% 14% .
1	C	368	 83% 16% .
1	E	368	 83% 16% .
1	G	368	 82% 17% .

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Mol	Chain	Length	Quality of chain
1	I	368	 84%15%.
1	K	368	 83%15%.
1	O	368	 85%14%.
1	Q	368	 82%17%.
2	B	337	 79%21%
2	D	337	 81%19%
2	F	337	 9%75%24%.
2	H	337	 7%80%19%.
2	J	337	 77%23%
2	L	337	 82%18%
2	P	337	 7%75%25%
2	R	337	 7%77%21%.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43184 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	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	Q	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	A	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	C	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	E	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	G	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	I	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		
1	K	368	Total	C	N	O	S	0	0
			2766	1748	476	531	11		

- Molecule 2 is a protein called 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		
2	B	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	D	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	F	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	H	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	J	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		

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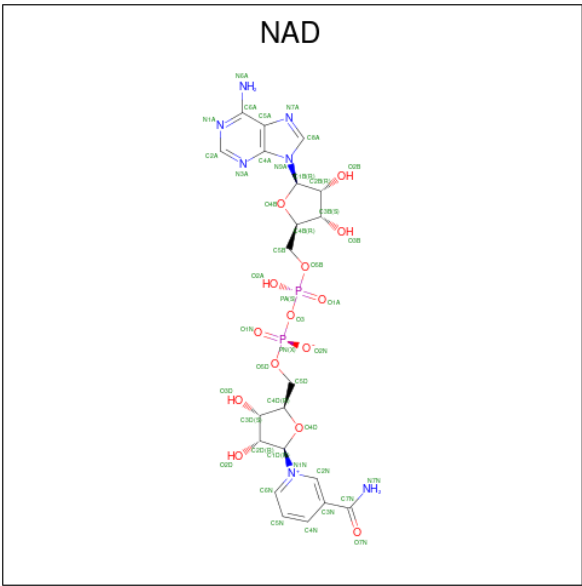
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	337	2544	1600	445	488	11	0	0

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (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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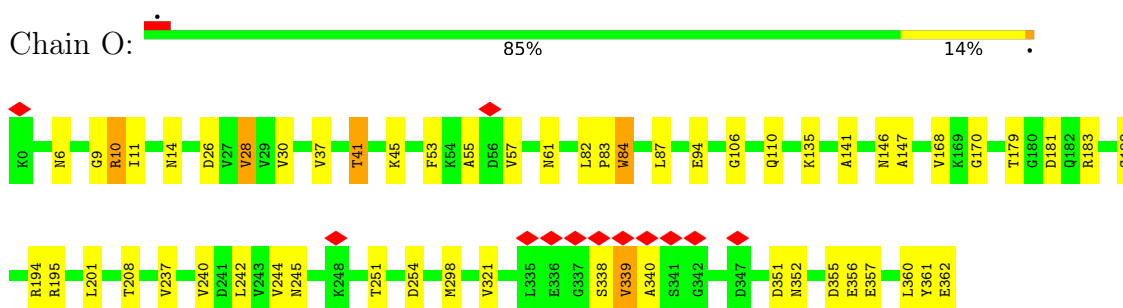
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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0
3	E	1	Total 44	C 21	N 7	O 14	P 2	0
3	F	1	Total 44	C 21	N 7	O 14	P 2	0
3	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

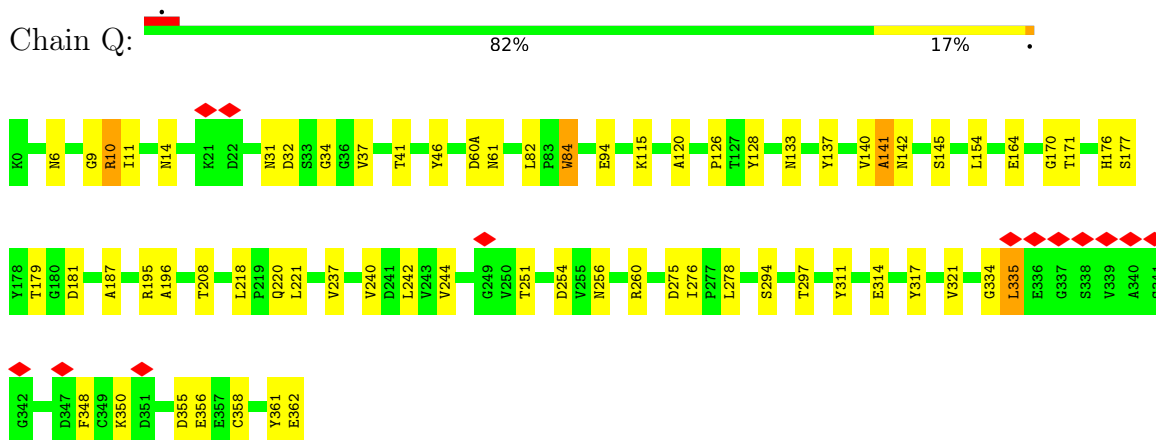
### 3 Residue-property plots [i](#)

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.

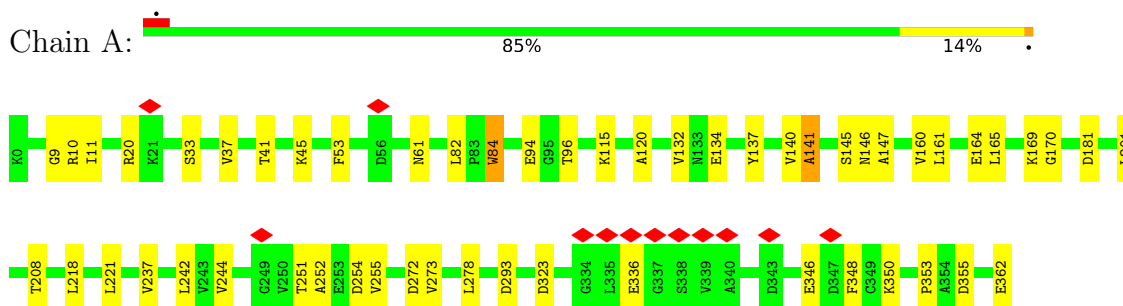
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic



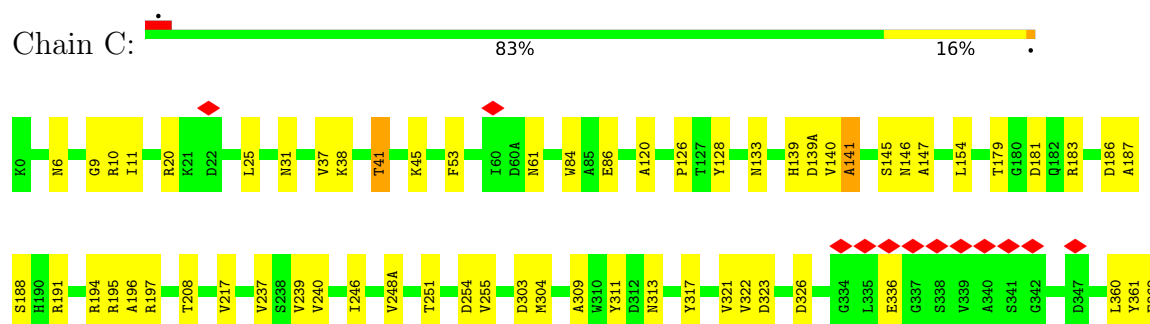
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic



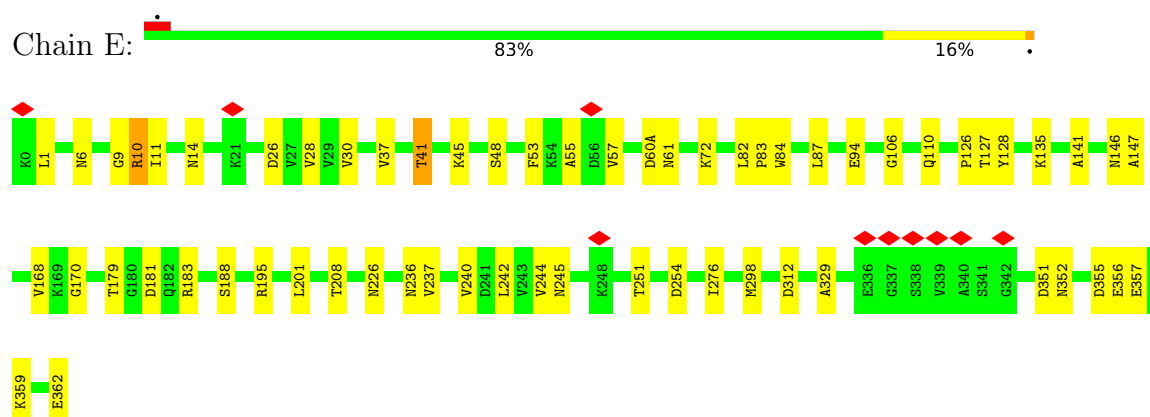
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic



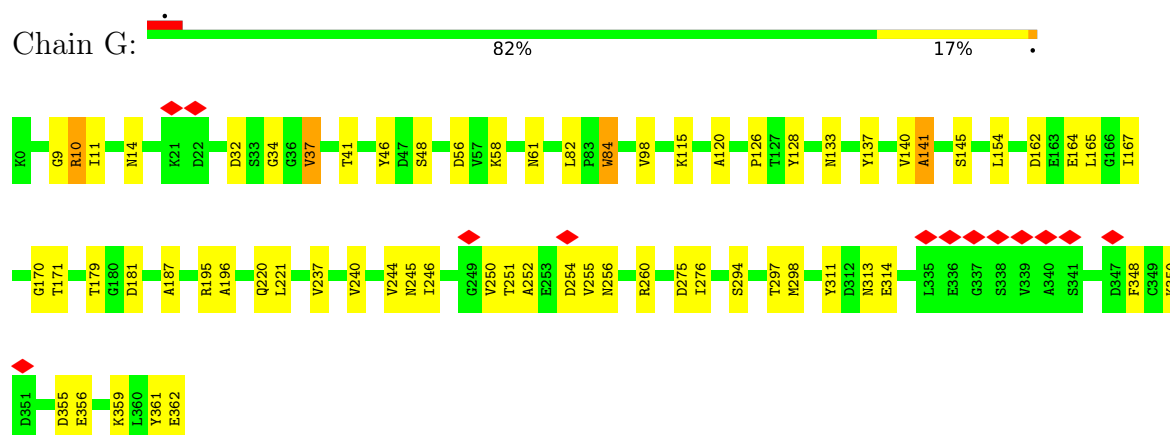
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplasic



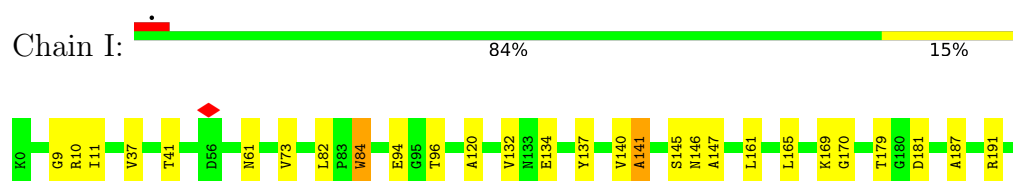
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplasic



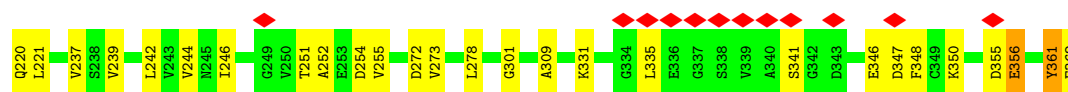
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplasic



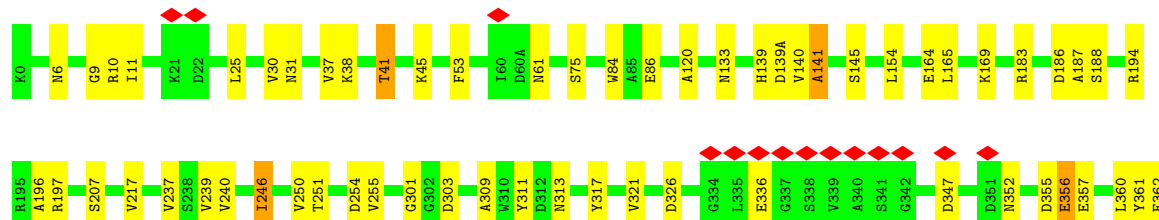
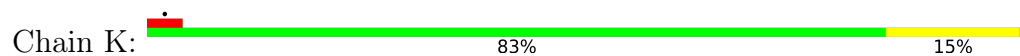
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplasic



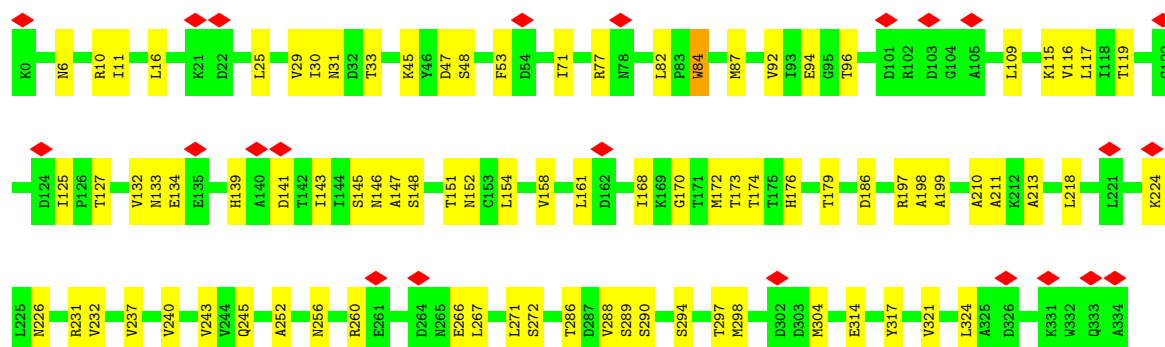
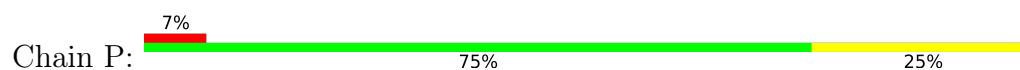




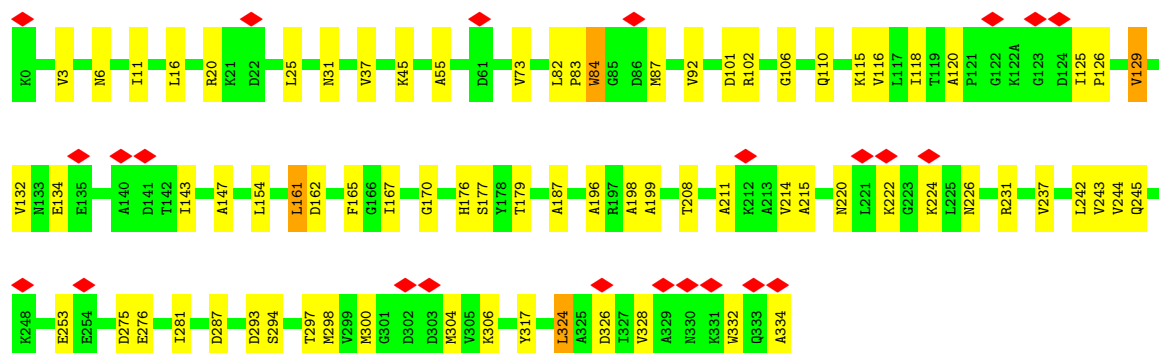
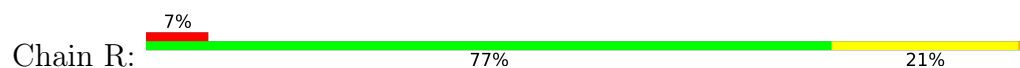
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic



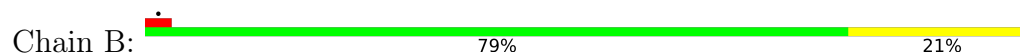
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

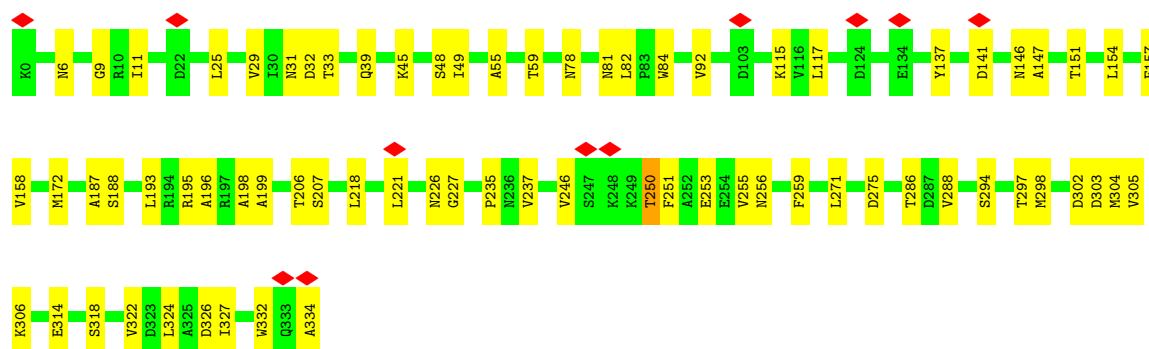


- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



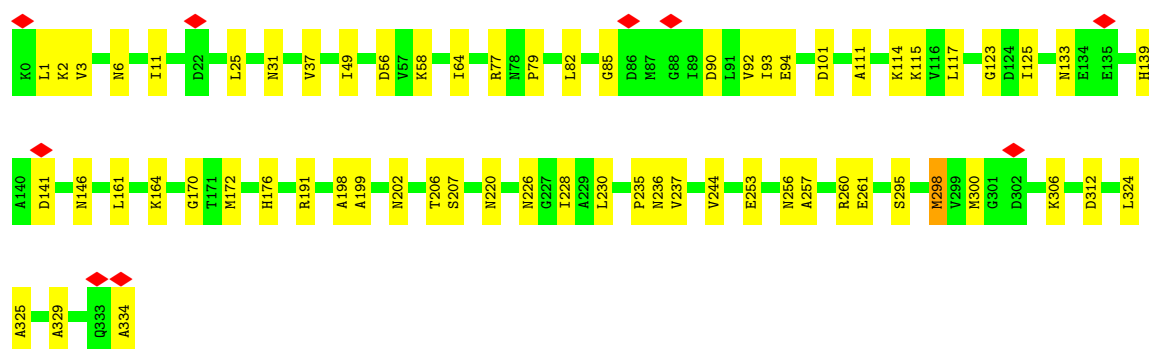
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic





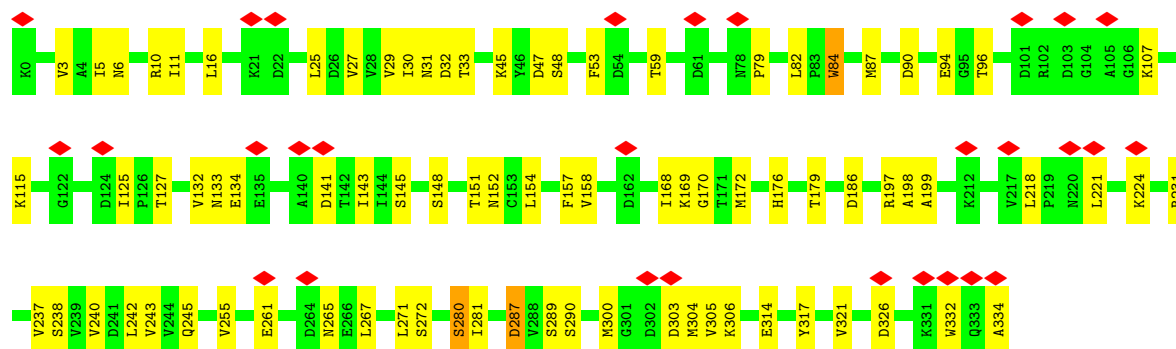
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

Chain D: 81% 19%



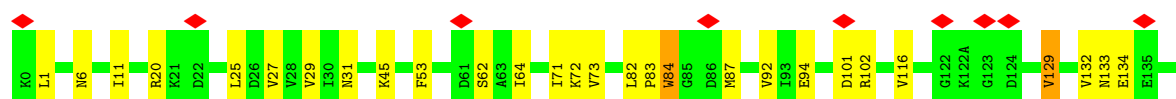
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

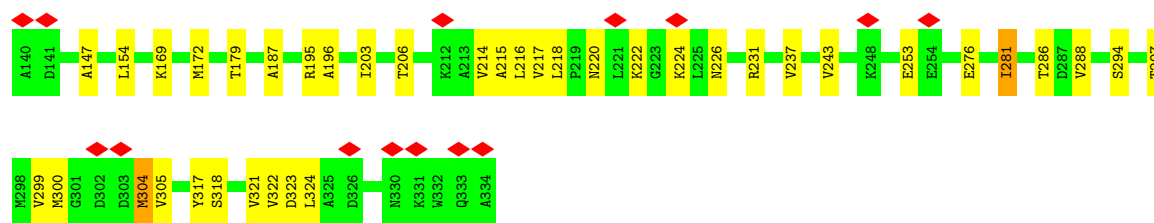
Chain F: 9% 75% 24%



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

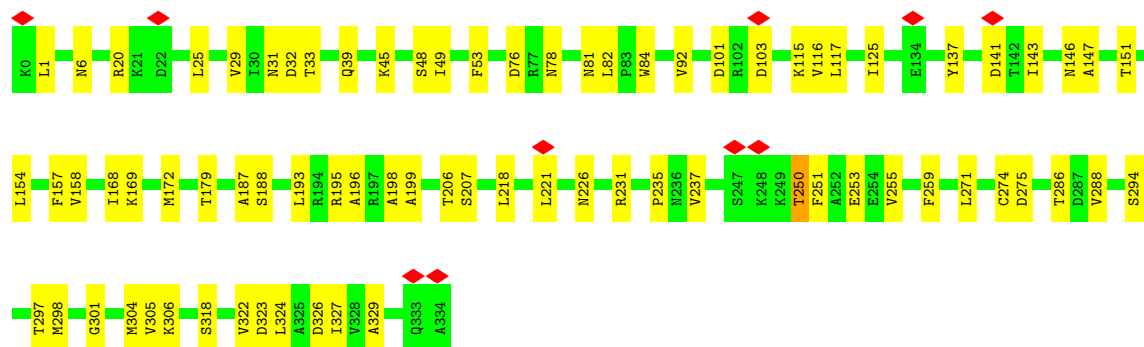
Chain H: 7% 80% 19%





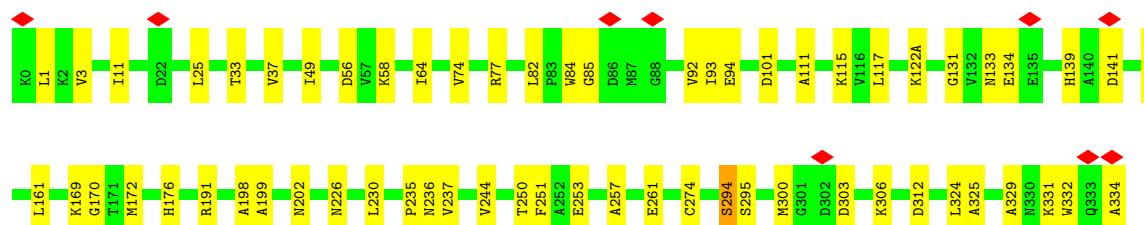
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

Chain J: 77% 23%



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

Chain L: 82% 18%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	55141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.283	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	301.172, 301.172, 301.172	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.28	0/2815	0.36	0/3826
1	C	0.27	0/2815	0.36	0/3826
1	E	0.28	0/2815	0.36	0/3826
1	G	0.27	0/2815	0.36	0/3826
1	I	0.28	0/2815	0.36	0/3826
1	K	0.27	0/2815	0.36	0/3826
1	O	0.27	0/2815	0.35	0/3826
1	Q	0.27	0/2815	0.37	0/3826
2	B	0.23	0/2585	0.34	0/3509
2	D	0.25	0/2585	0.34	0/3509
2	F	0.24	0/2585	0.37	0/3509
2	H	0.22	0/2585	0.32	0/3509
2	J	0.23	0/2585	0.34	0/3509
2	L	0.24	0/2585	0.34	0/3509
2	P	0.21	0/2585	0.33	0/3509
2	R	0.22	0/2585	0.33	0/3509
All	All	0.25	0/43200	0.35	0/58680

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

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	2766	0	2801	33	0
1	C	2766	0	2801	43	0
1	E	2766	0	2801	39	0
1	G	2766	0	2801	53	0
1	I	2766	0	2801	34	0
1	K	2766	0	2801	42	0
1	O	2766	0	2801	38	0
1	Q	2766	0	2801	55	0
2	B	2544	0	2580	49	0
2	D	2544	0	2580	41	0
2	F	2544	0	2580	56	0
2	H	2544	0	2580	46	0
2	J	2544	0	2580	51	0
2	L	2544	0	2580	49	0
2	P	2544	0	2580	60	0
2	R	2544	0	2580	50	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
3	C	44	0	26	0	0
3	D	44	0	26	1	0
3	E	44	0	26	1	0
3	F	44	0	26	2	0
3	G	44	0	26	0	0
3	H	44	0	26	1	0
3	I	44	0	26	1	0
3	J	44	0	26	0	0
3	K	44	0	26	0	0
3	L	44	0	26	2	0
3	O	44	0	26	1	0
3	P	44	0	26	2	0
3	Q	44	0	26	0	0
3	R	44	0	26	1	0
All	All	43184	0	43464	670	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 8.

All (670) 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:361:TYR:OH	1:C:208:THR:OG1	1.80	0.99
1:A:208:THR:OG1	1:G:361:TYR:OH	1.82	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:361:TYR:OH	1:I:208:THR:OG1	1.81	0.92
1:Q:208:THR:OG1	1:I:361:TYR:OH	1.88	0.91
1:I:94:GLU:OE2	1:I:96:THR:OG1	1.92	0.87
2:L:115:LYS:NZ	2:L:141:ASP:O	2.08	0.87
2:D:115:LYS:NZ	2:D:141:ASP:O	2.08	0.85
2:F:94:GLU:OE2	2:F:96:THR:OG1	1.94	0.85
1:O:37:VAL:O	1:O:41:THR:OG1	1.92	0.85
1:K:86:GLU:OE2	1:K:86:GLU:N	2.09	0.85
2:H:6:ASN:OD1	2:H:31:ASN:ND2	2.10	0.84
1:A:94:GLU:OE2	1:A:96:THR:OG1	1.93	0.84
1:C:86:GLU:OE1	1:C:86:GLU:N	2.09	0.84
2:P:6:ASN:OD1	2:P:31:ASN:ND2	2.11	0.84
2:P:94:GLU:OE2	2:P:96:THR:OG1	1.95	0.84
1:E:45:LYS:NZ	1:E:53:PHE:O	2.11	0.83
2:R:6:ASN:OD1	2:R:31:ASN:ND2	2.12	0.83
1:G:115:LYS:NZ	1:G:137:TYR:OH	2.12	0.83
2:J:172:MET:O	2:L:306:LYS:NZ	2.10	0.83
1:O:355:ASP:O	1:O:357:GLU:N	2.11	0.82
2:P:45:LYS:NZ	2:P:53:PHE:O	2.13	0.82
1:E:37:VAL:O	1:E:41:THR:OG1	1.96	0.82
2:J:45:LYS:NZ	2:J:53:PHE:O	2.12	0.81
2:B:172:MET:O	2:D:306:LYS:NZ	2.14	0.80
1:O:45:LYS:NZ	1:O:53:PHE:O	2.11	0.80
2:B:195:ARG:NH1	2:B:206:THR:OG1	2.15	0.80
2:F:45:LYS:NZ	2:F:53:PHE:O	2.14	0.80
2:F:6:ASN:OD1	2:F:31:ASN:ND2	2.14	0.79
2:P:92:VAL:HG12	2:P:116:VAL:HG22	1.65	0.78
1:E:355:ASP:O	1:E:357:GLU:N	2.17	0.78
2:H:220:ASN:O	2:H:224:LYS:NZ	2.17	0.78
1:I:9:GLY:O	1:I:11:ILE:N	2.17	0.78
2:R:179:THR:OG1	2:R:231:ARG:NH1	2.16	0.77
1:Q:9:GLY:O	1:Q:11:ILE:N	2.17	0.77
2:H:179:THR:OG1	2:H:231:ARG:NH1	2.17	0.77
2:F:280:SER:OG	2:H:203:ILE:N	2.18	0.77
2:L:56:ASP:OD2	2:L:58:LYS:NZ	2.18	0.77
1:G:9:GLY:O	1:G:11:ILE:N	2.19	0.76
1:A:9:GLY:O	1:A:11:ILE:N	2.18	0.76
2:D:56:ASP:OD1	2:D:58:LYS:NZ	2.19	0.76
2:F:169:LYS:NZ	2:F:245:GLN:OE1	2.15	0.74
2:F:115:LYS:NZ	2:F:141:ASP:O	2.19	0.74
2:R:294:SER:O	2:R:297:THR:HG22	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:ARG:NH2	1:G:275:ASP:OD1	2.21	0.73
1:G:154:LEU:HD13	1:G:240:VAL:HG11	1.70	0.73
1:K:9:GLY:O	1:K:11:ILE:N	2.22	0.73
1:C:9:GLY:O	1:C:11:ILE:N	2.22	0.73
2:H:134:GLU:N	2:H:134:GLU:OE1	2.22	0.73
2:P:139:HIS:O	2:P:139:HIS:ND1	2.21	0.73
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.24	0.72
1:K:154:LEU:HD13	1:K:240:VAL:HG11	1.69	0.72
1:G:256:ASN:OD1	1:G:297:THR:HG21	1.91	0.71
2:F:32:ASP:OD1	2:F:33:THR:N	2.24	0.71
2:P:179:THR:OG1	2:P:231:ARG:NH1	2.24	0.71
1:Q:294:SER:O	1:Q:297:THR:HG22	1.91	0.71
2:P:115:LYS:NZ	2:P:141:ASP:O	2.24	0.71
2:F:152:ASN:O	2:F:289:SER:OG	2.08	0.71
1:I:82:LEU:HD13	1:I:84:TRP:CZ2	2.24	0.71
1:C:154:LEU:HD13	1:C:240:VAL:HG11	1.71	0.70
1:E:208:THR:OG1	1:K:361:TYR:OH	2.09	0.70
2:R:332:TRP:NE1	2:R:334:ALA:OXT	2.24	0.70
1:O:208:THR:OG1	1:C:361:TYR:OH	2.09	0.70
2:F:179:THR:OG1	2:F:231:ARG:NH1	2.24	0.70
1:Q:154:LEU:HD13	1:Q:240:VAL:HG11	1.74	0.70
1:O:339:VAL:HG22	1:O:340:ALA:H	1.57	0.69
1:Q:251:THR:N	1:Q:254:ASP:OD2	2.25	0.69
1:O:183:ARG:NH1	1:O:188:SER:O	2.26	0.69
1:O:9:GLY:O	1:O:11:ILE:N	2.26	0.69
2:P:92:VAL:CG1	2:P:116:VAL:HG22	2.22	0.69
1:Q:260:ARG:NH2	1:Q:275:ASP:OD1	2.26	0.69
2:B:59:THR:O	2:B:59:THR:HG23	1.92	0.69
2:H:195:ARG:NH1	2:H:206:THR:OG1	2.25	0.69
2:H:294:SER:O	2:H:297:THR:HG22	1.92	0.69
1:Q:256:ASN:OD1	1:Q:297:THR:HG21	1.94	0.68
2:J:39:GLN:N	2:J:39:GLN:OE1	2.26	0.68
2:L:25:LEU:HD21	2:L:325:ALA:HB1	1.76	0.68
1:O:45:LYS:NZ	1:O:55:ALA:O	2.26	0.68
2:P:245:GLN:NE2	2:R:245:GLN:OE1	2.26	0.68
2:P:11:ILE:HD11	3:P:400:NAD:H71N	1.59	0.68
1:C:20:ARG:NH2	1:C:323:ASP:OD1	2.26	0.67
2:J:20:ARG:NH2	2:J:323:ASP:OD1	2.27	0.67
2:J:318:SER:O	2:J:322:VAL:HG23	1.94	0.67
2:B:39:GLN:OE1	2:B:39:GLN:N	2.27	0.67
2:F:11:ILE:HD11	3:F:400:NAD:H71N	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLY:O	1:E:11:ILE:N	2.28	0.67
2:H:92:VAL:CG1	2:H:116:VAL:HG22	2.26	0.66
1:I:134:GLU:N	1:I:134:GLU:OE1	2.29	0.66
1:K:6:ASN:OD1	1:K:31:ASN:ND2	2.28	0.66
1:I:272:ASP:OD1	1:I:273:VAL:N	2.28	0.66
1:I:278:LEU:O	1:K:194:ARG:NH1	2.28	0.66
2:B:294:SER:O	2:B:297:THR:HG22	1.95	0.66
2:J:294:SER:O	2:J:297:THR:HG22	1.95	0.66
2:L:11:ILE:HD11	3:L:400:NAD:H71N	1.60	0.66
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.31	0.66
2:B:318:SER:O	2:B:322:VAL:HG23	1.94	0.66
1:A:272:ASP:OD1	1:A:273:VAL:N	2.27	0.65
1:G:294:SER:O	1:G:297:THR:HG22	1.95	0.65
2:L:25:LEU:HD21	2:L:325:ALA:CB	2.26	0.65
1:A:134:GLU:N	1:A:134:GLU:OE1	2.29	0.65
1:A:278:LEU:O	1:C:194:ARG:NH1	2.30	0.65
2:R:220:ASN:O	2:R:224:LYS:NZ	2.30	0.65
2:P:252:ALA:O	2:P:256:ASN:ND2	2.30	0.65
2:P:134:GLU:N	2:P:134:GLU:OE1	2.28	0.65
1:E:183:ARG:NH1	1:E:188:SER:O	2.30	0.65
1:K:37:VAL:O	1:K:41:THR:OG1	2.12	0.65
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.32	0.64
2:D:170:GLY:HA3	2:D:244:VAL:HG12	1.78	0.64
1:E:45:LYS:NZ	1:E:55:ALA:O	2.28	0.64
2:H:286:THR:HG22	2:H:288:VAL:HG12	1.79	0.64
2:L:117:LEU:HD21	2:L:324:LEU:HD23	1.80	0.64
2:P:256:ASN:OD1	2:P:297:THR:HG21	1.98	0.64
2:B:32:ASP:OD1	2:B:33:THR:N	2.29	0.64
2:D:11:ILE:HD11	3:D:400:NAD:H71N	1.63	0.63
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.30	0.63
1:G:220:GLN:HG2	1:G:221:LEU:HD12	1.79	0.63
1:O:251:THR:N	1:O:254:ASP:OD2	2.30	0.63
1:G:181:ASP:OD2	1:G:195:ARG:NH1	2.31	0.63
1:O:179:THR:OG1	1:O:181:ASP:OD1	2.10	0.63
1:G:154:LEU:CD1	1:G:240:VAL:HG11	2.28	0.63
2:L:170:GLY:HA3	2:L:244:VAL:HG12	1.81	0.62
2:H:101:ASP:OD1	2:H:102:ARG:N	2.32	0.62
2:J:32:ASP:OD1	2:J:33:THR:N	2.32	0.62
2:P:173:THR:OG1	2:R:306:LYS:NZ	2.18	0.62
1:A:115:LYS:NZ	1:A:137:TYR:OH	2.22	0.62
2:H:6:ASN:ND2	2:H:94:GLU:OE2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:LYS:NZ	2:H:53:PHE:O	2.32	0.61
1:A:336:GLU:OE2	1:A:336:GLU:N	2.29	0.61
2:J:115:LYS:NZ	2:J:141:ASP:O	2.30	0.61
2:F:243:VAL:HG11	2:H:243:VAL:HG11	1.81	0.61
2:D:117:LEU:HD21	2:D:324:LEU:HD23	1.82	0.61
1:G:46:TYR:OH	2:H:276:GLU:OE2	2.11	0.61
2:R:82:LEU:HD13	2:R:84:TRP:CZ2	2.36	0.61
2:F:332:TRP:NE1	2:F:334:ALA:OXT	2.34	0.60
2:B:82:LEU:HD13	2:B:84:TRP:CZ2	2.36	0.60
2:L:303:ASP:OD1	2:L:303:ASP:N	2.34	0.60
1:C:37:VAL:O	1:C:41:THR:OG1	2.15	0.60
2:R:92:VAL:HG13	2:R:116:VAL:HG23	1.84	0.60
2:J:82:LEU:HD13	2:J:84:TRP:CZ2	2.36	0.59
1:G:355:ASP:N	1:G:355:ASP:OD1	2.35	0.59
1:I:355:ASP:OD1	1:I:356:GLU:N	2.35	0.59
1:K:186:ASP:OD1	1:K:197:ARG:NE	2.35	0.58
2:F:154:LEU:HD13	2:F:240:VAL:HG21	1.85	0.58
2:J:226:ASN:HB3	2:L:300:MET:HE1	1.84	0.58
2:D:146:ASN:O	2:D:146:ASN:ND2	2.36	0.58
2:J:154:LEU:HD22	2:J:158:VAL:HG21	1.84	0.58
2:L:257:ALA:O	2:L:261:GLU:HG3	2.03	0.58
2:P:304:MET:HE1	2:R:170:GLY:CA	2.34	0.58
1:Q:355:ASP:OD1	1:Q:355:ASP:N	2.34	0.58
1:A:170:GLY:HA2	1:C:304:MET:HE1	1.86	0.58
2:L:82:LEU:HD13	2:L:84:TRP:CZ2	2.38	0.58
2:P:304:MET:HE1	2:R:170:GLY:HA2	1.85	0.58
1:I:362:GLU:OE2	1:I:362:GLU:C	2.46	0.58
2:P:152:ASN:O	2:P:289:SER:OG	2.17	0.58
1:Q:154:LEU:CD1	1:Q:240:VAL:HG11	2.33	0.58
1:Q:276:ILE:N	1:Q:276:ILE:HD12	2.19	0.58
2:P:226:ASN:OD1	2:R:298:MET:HE1	2.05	0.57
1:G:165:LEU:HD11	1:G:250:VAL:HG21	1.87	0.57
1:I:341:SER:OG	1:I:347:ASP:OD2	2.20	0.57
1:K:336:GLU:OE1	1:K:336:GLU:N	2.37	0.57
2:H:1:LEU:HD23	2:H:25:LEU:CD1	2.35	0.57
1:O:208:THR:HG1	1:C:361:TYR:HH	1.49	0.57
2:L:85:GLY:N	2:L:111:ALA:O	2.37	0.57
1:O:10:ARG:O	1:O:14:ASN:ND2	2.36	0.56
1:G:179:THR:OG1	1:G:181:ASP:OD1	2.18	0.56
1:K:133:ASN:ND2	1:K:217:VAL:HG12	2.20	0.56
2:R:324:LEU:O	2:R:328:VAL:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:HIS:NE2	2:D:334:ALA:O	2.39	0.56
1:K:61:ASN:OD1	1:K:61:ASN:O	2.24	0.56
1:K:133:ASN:HD21	1:K:217:VAL:HG12	1.71	0.56
1:Q:335:LEU:HD22	1:Q:335:LEU:H	1.70	0.56
1:Q:358:CYS:HA	1:I:191:ARG:HD2	1.86	0.56
1:G:170:GLY:HA3	1:G:244:VAL:HG12	1.87	0.56
1:C:186:ASP:OD1	1:C:197:ARG:NE	2.36	0.56
1:I:251:THR:HG22	1:I:252:ALA:H	1.69	0.56
1:G:276:ILE:N	1:G:276:ILE:HD12	2.21	0.56
2:J:253:GLU:CD	2:J:253:GLU:H	2.13	0.56
1:O:41:THR:HG22	1:O:57:VAL:HG12	1.88	0.55
1:Q:220:GLN:HG2	1:Q:221:LEU:HD12	1.87	0.55
1:Q:10:ARG:O	1:Q:14:ASN:ND2	2.37	0.55
2:B:154:LEU:O	2:B:158:VAL:HG23	2.06	0.55
1:I:61:ASN:OD1	1:I:61:ASN:O	2.24	0.55
2:B:253:GLU:H	2:B:253:GLU:CD	2.14	0.55
1:E:181:ASP:OD2	1:E:195:ARG:NH1	2.33	0.55
2:B:115:LYS:NZ	2:B:137:TYR:OH	2.38	0.55
2:F:134:GLU:OE1	2:F:134:GLU:N	2.34	0.55
2:R:101:ASP:OD1	2:R:102:ARG:N	2.39	0.55
1:A:45:LYS:NZ	1:A:53:PHE:O	2.35	0.55
2:F:59:THR:HG23	2:F:59:THR:O	2.07	0.55
1:C:133:ASN:HD21	1:C:217:VAL:HG12	1.72	0.55
1:Q:350:LYS:HE2	1:Q:350:LYS:HA	1.88	0.55
2:R:129:VAL:HG13	2:R:132:VAL:HB	1.89	0.55
1:A:20:ARG:NH2	1:A:323:ASP:OD1	2.40	0.55
2:B:298:MET:SD	2:D:226:ASN:OD1	2.64	0.55
1:G:350:LYS:HE2	1:G:350:LYS:HA	1.89	0.55
2:B:6:ASN:OD1	2:B:31:ASN:ND2	2.38	0.55
1:E:10:ARG:O	1:E:14:ASN:ND2	2.38	0.55
1:E:61:ASN:OD1	1:E:61:ASN:O	2.24	0.55
2:H:318:SER:O	2:H:322:VAL:HG23	2.07	0.55
2:J:286:THR:HG22	2:J:288:VAL:HG22	1.89	0.55
1:K:45:LYS:NZ	1:K:53:PHE:O	2.37	0.55
1:C:183:ARG:NH1	1:C:188:SER:O	2.40	0.54
2:F:186:ASP:OD1	2:F:197:ARG:NE	2.41	0.54
2:J:48:SER:OG	1:K:186:ASP:OD2	2.18	0.54
1:K:183:ARG:NH1	1:K:188:SER:O	2.40	0.54
1:C:133:ASN:ND2	1:C:217:VAL:HG12	2.22	0.54
2:F:148:SER:N	2:F:151:THR:OG1	2.40	0.54
1:I:37:VAL:O	1:I:41:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:THR:OG1	2:D:207:SER:N	2.41	0.54
2:P:186:ASP:OD1	2:P:197:ARG:NE	2.39	0.53
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.43	0.53
1:A:132:VAL:HG13	1:A:218:LEU:HD21	1.88	0.53
2:B:286:THR:HG22	2:B:288:VAL:HG22	1.89	0.53
2:F:29:VAL:HB	2:F:87:MET:HE1	1.89	0.53
1:O:6:ASN:ND2	1:O:94:GLU:OE2	2.42	0.53
2:P:168:ILE:O	2:P:224:LYS:NZ	2.39	0.53
1:Q:6:ASN:OD1	1:Q:31:ASN:ND2	2.35	0.53
1:E:6:ASN:ND2	1:E:94:GLU:OE1	2.41	0.53
2:H:29:VAL:HG11	2:H:87:MET:SD	2.49	0.53
2:R:134:GLU:OE1	2:R:134:GLU:N	2.38	0.53
2:P:148:SER:N	2:P:151:THR:OG1	2.41	0.53
2:B:314:GLU:HG2	3:B:400:NAD:H72N	1.73	0.53
1:A:61:ASN:OD1	1:A:61:ASN:O	2.27	0.53
1:K:240:VAL:HG23	1:K:311:TYR:CE1	2.44	0.53
2:L:33:THR:HG22	2:L:77:ARG:CZ	2.39	0.53
2:L:139:HIS:O	2:L:139:HIS:ND1	2.40	0.53
2:J:306:LYS:NZ	2:L:172:MET:O	2.41	0.53
2:D:85:GLY:N	2:D:111:ALA:O	2.41	0.52
2:J:250:THR:OG1	2:J:251:PHE:N	2.41	0.52
1:K:313:ASN:OD1	1:K:313:ASN:N	2.42	0.52
2:P:132:VAL:HG13	2:P:218:LEU:HD21	1.91	0.52
2:P:243:VAL:HG11	2:R:243:VAL:HG11	1.91	0.52
2:F:168:ILE:O	2:F:224:LYS:NZ	2.43	0.52
2:F:267:LEU:HD23	2:F:271:LEU:CB	2.40	0.52
2:L:331:LYS:O	2:L:331:LYS:CG	2.57	0.52
2:P:29:VAL:HB	2:P:87:MET:HE1	1.91	0.52
2:L:133:ASN:C	2:L:133:ASN:OD1	2.53	0.52
1:I:242:LEU:HG	1:I:244:VAL:HG13	1.91	0.52
1:K:240:VAL:HG23	1:K:311:TYR:HE1	1.75	0.52
1:K:355:ASP:O	1:K:356:GLU:HB2	2.09	0.52
2:F:267:LEU:HD23	2:F:271:LEU:HB2	1.91	0.51
1:I:132:VAL:HG13	1:I:218:LEU:HD21	1.91	0.51
2:B:332:TRP:NE1	2:B:334:ALA:OXT	2.43	0.51
1:K:251:THR:O	1:K:255:VAL:HG23	2.10	0.51
2:B:250:THR:OG1	2:B:251:PHE:N	2.40	0.51
2:D:133:ASN:C	2:D:133:ASN:OD1	2.53	0.51
1:Q:61:ASN:ND2	1:Q:61:ASN:O	2.44	0.51
1:A:251:THR:HG22	1:A:252:ALA:H	1.76	0.51
1:I:120:ALA:O	1:I:145:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:101:ASP:OD1	2:J:103:ASP:N	2.42	0.51
2:B:115:LYS:NZ	2:B:141:ASP:O	2.36	0.51
2:H:82:LEU:HD13	2:H:84:TRP:CZ2	2.46	0.51
1:I:170:GLY:HA3	1:I:244:VAL:HG12	1.91	0.51
2:H:129:VAL:HG13	2:H:132:VAL:HB	1.93	0.51
1:G:120:ALA:O	1:G:145:SER:OG	2.29	0.51
1:A:346:GLU:O	1:A:350:LYS:HE2	2.11	0.50
2:B:29:VAL:HG11	2:B:84:TRP:HZ3	1.76	0.50
2:B:255:VAL:HG12	2:B:259:PHE:CE2	2.45	0.50
1:K:75:SER:O	1:K:75:SER:OG	2.23	0.50
1:E:135:LYS:HD2	1:E:135:LYS:N	2.27	0.50
1:O:351:ASP:O	1:O:352:ASN:C	2.55	0.50
2:B:306:LYS:NZ	2:D:172:MET:O	2.45	0.50
1:E:251:THR:N	1:E:254:ASP:OD2	2.45	0.50
1:G:37:VAL:O	1:G:41:THR:OG1	2.26	0.50
2:L:33:THR:HG22	2:L:77:ARG:NE	2.26	0.50
2:P:172:MET:O	2:R:306:LYS:NZ	2.45	0.50
2:B:193:LEU:HD11	1:C:38:LYS:HD2	1.94	0.50
1:C:45:LYS:NZ	1:C:53:PHE:O	2.36	0.50
2:R:161:LEU:CD2	2:R:244:VAL:HG21	2.41	0.50
2:J:255:VAL:HG12	2:J:259:PHE:CE2	2.47	0.50
2:P:266:GLU:HG3	2:P:267:LEU:HD12	1.93	0.50
2:P:272:SER:OG	2:P:288:VAL:HG11	2.12	0.50
2:J:6:ASN:OD1	2:J:31:ASN:ND2	2.42	0.50
1:Q:120:ALA:O	1:Q:145:SER:OG	2.28	0.49
2:B:117:LEU:HD11	2:B:324:LEU:HD23	1.93	0.49
1:C:139:HIS:O	1:C:139(A):ASP:CG	2.55	0.49
2:F:287:ASP:OD1	2:F:287:ASP:N	2.44	0.49
1:G:254:ASP:OD1	1:G:255:VAL:N	2.45	0.49
2:H:92:VAL:HG11	2:H:116:VAL:HG22	1.95	0.49
2:R:162:ASP:OD1	2:R:167:ILE:N	2.43	0.49
2:R:275:ASP:OD1	2:R:294:SER:OG	2.24	0.49
2:B:246:VAL:HG22	2:B:303:ASP:O	2.11	0.49
1:C:313:ASN:OD1	1:C:313:ASN:N	2.42	0.49
2:F:3:VAL:CG2	2:F:25:LEU:HD12	2.43	0.49
1:G:10:ARG:O	1:G:14:ASN:ND2	2.39	0.49
2:J:206:THR:HG22	2:J:207:SER:N	2.27	0.49
1:K:139:HIS:O	1:K:139(A):ASP:CG	2.55	0.49
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.35	0.49
2:P:294:SER:O	2:P:297:THR:HG22	2.12	0.49
2:R:198:ALA:O	2:R:199:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ASN:OD1	1:C:61:ASN:O	2.31	0.49
1:E:146:ASN:O	1:E:147:ALA:HB3	2.13	0.49
2:H:154:LEU:HD23	2:H:214:VAL:HG21	1.95	0.49
1:E:351:ASP:O	1:E:352:ASN:C	2.55	0.48
2:J:49:ILE:HD11	2:J:235:PRO:HB2	1.94	0.48
1:A:120:ALA:O	1:A:145:SER:OG	2.30	0.48
1:A:362:GLU:C	1:A:362:GLU:OE1	2.56	0.48
1:C:20:ARG:HE	1:C:322:VAL:HG11	1.78	0.48
1:C:240:VAL:HG23	1:C:311:TYR:CE1	2.47	0.48
2:F:5:ILE:HB	2:F:30:ILE:HD13	1.95	0.48
2:F:224:LYS:C	2:H:300:MET:HE1	2.38	0.48
2:J:301:GLY:HA3	2:L:169:LYS:HE2	1.94	0.48
1:C:240:VAL:HG23	1:C:311:TYR:HE1	1.77	0.48
1:E:179:THR:OG1	1:E:181:ASP:OD1	2.23	0.48
1:G:61:ASN:ND2	1:G:61:ASN:O	2.47	0.48
2:R:147:ALA:O	2:R:317:TYR:OH	2.29	0.48
2:B:298:MET:HE1	2:D:228:ILE:HG23	1.96	0.48
1:G:276:ILE:HD12	1:G:276:ILE:H	1.77	0.48
1:K:37:VAL:HG21	1:K:61:ASN:O	2.14	0.48
2:P:317:TYR:O	2:P:321:VAL:HG23	2.14	0.48
1:C:6:ASN:OD1	1:C:31:ASN:ND2	2.40	0.48
1:C:251:THR:O	1:C:255:VAL:HG23	2.14	0.48
2:F:198:ALA:O	2:F:199:ALA:HB3	2.14	0.48
2:F:304:MET:SD	2:H:169:LYS:HG3	2.54	0.48
1:I:346:GLU:O	1:I:350:LYS:HE2	2.14	0.48
2:P:109:LEU:HD11	2:P:143:ILE:HD13	1.96	0.47
2:R:287:ASP:OD1	2:R:287:ASP:N	2.47	0.47
1:Q:46:TYR:OH	2:R:276:GLU:OE2	2.17	0.47
1:C:120:ALA:O	1:C:145:SER:OG	2.32	0.47
1:Q:348:PHE:CE1	2:L:77:ARG:NH2	2.83	0.47
2:R:215:ALA:HB1	2:R:222:LYS:HA	1.96	0.47
2:B:226:ASN:OD1	2:D:298:MET:HE1	2.14	0.47
1:E:242:LEU:HG	1:E:244:VAL:HG13	1.96	0.47
2:P:133:ASN:OD1	2:P:133:ASN:C	2.58	0.47
2:P:224:LYS:C	2:R:300:MET:HE1	2.38	0.47
2:R:176:HIS:ND1	2:R:177:SER:O	2.41	0.47
2:P:11:ILE:CD1	3:P:400:NAD:H71N	2.27	0.47
1:C:181:ASP:OD2	1:C:195:ARG:NH1	2.46	0.47
2:B:25:LEU:HD21	2:B:326:ASP:OD2	2.15	0.47
2:B:49:ILE:HD11	2:B:235:PRO:HB2	1.97	0.47
2:B:147:ALA:HB1	2:B:151:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:ARG:NH2	1:G:348:PHE:CD1	2.82	0.47
2:D:220:ASN:OD1	2:D:220:ASN:C	2.58	0.47
1:E:359:LYS:HE3	1:E:362:GLU:OE2	2.15	0.47
1:K:355:ASP:O	1:K:356:GLU:CB	2.62	0.47
1:K:120:ALA:O	1:K:145:SER:OG	2.32	0.47
1:E:26:ASP:OD1	1:E:28:VAL:HG12	2.15	0.47
1:Q:115:LYS:NZ	1:Q:137:TYR:OH	2.34	0.47
1:A:37:VAL:O	1:A:41:THR:OG1	2.31	0.47
1:G:164:GLU:O	1:G:164:GLU:HG3	2.14	0.47
2:J:147:ALA:HB1	2:J:151:THR:HG21	1.97	0.47
1:A:242:LEU:HG	1:A:244:VAL:HG13	1.96	0.46
1:C:187:ALA:O	1:C:196:ALA:HB1	2.15	0.46
2:P:77:ARG:NH2	1:I:348:PHE:CZ	2.83	0.46
1:Q:32:ASP:OD1	1:Q:34:GLY:N	2.48	0.46
1:I:140:VAL:O	1:I:141:ALA:HB3	2.15	0.46
2:P:119:THR:O	2:P:119:THR:OG1	2.31	0.46
2:D:191:ARG:HB3	2:D:191:ARG:CZ	2.45	0.46
2:D:253:GLU:H	2:D:253:GLU:CD	2.23	0.46
1:E:276:ILE:HD13	1:E:276:ILE:N	2.31	0.46
1:K:357:GLU:CD	1:K:357:GLU:H	2.24	0.46
1:O:168:VAL:HB	1:O:245:ASN:OD1	2.15	0.46
1:Q:362:GLU:OE2	1:Q:362:GLU:C	2.59	0.46
2:D:49:ILE:HD11	2:D:235:PRO:HB2	1.98	0.46
2:H:133:ASN:OD1	2:H:133:ASN:C	2.59	0.46
1:A:254:ASP:OD1	1:A:255:VAL:N	2.48	0.46
2:F:127:THR:HG22	2:F:145:SER:OG	2.16	0.46
1:O:146:ASN:O	1:O:147:ALA:HB3	2.14	0.46
1:A:140:VAL:O	1:A:141:ALA:HB3	2.16	0.46
2:B:48:SER:HG	1:C:186:ASP:CG	2.19	0.46
1:C:360:LEU:O	1:C:361:TYR:HB2	2.16	0.46
2:H:27:VAL:HG12	2:H:71:ILE:HD13	1.97	0.46
2:H:216:LEU:HD12	2:H:216:LEU:O	2.15	0.46
2:J:275:ASP:OD1	2:J:275:ASP:N	2.48	0.46
2:D:1:LEU:HD22	2:D:329:ALA:HA	1.96	0.46
1:G:140:VAL:O	1:G:141:ALA:HB3	2.15	0.46
1:K:187:ALA:O	1:K:196:ALA:HB1	2.15	0.46
2:P:198:ALA:O	2:P:199:ALA:HB3	2.14	0.46
1:Q:164:GLU:O	1:Q:164:GLU:HG3	2.15	0.46
1:G:32:ASP:OD2	1:G:34:GLY:N	2.49	0.46
1:I:146:ASN:O	1:I:147:ALA:HB3	2.16	0.46
1:O:242:LEU:HG	1:O:244:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:140:VAL:O	1:Q:141:ALA:HB3	2.16	0.46
2:H:187:ALA:O	2:H:196:ALA:HB1	2.15	0.46
2:J:304:MET:HE1	2:L:170:GLY:HA2	1.98	0.45
2:F:11:ILE:CD1	3:F:400:NAD:H71N	2.28	0.45
2:F:25:LEU:HD23	2:F:326:ASP:OD2	2.16	0.45
2:J:226:ASN:HB3	2:L:300:MET:CE	2.46	0.45
1:K:165:LEU:HD22	1:K:250:VAL:HG11	1.98	0.45
2:L:191:ARG:HB3	2:L:191:ARG:CZ	2.45	0.45
1:Q:276:ILE:HD12	1:Q:276:ILE:H	1.81	0.45
1:E:170:GLY:HA3	1:E:244:VAL:HG12	1.97	0.45
2:P:82:LEU:HD13	2:P:84:TRP:CZ2	2.52	0.45
2:P:256:ASN:O	2:P:260:ARG:HG3	2.16	0.45
1:A:33:SER:O	1:A:33:SER:OG	2.32	0.45
1:A:146:ASN:O	1:A:147:ALA:HB3	2.16	0.45
1:G:240:VAL:HG23	1:G:311:TYR:HE1	1.80	0.45
2:L:250:THR:HG22	2:L:251:PHE:N	2.32	0.45
1:A:170:GLY:HA3	1:A:244:VAL:HG12	1.98	0.45
1:O:61:ASN:C	1:O:61:ASN:OD1	2.58	0.45
2:P:16:LEU:O	2:P:16:LEU:HD23	2.17	0.45
1:Q:170:GLY:HA3	1:Q:244:VAL:HG12	1.98	0.45
1:A:161:LEU:HD23	1:A:165:LEU:HD12	1.97	0.45
2:D:94:GLU:OE2	2:D:94:GLU:HA	2.16	0.45
1:G:251:THR:OG1	1:G:252:ALA:N	2.50	0.45
2:H:217:VAL:O	2:H:218:LEU:HD12	2.17	0.45
2:J:147:ALA:CB	2:J:151:THR:HG21	2.47	0.45
2:B:157:PHE:HB3	2:B:271:LEU:HD11	1.99	0.45
2:B:226:ASN:HB3	2:D:300:MET:CE	2.46	0.45
2:D:236:ASN:ND2	2:D:312:ASP:OD1	2.50	0.45
2:D:257:ALA:O	2:D:261:GLU:HG3	2.16	0.45
1:G:240:VAL:HG23	1:G:311:TYR:CE1	2.51	0.45
2:H:215:ALA:HB1	2:H:222:LYS:HA	1.99	0.45
2:L:94:GLU:OE2	2:L:94:GLU:HA	2.16	0.45
2:B:218:LEU:HB3	2:B:221:LEU:HD23	1.98	0.45
3:E:400:NAD:H3D	1:K:362:GLU:HA	1.98	0.45
2:F:261:GLU:O	2:F:265:ASN:OD1	2.35	0.45
2:J:274:CYS:O	2:J:294:SER:OG	2.35	0.45
2:P:30:ILE:HG12	2:P:71:ILE:HG21	1.98	0.45
1:Q:348:PHE:C	1:Q:348:PHE:CD2	2.95	0.45
1:Q:348:PHE:HE1	2:L:77:ARG:CZ	2.29	0.45
1:Q:362:GLU:HA	3:I:400:NAD:H3D	1.99	0.45
1:E:1:LEU:HD12	1:E:329:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:ILE:HG23	2:F:143:ILE:HG22	1.98	0.45
2:F:170:GLY:HA2	2:H:304:MET:HE1	1.99	0.45
1:G:165:LEU:HD23	1:G:246:ILE:HG12	1.98	0.45
1:G:244:VAL:HG23	1:G:246:ILE:HD11	1.99	0.45
2:J:195:ARG:NH2	2:J:206:THR:HG21	2.32	0.45
2:P:117:LEU:HD11	2:P:324:LEU:HD23	1.99	0.44
1:A:160:VAL:O	1:A:164:GLU:HG2	2.17	0.44
1:G:355:ASP:O	1:G:356:GLU:HB2	2.16	0.44
2:P:25:LEU:N	2:P:25:LEU:HD22	2.32	0.44
1:Q:335:LEU:HD13	1:Q:335:LEU:N	2.32	0.44
1:Q:355:ASP:O	1:Q:356:GLU:HB2	2.16	0.44
1:E:245:ASN:OD1	1:E:245:ASN:O	2.35	0.44
1:I:137:TYR:O	1:I:331:LYS:NZ	2.47	0.44
2:J:25:LEU:HD21	2:J:326:ASP:OD2	2.17	0.44
2:P:154:LEU:O	2:P:158:VAL:HG23	2.17	0.44
2:R:118:ILE:HG22	2:R:120:ALA:H	1.83	0.44
1:K:317:TYR:O	1:K:321:VAL:HG23	2.18	0.44
2:R:187:ALA:O	2:R:196:ALA:HB1	2.17	0.44
1:A:169:LYS:HG2	1:C:304:MET:HE2	1.99	0.44
2:D:37:VAL:HG13	2:D:64:ILE:HG23	2.00	0.44
1:C:254:ASP:OD1	1:C:254:ASP:N	2.43	0.44
1:E:41:THR:CG2	1:E:57:VAL:HG12	2.48	0.44
1:E:61:ASN:OD1	1:E:61:ASN:C	2.60	0.44
1:E:168:VAL:HB	1:E:245:ASN:OD1	2.17	0.44
1:G:48:SER:HA	2:H:281:ILE:HG21	1.99	0.44
2:H:253:GLU:N	2:H:253:GLU:CD	2.75	0.44
2:L:49:ILE:HD11	2:L:235:PRO:HB2	2.00	0.44
1:O:83:PRO:O	1:O:87:LEU:HD12	2.18	0.44
2:F:133:ASN:OD1	2:F:133:ASN:C	2.60	0.44
1:I:220:GLN:HG2	1:I:221:LEU:HD12	2.00	0.44
2:J:168:ILE:HG22	2:J:169:LYS:HD3	2.00	0.44
2:D:176:HIS:N	2:D:230:LEU:O	2.47	0.44
2:P:151:THR:HG21	2:P:213:ALA:HB3	2.00	0.44
1:Q:348:PHE:CD1	2:L:77:ARG:NH2	2.85	0.44
2:B:187:ALA:O	2:B:196:ALA:HB1	2.18	0.44
2:F:132:VAL:HG13	2:F:218:LEU:HD21	1.99	0.44
2:J:154:LEU:HD22	2:J:158:VAL:CG2	2.47	0.44
2:J:198:ALA:O	2:J:199:ALA:HB3	2.18	0.44
2:B:146:ASN:O	2:B:147:ALA:HB3	2.18	0.44
1:C:317:TYR:O	1:C:321:VAL:HG23	2.18	0.44
2:F:16:LEU:O	2:F:16:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:LEU:HD13	1:K:246:ILE:HG12	2.00	0.44
1:Q:179:THR:OG1	1:Q:181:ASP:OD1	2.19	0.43
2:R:37:VAL:HG22	2:R:73:VAL:CG2	2.48	0.43
2:R:253:GLU:N	2:R:253:GLU:CD	2.76	0.43
2:D:90:ASP:HA	2:D:114:LYS:HD2	2.00	0.43
1:E:298:MET:HE3	1:G:171:THR:HG22	2.00	0.43
2:F:10:ARG:NH2	2:F:314:GLU:OE1	2.43	0.43
1:O:245:ASN:OD1	1:O:245:ASN:O	2.36	0.43
2:R:165:PHE:N	2:R:165:PHE:CD2	2.84	0.43
3:A:400:NAD:H3D	1:G:362:GLU:HA	2.00	0.43
2:B:275:ASP:N	2:B:275:ASP:OD1	2.48	0.43
1:C:336:GLU:OE1	1:C:336:GLU:N	2.44	0.43
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.53	0.43
2:H:29:VAL:HG12	2:H:72:LYS:HB3	2.00	0.43
1:Q:6:ASN:HB3	1:Q:94:GLU:OE1	2.18	0.43
2:R:45:LYS:NZ	2:R:55:ALA:O	2.31	0.43
2:R:83:PRO:O	2:R:87:MET:HG3	2.17	0.43
1:E:236:ASN:ND2	1:E:312:ASP:OD1	2.51	0.43
1:O:61:ASN:OD1	1:O:61:ASN:O	2.37	0.43
2:D:198:ALA:O	2:D:199:ALA:HB3	2.19	0.43
1:I:161:LEU:HD23	1:I:244:VAL:HG21	2.01	0.43
2:J:29:VAL:HG11	2:J:84:TRP:HZ3	1.83	0.43
2:J:304:MET:HE2	2:L:169:LYS:NZ	2.33	0.43
1:K:140:VAL:O	1:K:141:ALA:HB3	2.18	0.43
2:R:115:LYS:HD2	2:R:328:VAL:HG11	1.99	0.43
1:A:251:THR:O	1:A:254:ASP:OD1	2.37	0.43
2:D:191:ARG:HB3	2:D:191:ARG:NH1	2.34	0.43
2:F:47:ASP:OD1	2:F:48:SER:N	2.51	0.43
2:H:11:ILE:HD11	3:H:400:NAD:H71N	1.84	0.43
2:J:125:ILE:HD12	2:J:143:ILE:HG21	2.01	0.43
2:D:6:ASN:OD1	2:D:31:ASN:ND2	2.51	0.43
1:I:179:THR:OG1	1:I:181:ASP:OD1	2.26	0.43
2:P:174:THR:O	2:P:174:THR:HG23	2.19	0.43
2:F:303:ASP:OD1	2:H:169:LYS:HE3	2.18	0.43
2:H:20:ARG:NH2	2:H:323:ASP:OD1	2.48	0.43
2:L:253:GLU:H	2:L:253:GLU:CD	2.25	0.43
2:R:11:ILE:CD1	3:R:400:NAD:H71N	2.32	0.43
2:B:147:ALA:CB	2:B:151:THR:HG21	2.48	0.43
2:B:198:ALA:O	2:B:199:ALA:HB3	2.18	0.43
2:B:298:MET:HE1	2:D:228:ILE:CG2	2.48	0.43
1:C:303:ASP:OD1	1:C:303:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82:LEU:HD13	2:F:84:TRP:CZ2	2.54	0.43
1:I:251:THR:O	1:I:254:ASP:OD1	2.37	0.43
1:A:353:PRO:HG2	1:G:98:VAL:HG13	2.01	0.43
2:D:253:GLU:CD	2:D:253:GLU:N	2.77	0.43
2:F:154:LEU:O	2:F:158:VAL:HG23	2.19	0.43
1:I:254:ASP:OD1	1:I:255:VAL:N	2.52	0.43
2:J:78:ASN:ND2	2:J:81:ASN:OD1	2.52	0.43
1:K:25:LEU:H	1:K:25:LEU:HD22	1.84	0.43
1:Q:32:ASP:OD1	1:Q:32:ASP:C	2.61	0.43
1:C:248(A):VAL:O	1:C:248(A):VAL:HG22	2.19	0.43
1:G:362:GLU:C	1:G:362:GLU:OE1	2.62	0.43
2:P:47:ASP:OD1	2:P:48:SER:N	2.52	0.42
1:A:355:ASP:OD1	1:A:355:ASP:C	2.62	0.42
1:E:83:PRO:O	1:E:87:LEU:HD12	2.19	0.42
1:E:226:ASN:ND2	1:G:298:MET:SD	2.92	0.42
2:F:218:LEU:HB3	2:F:221:LEU:HD23	2.00	0.42
2:J:117:LEU:HD11	2:J:324:LEU:HD23	2.00	0.42
2:P:146:ASN:HD22	2:P:321:VAL:HG22	1.84	0.42
1:G:126:PRO:HB2	1:G:128:TYR:CE2	2.54	0.42
1:I:169:LYS:HD3	1:K:301:GLY:HA3	2.00	0.42
1:O:26:ASP:O	1:O:28:VAL:HG13	2.19	0.42
1:O:360:LEU:HD11	1:C:191:ARG:HD3	2.01	0.42
1:A:348:PHE:HE1	1:A:355:ASP:OD2	2.02	0.42
2:B:82:LEU:HD13	2:B:84:TRP:HZ2	1.81	0.42
2:R:20:ARG:HG3	2:R:20:ARG:HH11	1.85	0.42
2:R:208:THR:HG23	2:R:211:ALA:H	1.84	0.42
1:E:48:SER:HA	2:F:281:ILE:HG21	2.00	0.42
2:F:304:MET:HG3	2:H:169:LYS:HE3	2.01	0.42
1:G:245:ASN:C	1:G:246:ILE:HD12	2.43	0.42
2:H:83:PRO:O	2:H:87:MET:HG2	2.19	0.42
2:J:115:LYS:NZ	2:J:137:TYR:OH	2.48	0.42
2:J:146:ASN:O	2:J:147:ALA:HB3	2.19	0.42
2:L:191:ARG:HB3	2:L:191:ARG:NH1	2.34	0.42
2:F:255:VAL:HG11	2:F:305:VAL:HG11	2.01	0.42
1:G:56:ASP:OD2	1:G:58:LYS:HE3	2.20	0.42
2:H:147:ALA:O	2:H:317:TYR:OH	2.36	0.42
2:J:157:PHE:HB3	2:J:271:LEU:HD11	2.01	0.42
1:O:146:ASN:HD22	1:O:321:VAL:HG22	1.84	0.42
1:O:170:GLY:HA3	1:O:244:VAL:HG12	1.99	0.42
2:P:125:ILE:HD12	2:P:143:ILE:HG21	2.02	0.42
2:P:298:MET:HE1	2:R:226:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:PRO:HB2	1:Q:128:TYR:CE2	2.54	0.42
2:B:92:VAL:O	2:B:92:VAL:HG13	2.20	0.42
1:C:146:ASN:O	1:C:147:ALA:HB3	2.20	0.42
2:D:79:PRO:HA	2:D:82:LEU:HD12	2.02	0.42
1:I:165:LEU:HD23	1:I:246:ILE:HG21	2.01	0.42
2:J:154:LEU:HD11	2:J:172:MET:SD	2.60	0.42
1:K:239:VAL:HG23	1:K:309:ALA:O	2.20	0.42
2:L:154:LEU:HD22	2:L:172:MET:CE	2.50	0.42
2:L:198:ALA:O	2:L:199:ALA:HB3	2.19	0.42
1:E:106:GLY:O	1:E:110:GLN:HG3	2.20	0.42
2:F:218:LEU:CB	2:F:221:LEU:HD23	2.50	0.42
1:K:165:LEU:HB3	1:K:246:ILE:CG1	2.50	0.42
2:R:25:LEU:HD23	2:R:326:ASP:OD1	2.20	0.42
1:C:179:THR:OG1	1:C:181:ASP:OD1	2.30	0.42
2:D:256:ASN:O	2:D:260:ARG:HG3	2.20	0.42
1:E:352:ASN:OD1	1:E:352:ASN:N	2.52	0.42
2:J:82:LEU:HD13	2:J:84:TRP:HZ2	1.81	0.42
2:J:92:VAL:HG13	2:J:92:VAL:O	2.20	0.42
2:J:298:MET:HE3	2:L:226:ASN:OD1	2.19	0.42
2:L:3:VAL:HG13	2:L:93:ILE:CD1	2.50	0.42
2:R:73:VAL:O	2:R:73:VAL:HG23	2.19	0.42
1:G:32:ASP:OD2	1:G:32:ASP:C	2.63	0.42
2:L:154:LEU:HD22	2:L:172:MET:HE3	2.01	0.42
1:O:135:LYS:HA	1:O:135:LYS:HE2	2.01	0.42
1:O:194:ARG:NH1	1:Q:278:LEU:O	2.53	0.42
2:P:151:THR:CG2	2:P:213:ALA:HB3	2.49	0.42
1:Q:10:ARG:NH2	1:Q:314:GLU:OE1	2.41	0.42
1:Q:142:ASN:OD1	1:Q:142:ASN:N	2.47	0.42
1:C:239:VAL:HG23	1:C:309:ALA:O	2.20	0.42
2:F:157:PHE:CE1	2:F:242:LEU:HD23	2.54	0.42
1:G:10:ARG:NH2	1:G:314:GLU:OE1	2.39	0.42
2:R:242:LEU:HD11	2:R:244:VAL:HG13	2.01	0.41
2:D:92:VAL:O	2:D:92:VAL:HG13	2.20	0.41
1:E:60(A):ASP:OD1	1:E:61:ASN:N	2.43	0.41
1:E:72:LYS:HA	1:E:72:LYS:HE2	2.02	0.41
1:K:25:LEU:CD2	1:K:326:ASP:OD2	2.68	0.41
1:O:84:TRP:HA	1:O:84:TRP:CE3	2.55	0.41
1:I:187:ALA:O	1:I:196:ALA:HB1	2.20	0.41
2:J:206:THR:HG22	2:J:207:SER:H	1.85	0.41
1:K:251:THR:O	1:K:254:ASP:OD1	2.38	0.41
1:K:360:LEU:O	1:K:361:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:170:GLY:HA2	2:R:304:MET:HE1	2.01	0.41
1:Q:334:GLY:C	1:Q:335:LEU:HD13	2.46	0.41
1:Q:362:GLU:C	1:Q:362:GLU:CD	2.88	0.41
2:B:304:MET:HE1	2:D:170:GLY:HA2	2.02	0.41
1:G:133:ASN:OD1	1:G:133:ASN:C	2.63	0.41
1:G:187:ALA:O	1:G:196:ALA:HB1	2.19	0.41
2:J:1:LEU:HD22	2:J:329:ALA:HA	2.02	0.41
2:L:25:LEU:HD21	2:L:325:ALA:HB3	2.00	0.41
2:L:92:VAL:O	2:L:92:VAL:HG13	2.20	0.41
1:O:106:GLY:O	1:O:110:GLN:HG3	2.20	0.41
2:P:210:ALA:O	2:P:211:ALA:C	2.64	0.41
2:J:218:LEU:HB3	2:J:221:LEU:HD23	2.01	0.41
1:O:352:ASN:OD1	1:O:352:ASN:N	2.51	0.41
2:R:106:GLY:O	2:R:110:GLN:HG3	2.20	0.41
2:F:306:LYS:NZ	2:H:172:MET:O	2.54	0.41
2:L:176:HIS:N	2:L:230:LEU:O	2.53	0.41
1:O:338:SER:O	1:O:339:VAL:HG12	2.20	0.41
1:Q:60(A):ASP:CG	1:Q:61:ASN:H	2.28	0.41
1:Q:240:VAL:HG23	1:Q:311:TYR:HE1	1.85	0.41
2:R:126:PRO:HD2	2:R:143:ILE:O	2.21	0.41
2:B:172:MET:HG3	2:B:227:GLY:HA3	2.02	0.41
2:D:123:GLY:C	2:D:125:ILE:HD12	2.45	0.41
2:F:3:VAL:HG22	2:F:25:LEU:HD12	2.02	0.41
2:P:10:ARG:NH2	2:P:314:GLU:OE1	2.44	0.41
2:P:176:HIS:O	2:P:232:VAL:HG22	2.21	0.41
2:R:293:ASP:C	2:R:293:ASP:OD1	2.63	0.41
2:B:78:ASN:ND2	2:B:81:ASN:OD1	2.53	0.41
1:C:25:LEU:CD2	1:C:326:ASP:OD2	2.69	0.41
1:C:140:VAL:O	1:C:141:ALA:HB3	2.19	0.41
1:I:301:GLY:HA3	1:K:169:LYS:HD3	2.02	0.41
2:J:187:ALA:O	2:J:196:ALA:HB1	2.21	0.41
1:O:84:TRP:HA	1:O:84:TRP:HE3	1.86	0.41
3:O:400:NAD:H3D	1:C:362:GLU:HA	2.01	0.41
1:Q:218:LEU:CB	1:Q:221:LEU:HD13	2.51	0.41
2:R:16:LEU:C	2:R:16:LEU:HD23	2.46	0.41
2:H:92:VAL:HG13	2:H:92:VAL:O	2.20	0.41
1:I:239:VAL:HG23	1:I:309:ALA:O	2.21	0.41
2:L:11:ILE:CD1	3:L:400:NAD:H71N	2.33	0.41
2:L:131:GLY:N	2:L:134:GLU:OE2	2.53	0.41
2:L:236:ASN:ND2	2:L:312:ASP:OD1	2.51	0.41
1:O:362:GLU:C	1:O:362:GLU:CD	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:148:SER:O	2:P:151:THR:OG1	2.38	0.41
2:P:267:LEU:HD23	2:P:271:LEU:HB2	2.01	0.41
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.19	0.41
2:R:161:LEU:HD21	2:R:244:VAL:HG21	2.02	0.41
2:B:154:LEU:HD22	2:B:172:MET:HE2	2.02	0.41
2:B:206:THR:OG1	2:B:207:SER:N	2.54	0.41
1:E:126:PRO:HB2	1:E:128:TYR:CZ	2.56	0.41
2:F:176:HIS:HA	2:F:238:SER:HB3	2.02	0.41
2:F:317:TYR:O	2:F:321:VAL:HG23	2.20	0.41
2:H:1:LEU:HD23	2:H:25:LEU:HD12	2.02	0.41
2:J:193:LEU:HD11	1:K:38:LYS:HD2	2.03	0.41
1:K:303:ASP:OD1	1:K:303:ASP:N	2.54	0.41
2:L:122(A):LYS:HE3	2:L:122(A):LYS:HA	2.02	0.41
2:L:253:GLU:CD	2:L:253:GLU:N	2.79	0.41
2:L:332:TRP:NE1	2:L:334:ALA:OXT	2.54	0.41
1:Q:133:ASN:OD1	1:Q:133:ASN:C	2.63	0.41
2:F:3:VAL:HB	2:F:27:VAL:HA	2.03	0.41
2:H:299:VAL:HG13	2:H:305:VAL:HG22	2.03	0.41
2:L:37:VAL:HG13	2:L:64:ILE:HG23	2.03	0.41
1:O:298:MET:HE3	1:Q:171:THR:HG22	2.03	0.40
2:P:154:LEU:HD13	2:P:240:VAL:HG21	2.04	0.40
2:R:154:LEU:HD23	2:R:214:VAL:HG21	2.03	0.40
2:B:9:GLY:HA3	3:B:400:NAD:H4B	2.03	0.40
2:B:256:ASN:OD1	2:B:297:THR:HG21	2.20	0.40
2:F:90:ASP:OD1	2:F:90:ASP:N	2.54	0.40
2:F:300:MET:HE1	2:H:226:ASN:N	2.36	0.40
2:H:317:TYR:O	2:H:321:VAL:HG23	2.21	0.40
1:Q:37:VAL:O	1:Q:41:THR:OG1	2.36	0.40
1:A:181:ASP:OD1	1:A:181:ASP:N	2.51	0.40
2:D:1:LEU:HD12	2:D:2:LYS:H	1.86	0.40
2:D:3:VAL:HG13	2:D:93:ILE:CD1	2.50	0.40
2:P:127:THR:HG22	2:P:145:SER:OG	2.22	0.40
1:Q:317:TYR:O	1:Q:321:VAL:HG23	2.21	0.40
2:B:45:LYS:NZ	2:B:55:ALA:O	2.37	0.40
1:C:126:PRO:HB2	1:C:128:TYR:CZ	2.57	0.40
1:G:251:THR:O	1:G:255:VAL:HG23	2.22	0.40
2:J:179:THR:OG1	2:J:231:ARG:NH1	2.55	0.40
2:L:1:LEU:HD22	2:L:329:ALA:HA	2.02	0.40
2:L:274:CYS:O	2:L:294:SER:OG	2.40	0.40
2:P:147:ALA:HB1	2:P:151:THR:OG1	2.22	0.40
1:Q:176:HIS:HD2	1:Q:177:SER:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:242:LEU:HG	1:Q:244:VAL:HG13	2.04	0.40
2:D:25:LEU:HD11	2:D:325:ALA:HB3	2.02	0.40
1:E:127:THR:CG2	1:E:147:ALA:HB2	2.52	0.40
1:E:298:MET:CE	1:G:171:THR:HG22	2.51	0.40
2:F:271:LEU:HD12	2:F:272:SER:H	1.86	0.40
1:G:254:ASP:OD1	1:G:254:ASP:C	2.64	0.40
1:G:359:LYS:HB3	1:G:362:GLU:HB3	2.03	0.40
2:H:64:ILE:HG23	2:H:73:VAL:HG21	2.03	0.40
2:P:33:THR:OG1	2:P:77:ARG:NH1	2.55	0.40
2:F:79:PRO:HD2	2:F:107:LYS:HD3	2.04	0.40
1:G:162:ASP:HB2	1:G:167:ILE:HD12	2.04	0.40
1:G:313:ASN:OD1	1:G:313:ASN:N	2.52	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	366/368 (100%)	342 (93%)	21 (6%)	3 (1%)	16	47
1	C	366/368 (100%)	335 (92%)	28 (8%)	3 (1%)	16	47
1	E	366/368 (100%)	335 (92%)	27 (7%)	4 (1%)	11	39
1	G	366/368 (100%)	332 (91%)	31 (8%)	3 (1%)	16	47
1	I	366/368 (100%)	337 (92%)	25 (7%)	4 (1%)	11	39
1	K	366/368 (100%)	336 (92%)	26 (7%)	4 (1%)	11	39
1	O	366/368 (100%)	330 (90%)	31 (8%)	5 (1%)	9	34
1	Q	366/368 (100%)	338 (92%)	25 (7%)	3 (1%)	16	47
2	B	335/337 (99%)	317 (95%)	17 (5%)	1 (0%)	36	67
2	D	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	335/337 (99%)	315 (94%)	19 (6%)	1 (0%)	36	67
2	H	335/337 (99%)	317 (95%)	17 (5%)	1 (0%)	36	67
2	J	335/337 (99%)	315 (94%)	19 (6%)	1 (0%)	36	67
2	L	335/337 (99%)	317 (95%)	17 (5%)	1 (0%)	36	67
2	P	335/337 (99%)	317 (95%)	17 (5%)	1 (0%)	36	67
2	R	335/337 (99%)	315 (94%)	19 (6%)	1 (0%)	36	67
All	All	5608/5640 (99%)	5216 (93%)	355 (6%)	37 (1%)	20	49

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	10	ARG
1	O	356	GLU
1	Q	10	ARG
1	A	10	ARG
1	C	10	ARG
1	E	10	ARG
1	E	356	GLU
1	G	10	ARG
1	I	10	ARG
1	I	356	GLU
1	K	10	ARG
1	O	339	VAL
1	G	237	VAL
1	K	356	GLU
1	O	141	ALA
2	P	237	VAL
1	Q	237	VAL
2	R	237	VAL
1	A	237	VAL
1	C	141	ALA
1	C	237	VAL
1	E	141	ALA
2	F	237	VAL
2	H	237	VAL
1	I	237	VAL
1	K	141	ALA
1	O	237	VAL
1	A	141	ALA
2	B	237	VAL

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Mol	Chain	Res	Type
2	D	237	VAL
1	E	237	VAL
2	J	237	VAL
1	K	237	VAL
2	L	237	VAL
1	Q	141	ALA
1	G	141	ALA
1	I	141	ALA

### 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	A	304/304 (100%)	300 (99%)	4 (1%)	61	77
1	C	304/304 (100%)	301 (99%)	3 (1%)	68	79
1	E	304/304 (100%)	300 (99%)	4 (1%)	61	77
1	G	304/304 (100%)	302 (99%)	2 (1%)	76	82
1	I	304/304 (100%)	300 (99%)	4 (1%)	61	77
1	K	304/304 (100%)	296 (97%)	8 (3%)	40	68
1	O	304/304 (100%)	298 (98%)	6 (2%)	48	72
1	Q	304/304 (100%)	302 (99%)	2 (1%)	76	82
2	B	279/279 (100%)	273 (98%)	6 (2%)	45	71
2	D	279/279 (100%)	273 (98%)	6 (2%)	45	71
2	F	279/279 (100%)	274 (98%)	5 (2%)	51	73
2	H	279/279 (100%)	273 (98%)	6 (2%)	45	71
2	J	279/279 (100%)	273 (98%)	6 (2%)	45	71
2	L	279/279 (100%)	273 (98%)	6 (2%)	45	71
2	P	279/279 (100%)	275 (99%)	4 (1%)	59	76
2	R	279/279 (100%)	272 (98%)	7 (2%)	42	69
All	All	4664/4664 (100%)	4585 (98%)	79 (2%)	52	74

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	28	VAL
1	O	30	VAL
1	O	41	THR
1	O	84	TRP
1	O	201	LEU
1	O	240	VAL
2	P	84	TRP
2	P	161	LEU
2	P	286	THR
2	P	290	SER
1	Q	84	TRP
1	Q	335	LEU
2	R	3	VAL
2	R	84	TRP
2	R	125	ILE
2	R	129	VAL
2	R	161	LEU
2	R	281	ILE
2	R	324	LEU
1	A	84	TRP
1	A	201	LEU
1	A	221	LEU
1	A	293	ASP
2	B	11	ILE
2	B	188	SER
2	B	250	THR
2	B	302	ASP
2	B	305	VAL
2	B	327	ILE
1	C	41	THR
1	C	84	TRP
1	C	246	ILE
2	D	101	ASP
2	D	161	LEU
2	D	164	LYS
2	D	202	ASN
2	D	295	SER
2	D	298	MET
1	E	30	VAL
1	E	41	THR
1	E	201	LEU
1	E	240	VAL

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Mol	Chain	Res	Type
2	F	84	TRP
2	F	172	MET
2	F	280	SER
2	F	287	ASP
2	F	290	SER
1	G	37	VAL
1	G	84	TRP
2	H	62	SER
2	H	84	TRP
2	H	129	VAL
2	H	281	ILE
2	H	304	MET
2	H	324	LEU
1	I	73	VAL
1	I	84	TRP
1	I	335	LEU
1	I	361	TYR
2	J	76	ASP
2	J	116	VAL
2	J	188	SER
2	J	250	THR
2	J	305	VAL
2	J	327	ILE
1	K	30	VAL
1	K	41	THR
1	K	84	TRP
1	K	164	GLU
1	K	207	SER
1	K	246	ILE
1	K	347	ASP
1	K	352	ASN
2	L	74	VAL
2	L	101	ASP
2	L	161	LEU
2	L	202	ASN
2	L	294	SER
2	L	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	18(B)	HIS

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Mol	Chain	Res	Type
1	O	146	ASN
1	O	176	HIS
1	O	245	ASN
2	P	146	ASN
2	P	152	ASN
2	P	202	ASN
1	Q	18(B)	HIS
1	Q	42	HIS
1	Q	61	ASN
1	Q	176	HIS
1	Q	202	ASN
2	R	31	ASN
2	R	139	HIS
2	R	146	ASN
2	R	202	ASN
1	A	18(B)	HIS
1	A	61	ASN
1	A	139	HIS
1	A	146	ASN
1	A	176	HIS
1	A	182	GLN
1	A	245	ASN
2	B	18(B)	HIS
2	B	78	ASN
2	B	139	HIS
2	B	202	ASN
2	B	220	ASN
2	B	333	GLN
1	C	18(B)	HIS
1	C	61	ASN
1	C	76	ASN
1	C	133	ASN
1	C	146	ASN
1	C	176	HIS
1	C	245	ASN
1	C	352	ASN
2	D	226	ASN
1	E	18(B)	HIS
1	E	152	ASN
1	E	176	HIS
1	E	245	ASN
2	F	139	HIS

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Mol	Chain	Res	Type
2	F	146	ASN
2	F	202	ASN
2	F	256	ASN
1	G	61	ASN
1	G	176	HIS
1	G	330	ASN
2	H	42	HIS
2	H	265	ASN
1	I	18(B)	HIS
1	I	61	ASN
1	I	146	ASN
1	I	176	HIS
1	I	182	GLN
1	I	245	ASN
2	J	18(B)	HIS
2	J	42	HIS
2	J	78	ASN
2	J	133	ASN
2	J	152	ASN
2	J	202	ASN
2	J	220	ASN
1	K	18(B)	HIS
1	K	76	ASN
1	K	133	ASN
1	K	176	HIS
1	K	245	ASN
2	L	78	ASN
2	L	202	ASN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	J	400	-	46,48,48	0.62	1 (2%)	64,73,73	0.59	0
3	NAD	G	400	-	46,48,48	0.63	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	H	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.61	1 (1%)
3	NAD	D	400	-	46,48,48	0.62	1 (2%)	64,73,73	0.64	1 (1%)
3	NAD	F	400	-	46,48,48	0.62	1 (2%)	64,73,73	0.61	1 (1%)
3	NAD	E	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	P	400	-	46,48,48	0.63	1 (2%)	64,73,73	0.63	1 (1%)
3	NAD	C	400	-	46,48,48	0.66	1 (2%)	64,73,73	0.61	0
3	NAD	B	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.63	1 (1%)
3	NAD	L	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.60	1 (1%)
3	NAD	R	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.60	1 (1%)
3	NAD	Q	400	-	46,48,48	0.64	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	A	400	-	46,48,48	0.63	1 (2%)	64,73,73	0.55	1 (1%)
3	NAD	O	400	-	46,48,48	0.61	1 (2%)	64,73,73	0.57	1 (1%)
3	NAD	K	400	-	46,48,48	0.66	1 (2%)	64,73,73	0.58	1 (1%)
3	NAD	I	400	-	46,48,48	0.69	1 (2%)	64,73,73	0.56	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	J	400	-	-	19/30/62/62	0/5/5/5
3	NAD	G	400	-	-	18/30/62/62	0/5/5/5
3	NAD	H	400	-	-	15/30/62/62	0/5/5/5
3	NAD	D	400	-	-	17/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	F	400	-	-	15/30/62/62	0/5/5/5
3	NAD	E	400	-	-	15/30/62/62	0/5/5/5
3	NAD	P	400	-	-	20/30/62/62	0/5/5/5
3	NAD	C	400	-	-	13/30/62/62	0/5/5/5
3	NAD	B	400	-	-	16/30/62/62	0/5/5/5
3	NAD	L	400	-	-	18/30/62/62	0/5/5/5
3	NAD	R	400	-	-	12/30/62/62	0/5/5/5
3	NAD	Q	400	-	-	18/30/62/62	0/5/5/5
3	NAD	A	400	-	-	14/30/62/62	0/5/5/5
3	NAD	O	400	-	-	15/30/62/62	0/5/5/5
3	NAD	K	400	-	-	13/30/62/62	0/5/5/5
3	NAD	I	400	-	-	19/30/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	400	NAD	C2N-N1N	2.87	1.38	1.35
3	F	400	NAD	C2N-N1N	2.87	1.38	1.35
3	J	400	NAD	C2N-N1N	2.69	1.37	1.35
3	G	400	NAD	C2N-N1N	2.67	1.37	1.35
3	K	400	NAD	C2N-N1N	2.66	1.37	1.35
3	A	400	NAD	C2N-N1N	2.66	1.37	1.35
3	B	400	NAD	C2N-N1N	2.63	1.37	1.35
3	L	400	NAD	C2N-N1N	2.60	1.37	1.35
3	Q	400	NAD	C2N-N1N	2.60	1.37	1.35
3	R	400	NAD	C2N-N1N	2.59	1.37	1.35
3	D	400	NAD	C2N-N1N	2.58	1.37	1.35
3	C	400	NAD	C2N-N1N	2.57	1.37	1.35
3	I	400	NAD	C2N-N1N	2.57	1.37	1.35
3	H	400	NAD	C2N-N1N	2.56	1.37	1.35
3	E	400	NAD	C2N-N1N	2.55	1.37	1.35
3	O	400	NAD	C2N-N1N	2.52	1.37	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	400	NAD	C6N-N1N-C2N	-2.36	119.87	121.88
3	R	400	NAD	C6N-N1N-C2N	-2.30	119.92	121.88
3	E	400	NAD	C6N-N1N-C2N	-2.30	119.92	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	400	NAD	C6N-N1N-C2N	-2.25	119.96	121.88
3	A	400	NAD	C6N-N1N-C2N	-2.24	119.97	121.88
3	H	400	NAD	C6N-N1N-C2N	-2.23	119.98	121.88
3	I	400	NAD	C6N-N1N-C2N	-2.22	119.98	121.88
3	G	400	NAD	C6N-N1N-C2N	-2.21	120.00	121.88
3	L	400	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
3	P	400	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
3	Q	400	NAD	C6N-N1N-C2N	-2.10	120.09	121.88
3	D	400	NAD	C6N-N1N-C2N	-2.05	120.13	121.88
3	B	400	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
3	K	400	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	400	NAD	C5B-O5B-PA-O1A
3	O	400	NAD	C5B-O5B-PA-O2A
3	O	400	NAD	C5B-O5B-PA-O3
3	O	400	NAD	C5D-O5D-PN-O3
3	O	400	NAD	C5D-O5D-PN-O2N
3	O	400	NAD	O4D-C1D-N1N-C2N
3	P	400	NAD	C5B-O5B-PA-O2A
3	P	400	NAD	C5B-O5B-PA-O3
3	P	400	NAD	C5D-O5D-PN-O3
3	P	400	NAD	C5D-O5D-PN-O1N
3	P	400	NAD	C5D-O5D-PN-O2N
3	P	400	NAD	O4D-C1D-N1N-C2N
3	P	400	NAD	O4D-C1D-N1N-C6N
3	P	400	NAD	C2D-C1D-N1N-C2N
3	P	400	NAD	C2D-C1D-N1N-C6N
3	P	400	NAD	C2N-C3N-C7N-O7N
3	P	400	NAD	C2N-C3N-C7N-N7N
3	Q	400	NAD	C5B-O5B-PA-O1A
3	Q	400	NAD	C5B-O5B-PA-O3
3	Q	400	NAD	PN-O3-PA-O5B
3	Q	400	NAD	C5D-O5D-PN-O3
3	Q	400	NAD	C5D-O5D-PN-O2N
3	Q	400	NAD	O4D-C1D-N1N-C2N
3	R	400	NAD	C5D-O5D-PN-O3
3	R	400	NAD	C5D-O5D-PN-O2N
3	R	400	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	R	400	NAD	O4D-C1D-N1N-C6N
3	R	400	NAD	C2D-C1D-N1N-C6N
3	R	400	NAD	C2N-C3N-C7N-N7N
3	A	400	NAD	C5B-O5B-PA-O1A
3	A	400	NAD	C5B-O5B-PA-O3
3	A	400	NAD	PN-O3-PA-O5B
3	A	400	NAD	O4D-C1D-N1N-C2N
3	B	400	NAD	C5D-O5D-PN-O3
3	B	400	NAD	C5D-O5D-PN-O1N
3	B	400	NAD	O4D-C4D-C5D-O5D
3	B	400	NAD	C3D-C4D-C5D-O5D
3	B	400	NAD	C2N-C3N-C7N-O7N
3	B	400	NAD	C2N-C3N-C7N-N7N
3	C	400	NAD	C5B-O5B-PA-O2A
3	C	400	NAD	C5B-O5B-PA-O3
3	C	400	NAD	O4B-C4B-C5B-O5B
3	C	400	NAD	O4D-C1D-N1N-C2N
3	D	400	NAD	C5B-O5B-PA-O1A
3	D	400	NAD	C5B-O5B-PA-O2A
3	D	400	NAD	C5B-O5B-PA-O3
3	D	400	NAD	PN-O3-PA-O5B
3	D	400	NAD	C5D-O5D-PN-O3
3	D	400	NAD	C5D-O5D-PN-O1N
3	D	400	NAD	C5D-O5D-PN-O2N
3	D	400	NAD	O4D-C1D-N1N-C2N
3	D	400	NAD	C2N-C3N-C7N-O7N
3	D	400	NAD	C2N-C3N-C7N-N7N
3	E	400	NAD	C5B-O5B-PA-O1A
3	E	400	NAD	C5B-O5B-PA-O2A
3	E	400	NAD	C5B-O5B-PA-O3
3	E	400	NAD	C5D-O5D-PN-O3
3	E	400	NAD	C5D-O5D-PN-O1N
3	E	400	NAD	C5D-O5D-PN-O2N
3	E	400	NAD	O4D-C1D-N1N-C2N
3	F	400	NAD	C5D-O5D-PN-O3
3	F	400	NAD	O4D-C1D-N1N-C2N
3	F	400	NAD	O4D-C1D-N1N-C6N
3	F	400	NAD	C2D-C1D-N1N-C2N
3	F	400	NAD	C2D-C1D-N1N-C6N
3	F	400	NAD	C2N-C3N-C7N-O7N
3	F	400	NAD	C2N-C3N-C7N-N7N
3	G	400	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	G	400	NAD	C5B-O5B-PA-O3
3	G	400	NAD	C5D-O5D-PN-O2N
3	G	400	NAD	O4D-C1D-N1N-C2N
3	H	400	NAD	C5D-O5D-PN-O3
3	H	400	NAD	C5D-O5D-PN-O1N
3	H	400	NAD	C5D-O5D-PN-O2N
3	H	400	NAD	O4D-C1D-N1N-C2N
3	H	400	NAD	O4D-C1D-N1N-C6N
3	H	400	NAD	C2D-C1D-N1N-C2N
3	H	400	NAD	C2D-C1D-N1N-C6N
3	H	400	NAD	C2N-C3N-C7N-O7N
3	H	400	NAD	C2N-C3N-C7N-N7N
3	I	400	NAD	C5B-O5B-PA-O1A
3	I	400	NAD	C5B-O5B-PA-O2A
3	I	400	NAD	C5B-O5B-PA-O3
3	I	400	NAD	C5D-O5D-PN-O3
3	I	400	NAD	C5D-O5D-PN-O2N
3	I	400	NAD	O4D-C1D-N1N-C2N
3	I	400	NAD	C2N-C3N-C7N-N7N
3	J	400	NAD	C5B-O5B-PA-O2A
3	J	400	NAD	C5B-O5B-PA-O3
3	J	400	NAD	C5D-O5D-PN-O3
3	J	400	NAD	C5D-O5D-PN-O1N
3	J	400	NAD	C5D-O5D-PN-O2N
3	J	400	NAD	O4D-C1D-N1N-C2N
3	J	400	NAD	O4D-C1D-N1N-C6N
3	J	400	NAD	C2D-C1D-N1N-C6N
3	K	400	NAD	C5B-O5B-PA-O3
3	K	400	NAD	O4B-C4B-C5B-O5B
3	K	400	NAD	O4D-C1D-N1N-C2N
3	K	400	NAD	O4D-C1D-N1N-C6N
3	L	400	NAD	C5B-O5B-PA-O1A
3	L	400	NAD	C5B-O5B-PA-O2A
3	L	400	NAD	C5B-O5B-PA-O3
3	L	400	NAD	C5D-O5D-PN-O3
3	L	400	NAD	C5D-O5D-PN-O1N
3	L	400	NAD	C5D-O5D-PN-O2N
3	L	400	NAD	O4D-C1D-N1N-C2N
3	L	400	NAD	C2N-C3N-C7N-O7N
3	L	400	NAD	C2N-C3N-C7N-N7N
3	P	400	NAD	C4N-C3N-C7N-O7N
3	P	400	NAD	C4N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
3	D	400	NAD	C4N-C3N-C7N-O7N
3	D	400	NAD	C4N-C3N-C7N-N7N
3	F	400	NAD	C4N-C3N-C7N-O7N
3	F	400	NAD	C4N-C3N-C7N-N7N
3	H	400	NAD	C4N-C3N-C7N-O7N
3	H	400	NAD	C4N-C3N-C7N-N7N
3	L	400	NAD	C4N-C3N-C7N-N7N
3	R	400	NAD	C4N-C3N-C7N-O7N
3	L	400	NAD	C4N-C3N-C7N-O7N
3	R	400	NAD	C4N-C3N-C7N-N7N
3	I	400	NAD	C4N-C3N-C7N-N7N
3	R	400	NAD	C2N-C3N-C7N-O7N
3	A	400	NAD	C2N-C3N-C7N-O7N
3	A	400	NAD	C2N-C3N-C7N-N7N
3	I	400	NAD	C2N-C3N-C7N-O7N
3	B	400	NAD	C4N-C3N-C7N-N7N
3	B	400	NAD	C4N-C3N-C7N-O7N
3	I	400	NAD	C4N-C3N-C7N-O7N
3	B	400	NAD	O4B-C4B-C5B-O5B
3	A	400	NAD	C4N-C3N-C7N-N7N
3	A	400	NAD	C4N-C3N-C7N-O7N
3	B	400	NAD	C3B-C4B-C5B-O5B
3	C	400	NAD	C3B-C4B-C5B-O5B
3	F	400	NAD	O4B-C4B-C5B-O5B
3	J	400	NAD	O4B-C4B-C5B-O5B
3	K	400	NAD	C3B-C4B-C5B-O5B
3	F	400	NAD	C3B-C4B-C5B-O5B
3	J	400	NAD	C3B-C4B-C5B-O5B
3	I	400	NAD	O4B-C4B-C5B-O5B
3	I	400	NAD	C3B-C4B-C5B-O5B
3	G	400	NAD	C4N-C3N-C7N-O7N
3	G	400	NAD	C4N-C3N-C7N-N7N
3	K	400	NAD	C4N-C3N-C7N-N7N
3	K	400	NAD	C4N-C3N-C7N-O7N
3	O	400	NAD	O4B-C4B-C5B-O5B
3	O	400	NAD	C3B-C4B-C5B-O5B
3	A	400	NAD	O4B-C4B-C5B-O5B
3	A	400	NAD	C3B-C4B-C5B-O5B
3	E	400	NAD	C3B-C4B-C5B-O5B
3	G	400	NAD	C3B-C4B-C5B-O5B
3	C	400	NAD	C4N-C3N-C7N-O7N
3	C	400	NAD	C4N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
3	C	400	NAD	C2N-C3N-C7N-O7N
3	G	400	NAD	C2N-C3N-C7N-O7N
3	K	400	NAD	C2N-C3N-C7N-O7N
3	P	400	NAD	O4B-C4B-C5B-O5B
3	Q	400	NAD	O4B-C4B-C5B-O5B
3	D	400	NAD	O4B-C4B-C5B-O5B
3	E	400	NAD	O4B-C4B-C5B-O5B
3	G	400	NAD	O4B-C4B-C5B-O5B
3	L	400	NAD	O4B-C4B-C5B-O5B
3	G	400	NAD	C2N-C3N-C7N-N7N
3	K	400	NAD	C2N-C3N-C7N-N7N
3	P	400	NAD	C3B-C4B-C5B-O5B
3	D	400	NAD	C3B-C4B-C5B-O5B
3	O	400	NAD	PN-O3-PA-O1A
3	Q	400	NAD	PA-O3-PN-O1N
3	E	400	NAD	PN-O3-PA-O1A
3	I	400	NAD	PN-O3-PA-O1A
3	J	400	NAD	PN-O3-PA-O1A
3	C	400	NAD	C2N-C3N-C7N-N7N
3	Q	400	NAD	C3B-C4B-C5B-O5B
3	L	400	NAD	C3B-C4B-C5B-O5B
3	Q	400	NAD	C4N-C3N-C7N-N7N
3	O	400	NAD	PN-O3-PA-O5B
3	P	400	NAD	PN-O3-PA-O5B
3	R	400	NAD	PN-O3-PA-O5B
3	E	400	NAD	PN-O3-PA-O5B
3	F	400	NAD	PN-O3-PA-O5B
3	G	400	NAD	PN-O3-PA-O5B
3	H	400	NAD	PN-O3-PA-O5B
3	I	400	NAD	PN-O3-PA-O5B
3	L	400	NAD	PN-O3-PA-O5B
3	Q	400	NAD	C4N-C3N-C7N-O7N
3	P	400	NAD	C2B-C1B-N9A-C8A
3	B	400	NAD	C2B-C1B-N9A-C8A
3	J	400	NAD	C2B-C1B-N9A-C8A
3	C	400	NAD	PA-O3-PN-O1N
3	I	400	NAD	PA-O3-PN-O1N
3	B	400	NAD	C4B-C5B-O5B-PA
3	Q	400	NAD	C2N-C3N-C7N-N7N
3	O	400	NAD	C5D-O5D-PN-O1N
3	Q	400	NAD	C5B-O5B-PA-O2A
3	Q	400	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
3	R	400	NAD	C5D-O5D-PN-O1N
3	A	400	NAD	C5B-O5B-PA-O2A
3	B	400	NAD	C5D-O5D-PN-O2N
3	C	400	NAD	C5B-O5B-PA-O1A
3	F	400	NAD	C5D-O5D-PN-O1N
3	G	400	NAD	C5B-O5B-PA-O2A
3	G	400	NAD	C5D-O5D-PN-O3
3	G	400	NAD	C5D-O5D-PN-O1N
3	I	400	NAD	C5D-O5D-PN-O1N
3	K	400	NAD	C5B-O5B-PA-O2A
3	P	400	NAD	C4B-C5B-O5B-PA
3	F	400	NAD	C4B-C5B-O5B-PA
3	J	400	NAD	C4B-C5B-O5B-PA
3	Q	400	NAD	C2N-C3N-C7N-O7N
3	Q	400	NAD	PA-O3-PN-O2N
3	A	400	NAD	PA-O3-PN-O2N
3	F	400	NAD	PN-O3-PA-O1A
3	G	400	NAD	PA-O3-PN-O2N
3	K	400	NAD	PA-O3-PN-O1N
3	E	400	NAD	C4B-C5B-O5B-PA
3	R	400	NAD	C2D-C1D-N1N-C2N
3	D	400	NAD	C2D-C1D-N1N-C6N
3	J	400	NAD	C2D-C1D-N1N-C2N
3	K	400	NAD	C2D-C1D-N1N-C6N
3	O	400	NAD	C4B-C5B-O5B-PA
3	B	400	NAD	C2B-C1B-N9A-C4A
3	B	400	NAD	O4B-C1B-N9A-C8A
3	Q	400	NAD	C4B-C5B-O5B-PA
3	I	400	NAD	C4B-C5B-O5B-PA
3	O	400	NAD	O4D-C1D-N1N-C6N
3	Q	400	NAD	O4D-C1D-N1N-C6N
3	A	400	NAD	O4D-C1D-N1N-C6N
3	C	400	NAD	O4D-C1D-N1N-C6N
3	D	400	NAD	O4D-C1D-N1N-C6N
3	E	400	NAD	O4D-C1D-N1N-C6N
3	G	400	NAD	O4D-C1D-N1N-C6N
3	I	400	NAD	O4D-C1D-N1N-C6N
3	L	400	NAD	O4D-C1D-N1N-C6N
3	P	400	NAD	PN-O3-PA-O1A
3	G	400	NAD	PA-O3-PN-O1N
3	H	400	NAD	PN-O3-PA-O1A
3	H	400	NAD	PA-O3-PN-O2N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	J	400	NAD	PA-O3-PN-O1N
3	J	400	NAD	PA-O3-PN-O2N
3	L	400	NAD	PA-O3-PN-O1N
3	J	400	NAD	PN-O3-PA-O5B
3	G	400	NAD	C4B-C5B-O5B-PA
3	B	400	NAD	C4D-C5D-O5D-PN
3	J	400	NAD	O4B-C1B-N9A-C8A
3	A	400	NAD	C4B-C5B-O5B-PA
3	P	400	NAD	PA-O3-PN-O2N
3	C	400	NAD	PA-O3-PN-O2N
3	I	400	NAD	PA-O3-PN-O2N
3	L	400	NAD	PN-O3-PA-O1A
3	L	400	NAD	PA-O3-PN-O2N
3	J	400	NAD	C2B-C1B-N9A-C4A
3	O	400	NAD	C2B-C1B-N9A-C8A
3	O	400	NAD	PA-O3-PN-O2N
3	D	400	NAD	PN-O3-PA-O1A
3	E	400	NAD	PA-O3-PN-O1N
3	E	400	NAD	PA-O3-PN-O2N
3	H	400	NAD	PA-O3-PN-O1N
3	K	400	NAD	PA-O3-PN-O2N

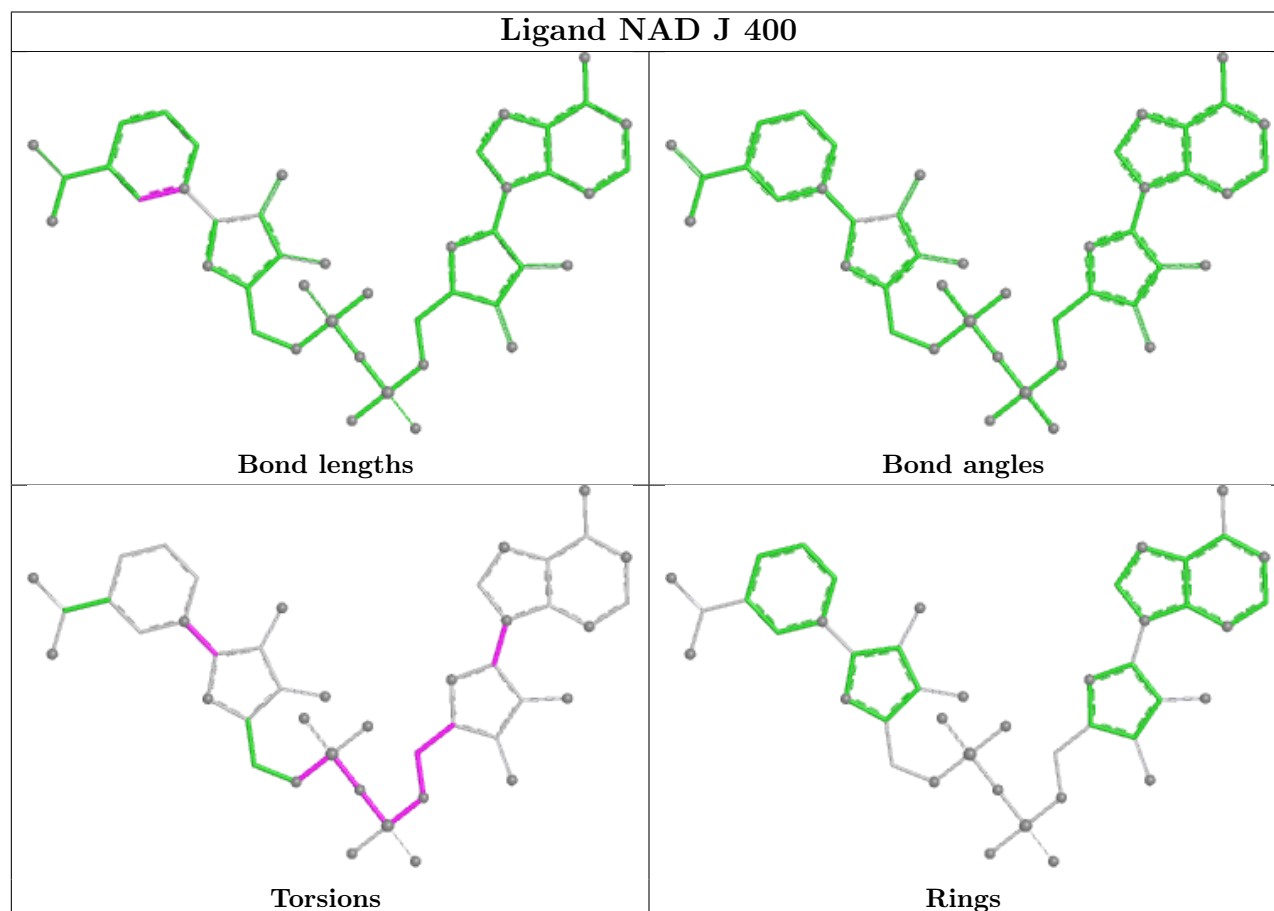
There are no ring outliers.

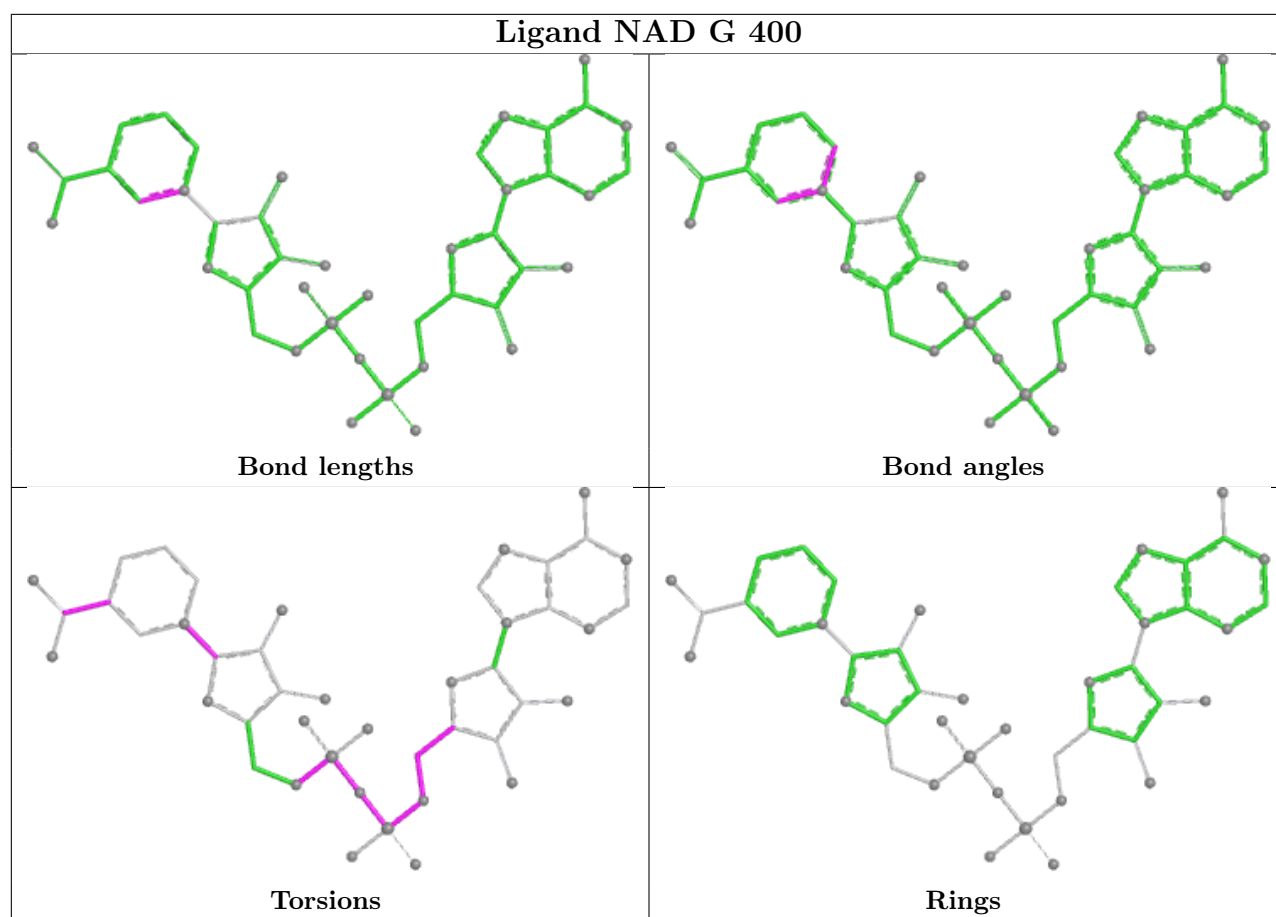
11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	400	NAD	1	0
3	D	400	NAD	1	0
3	F	400	NAD	2	0
3	E	400	NAD	1	0
3	P	400	NAD	2	0
3	B	400	NAD	2	0
3	L	400	NAD	2	0
3	R	400	NAD	1	0
3	A	400	NAD	1	0
3	O	400	NAD	1	0
3	I	400	NAD	1	0

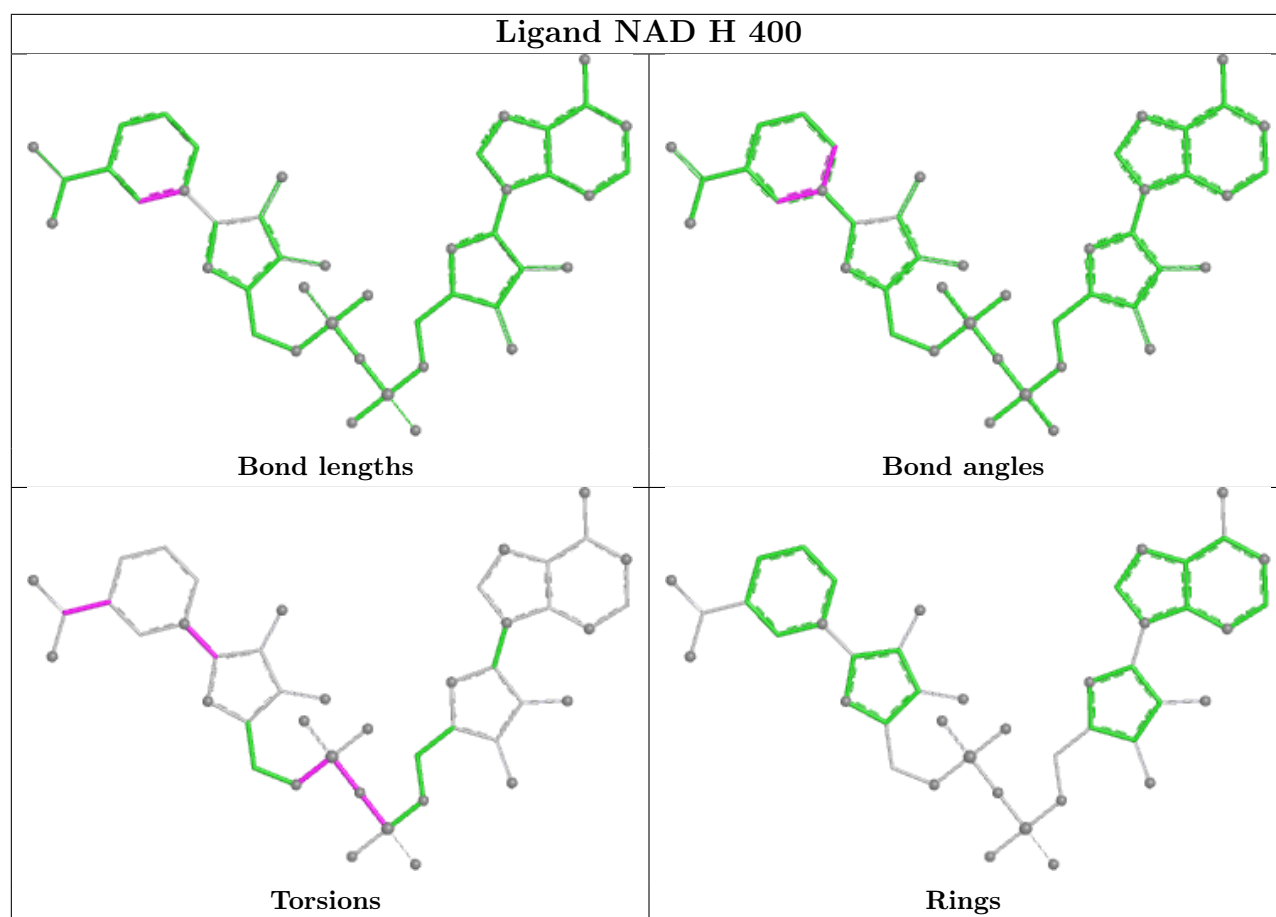
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

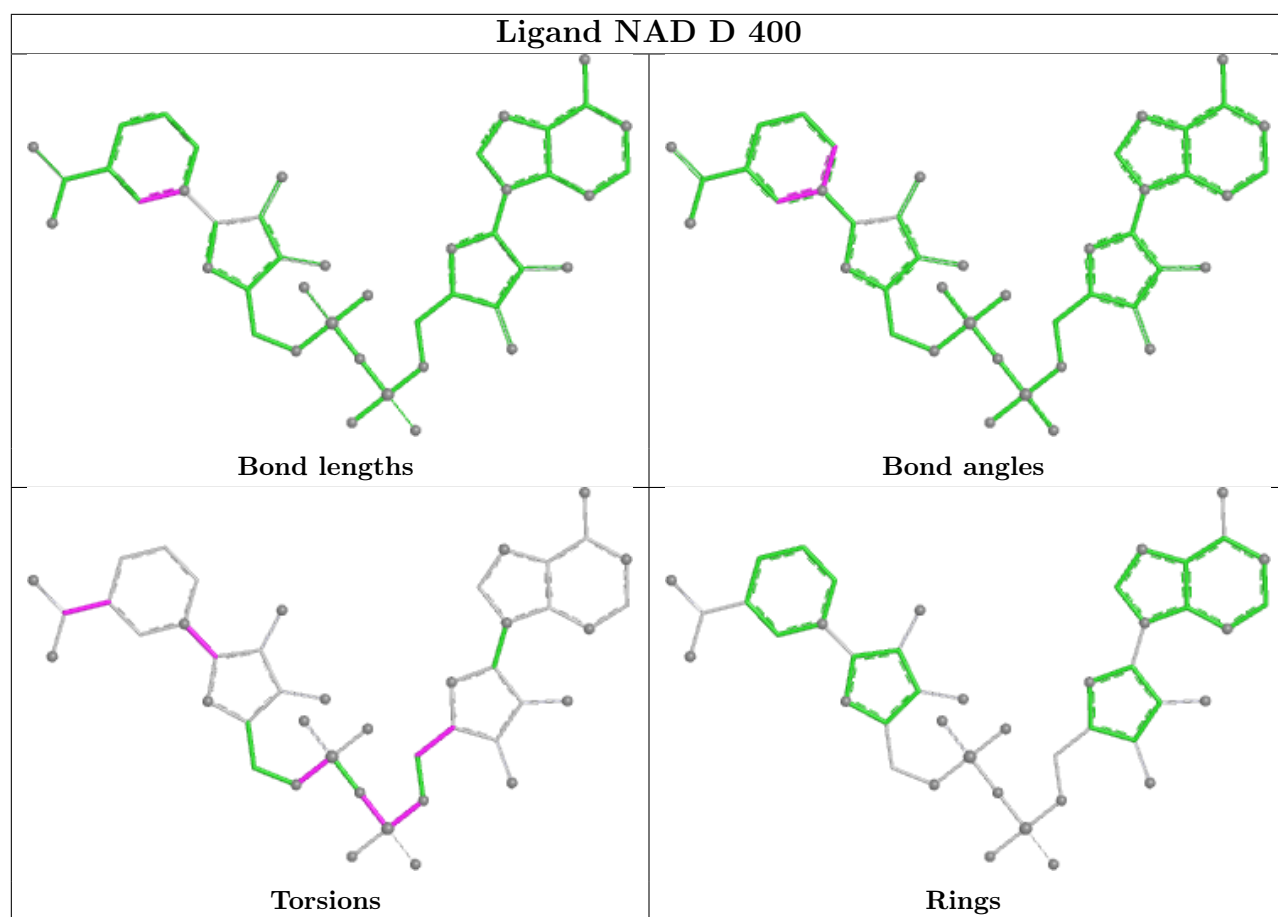
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

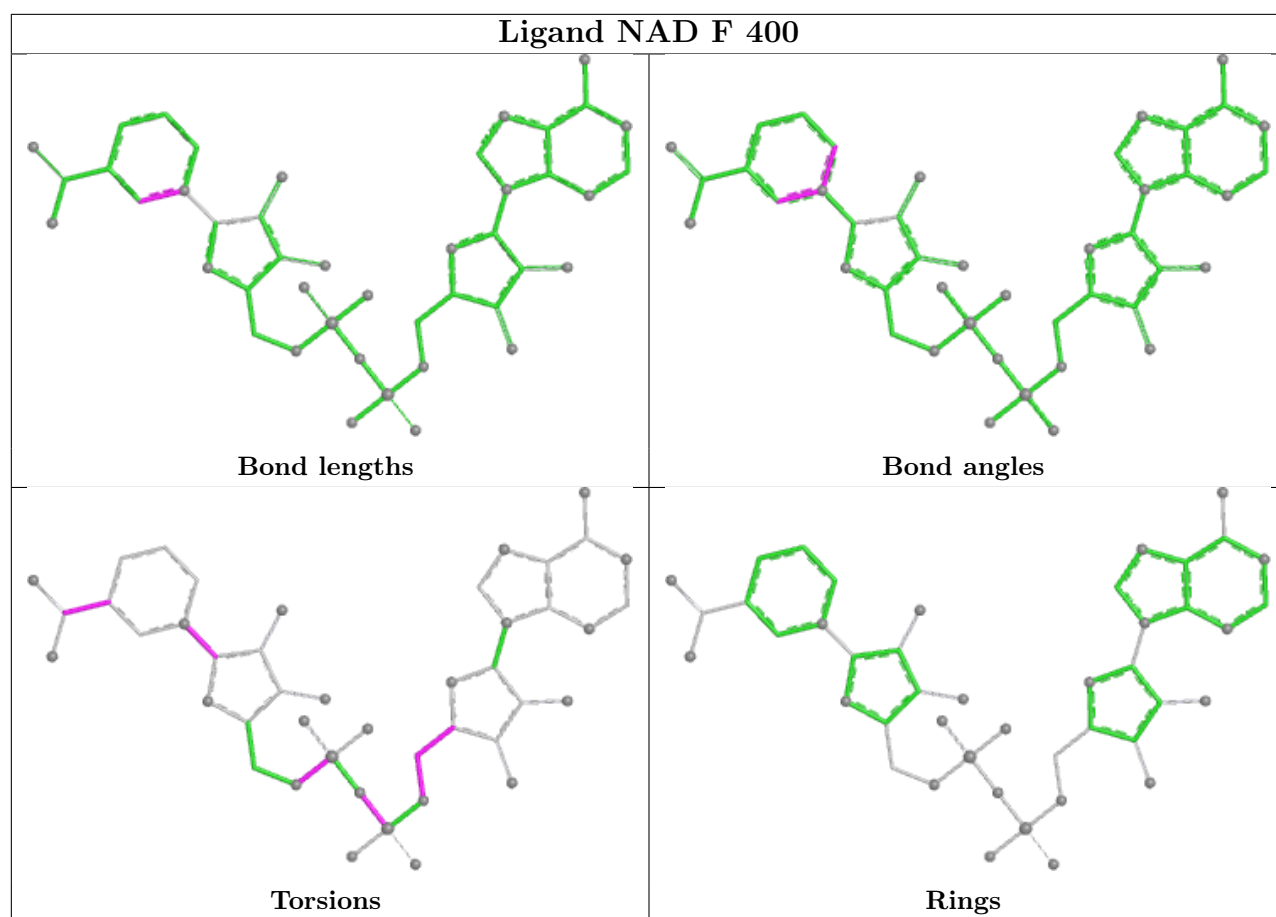


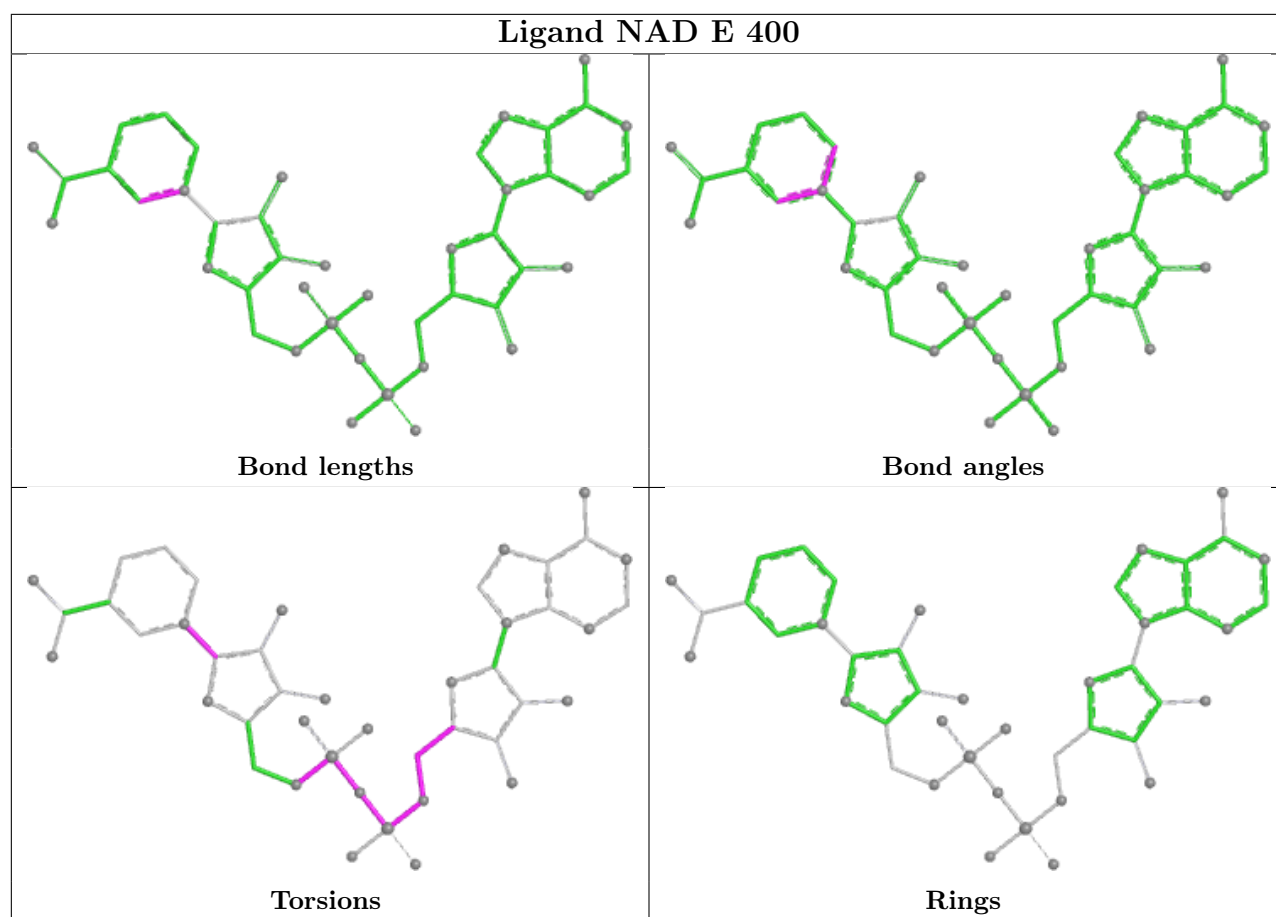


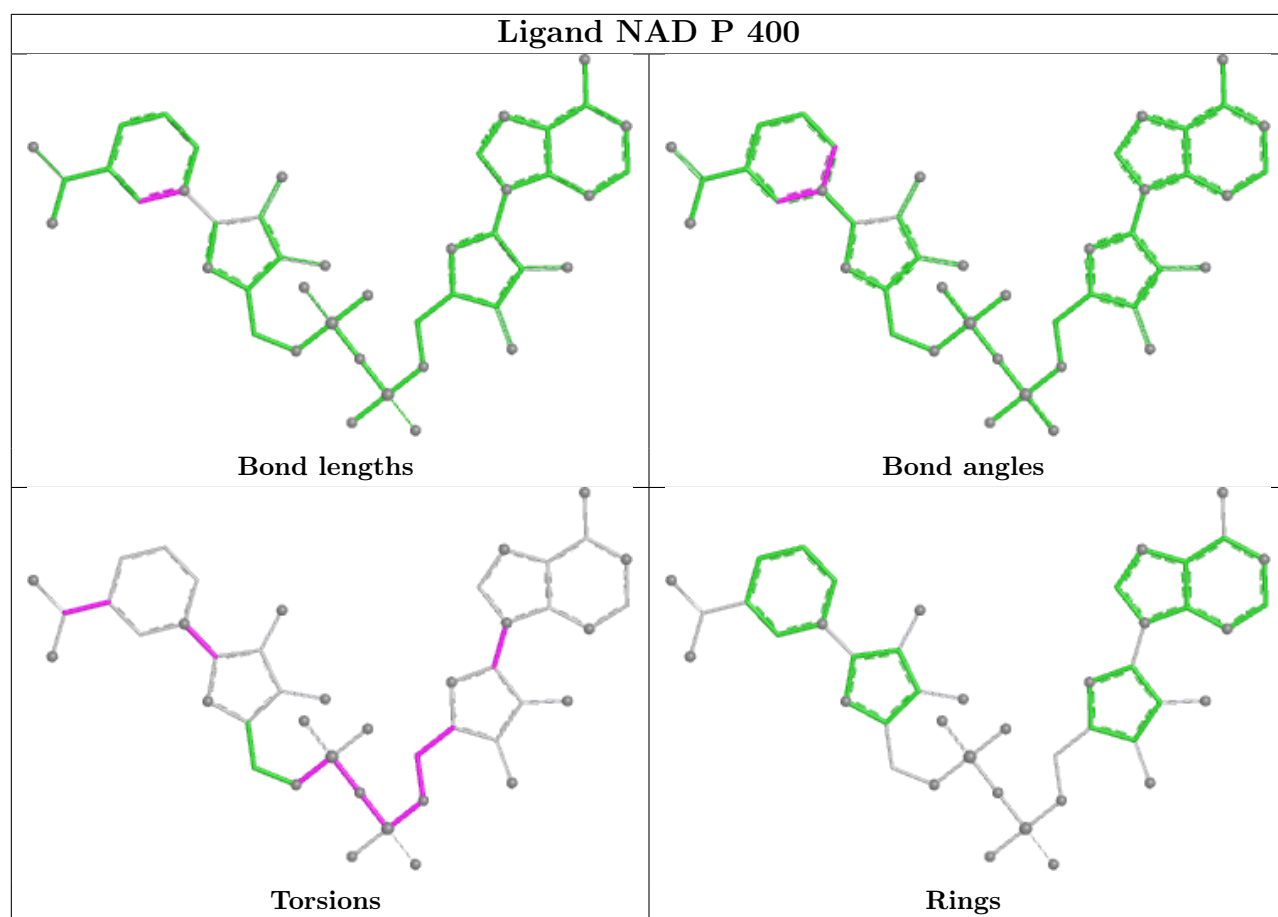


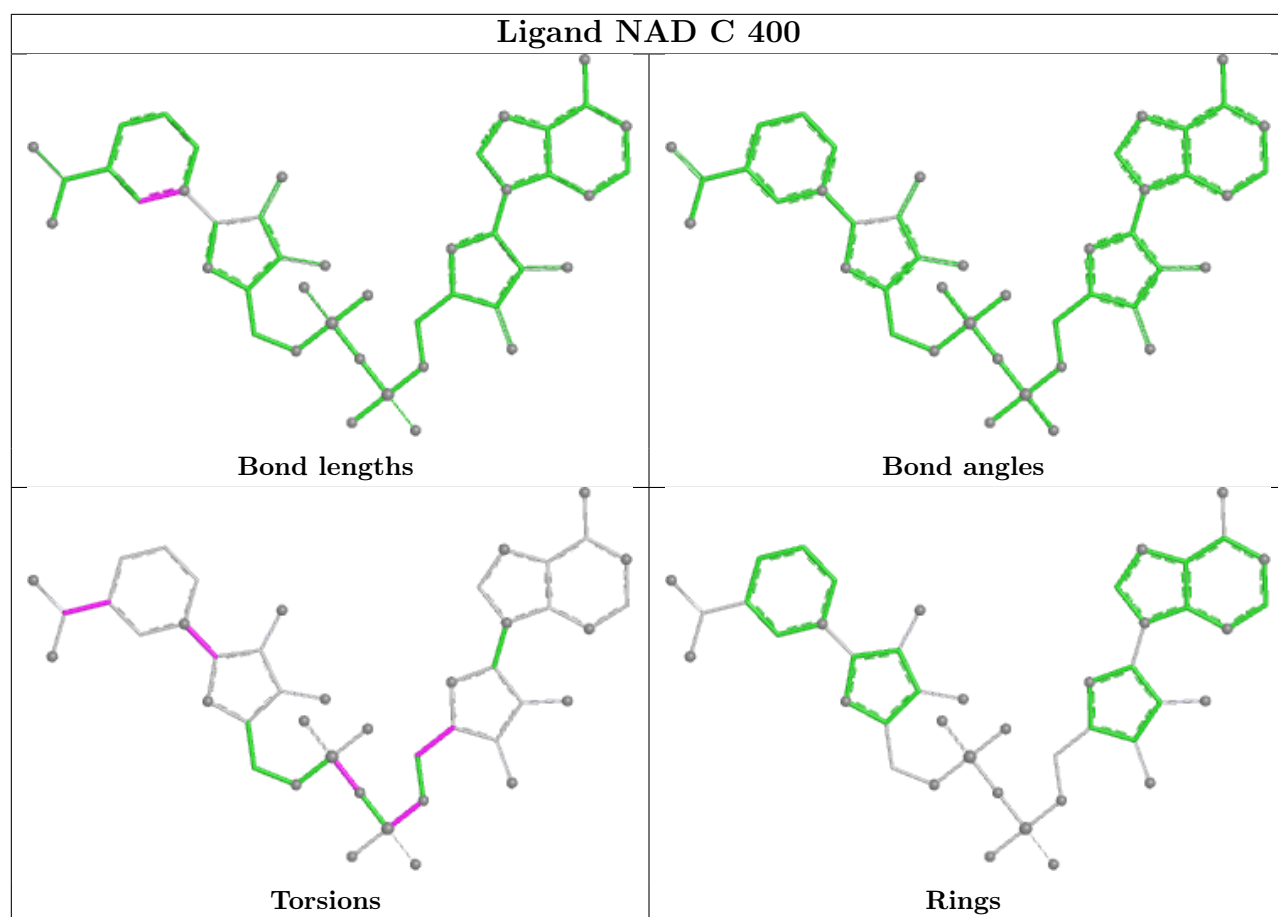


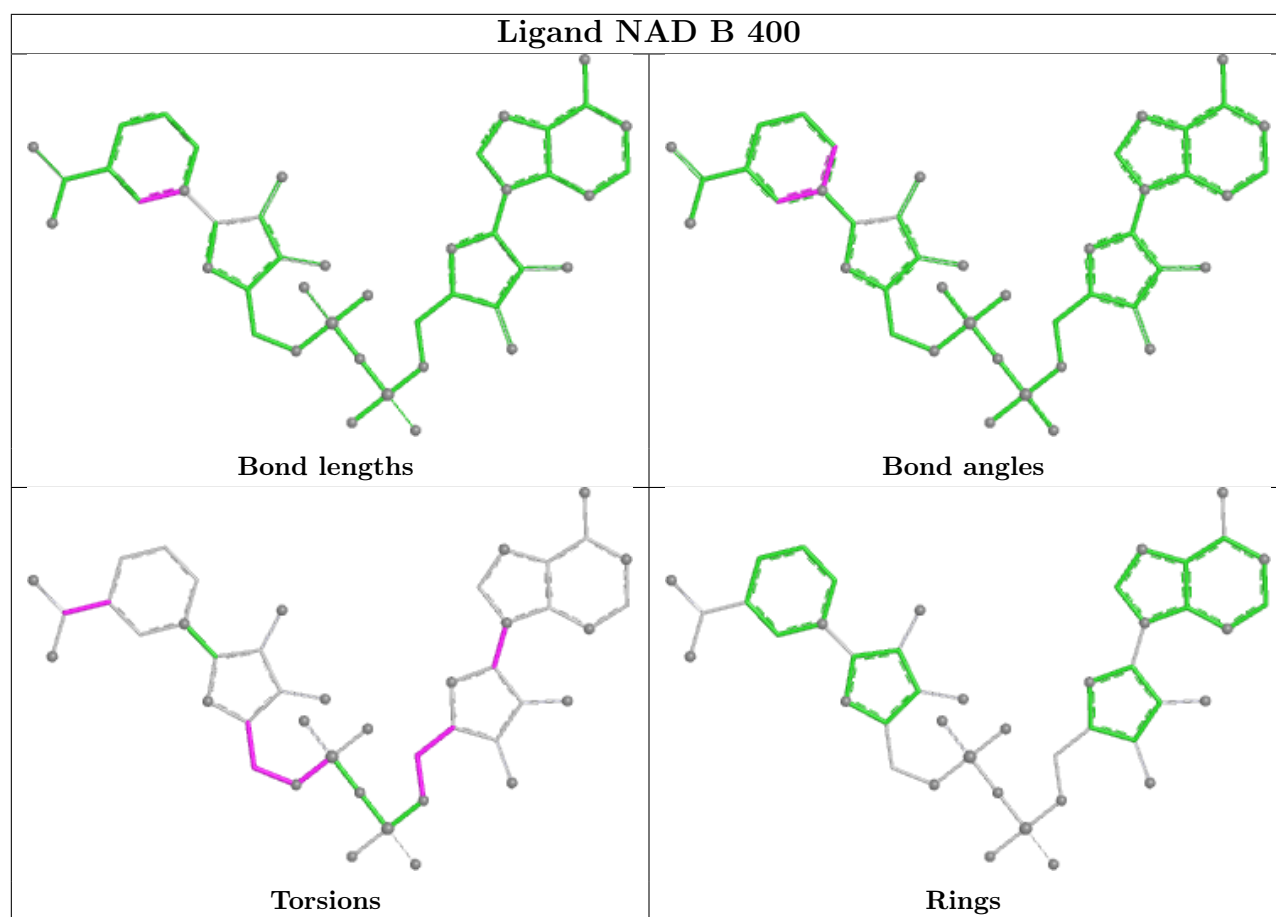


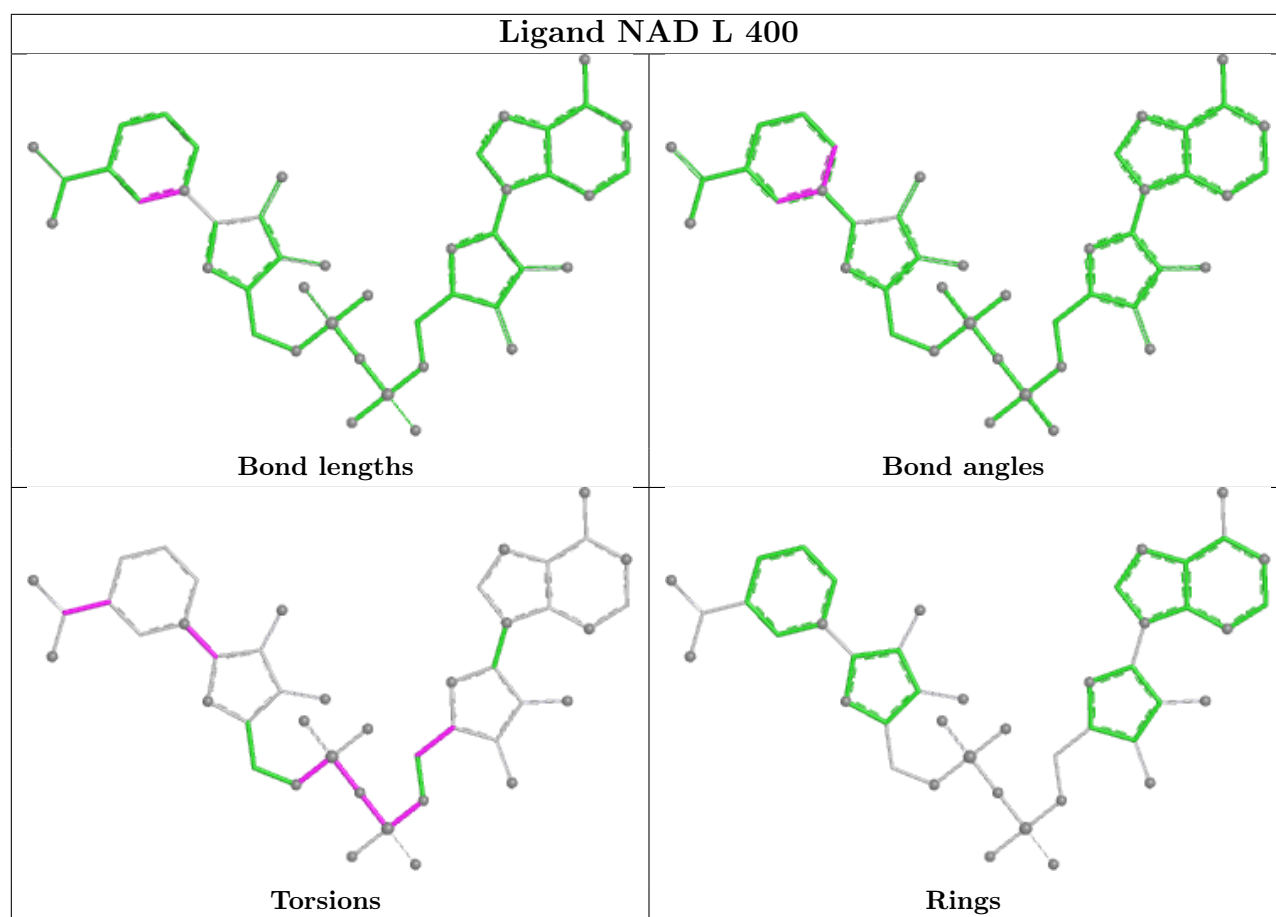




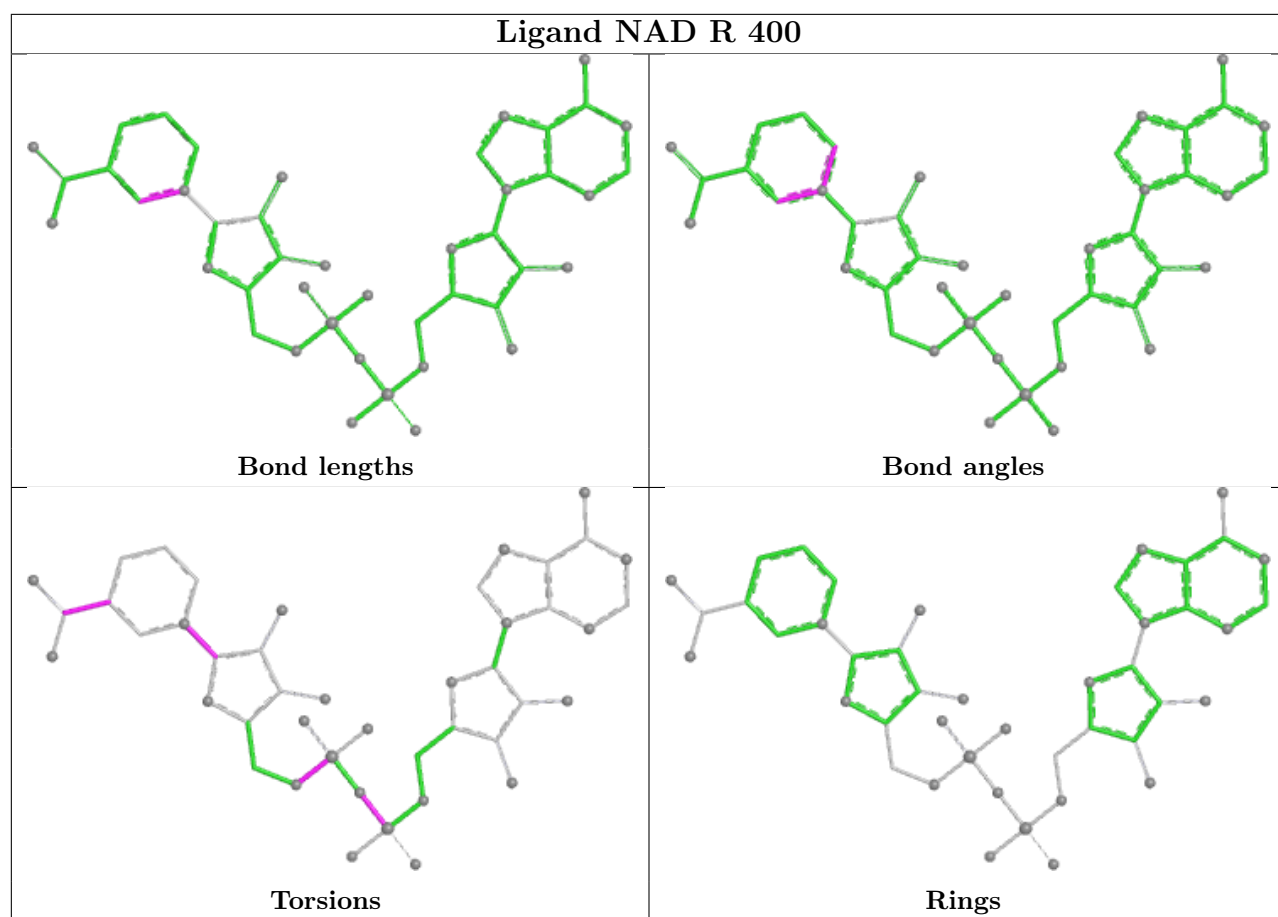


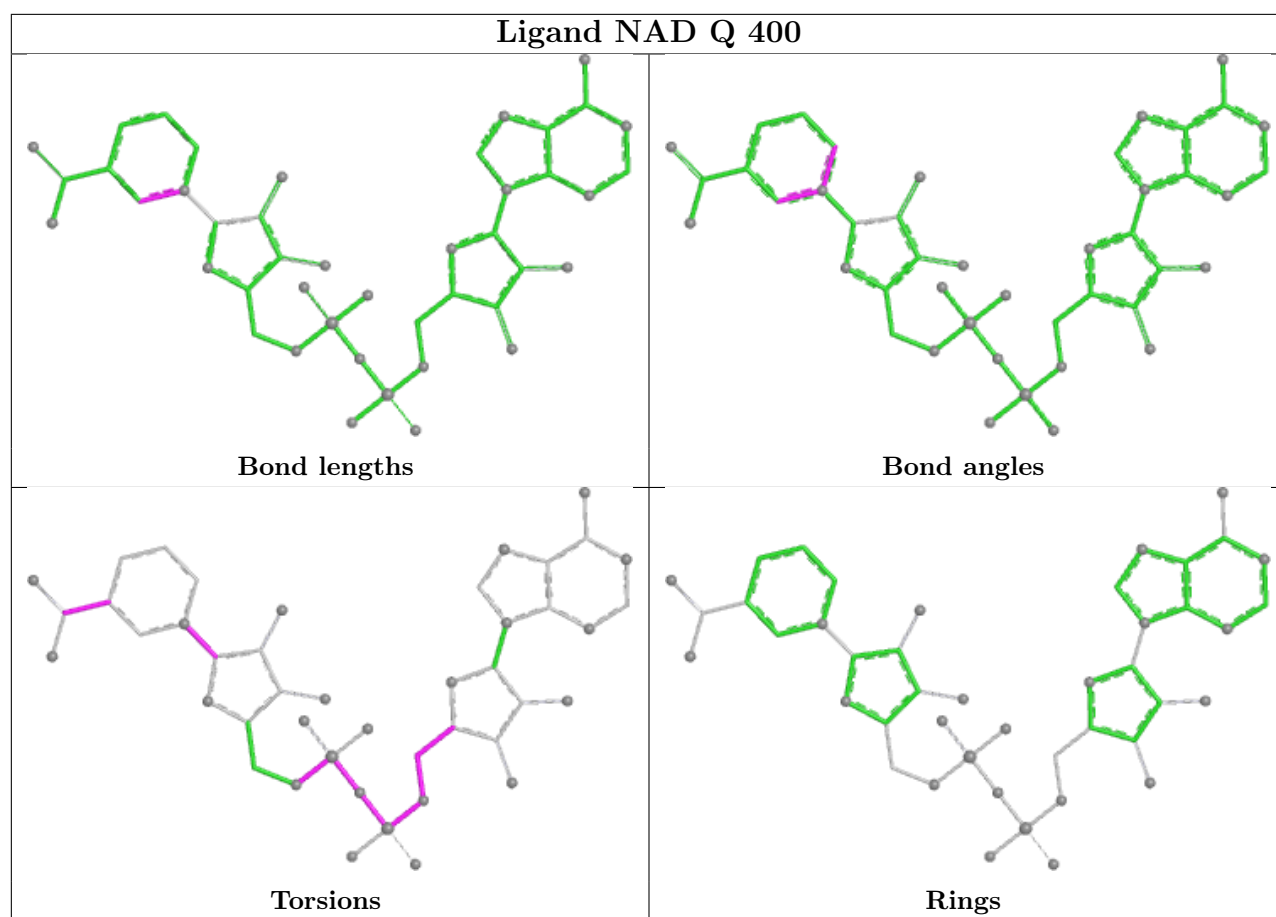


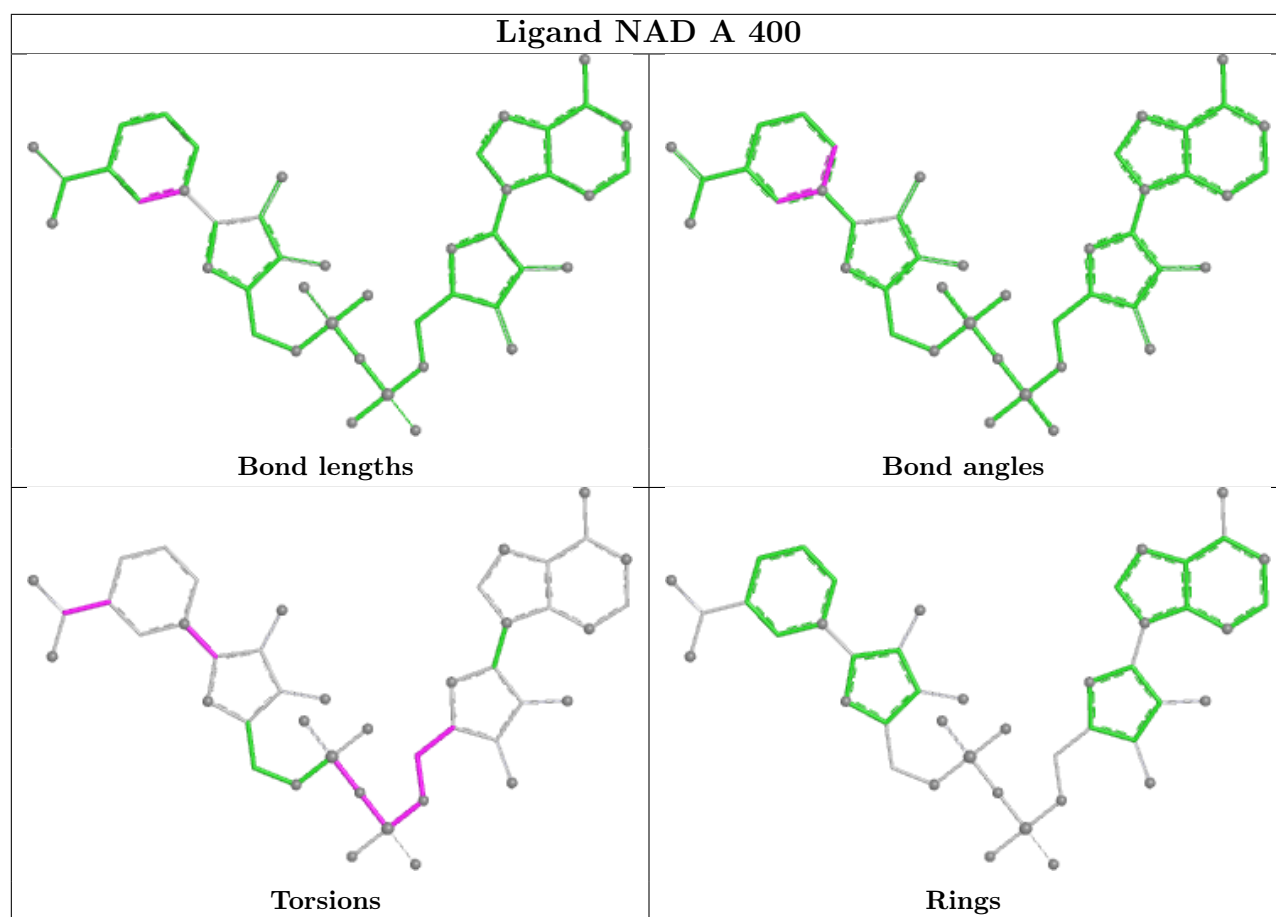


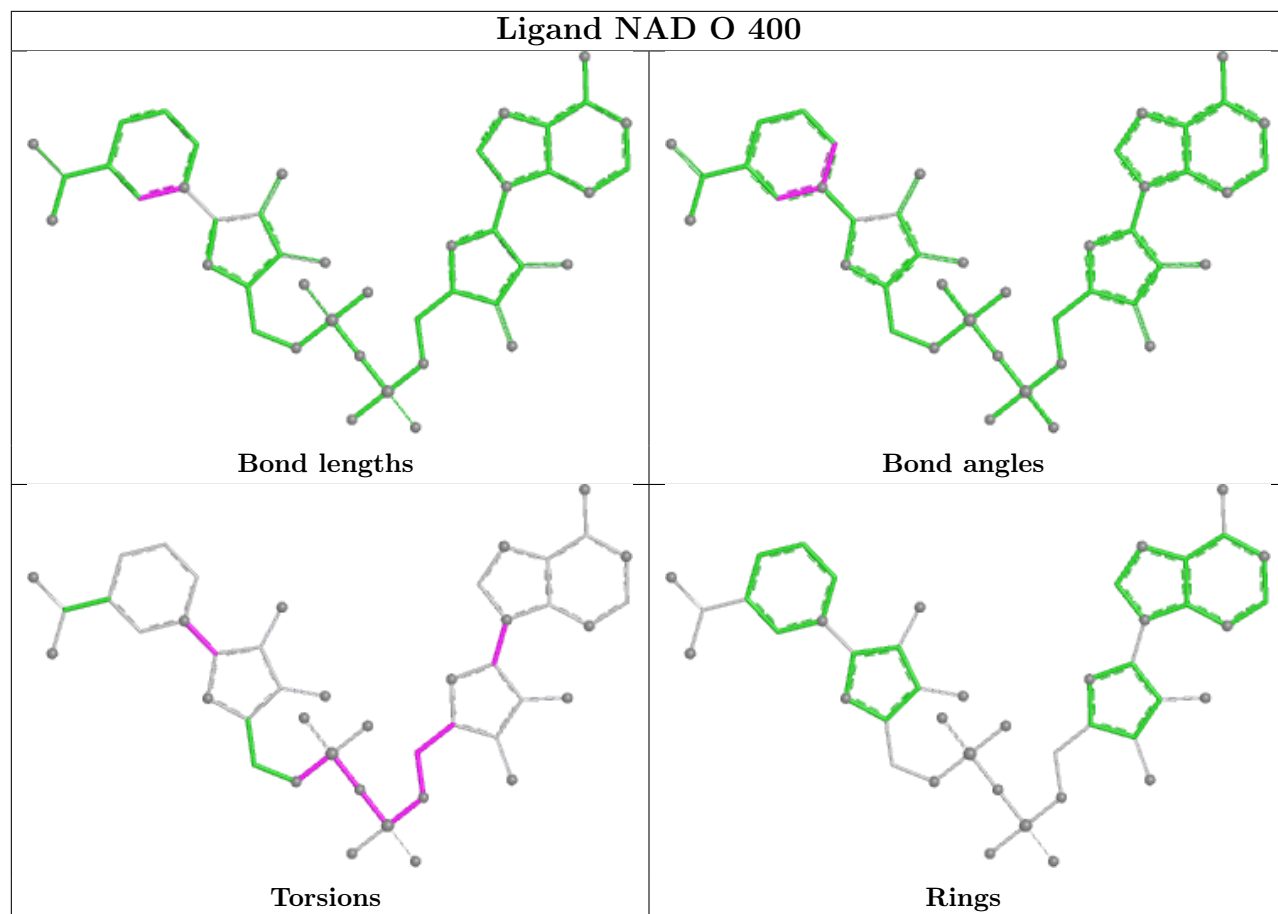


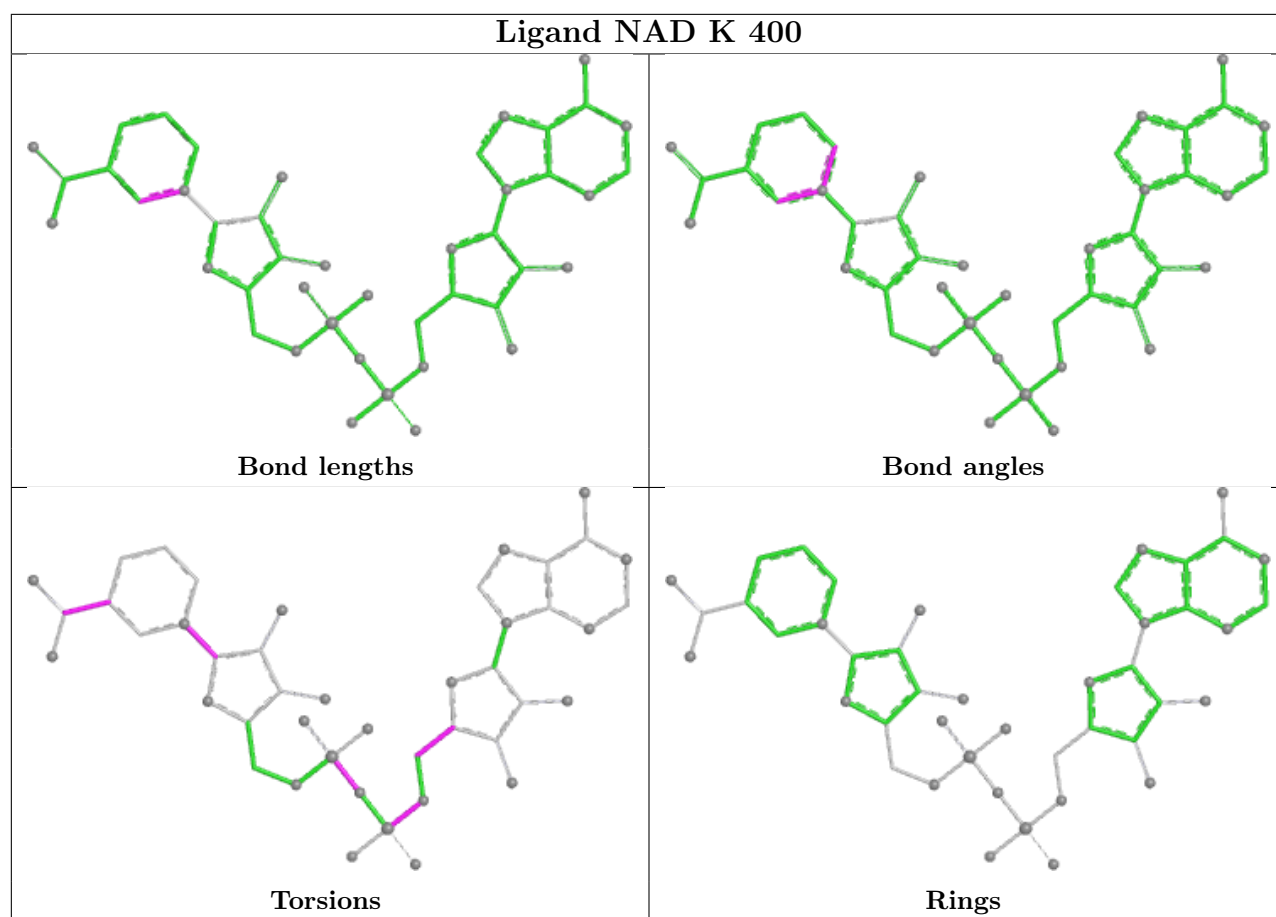


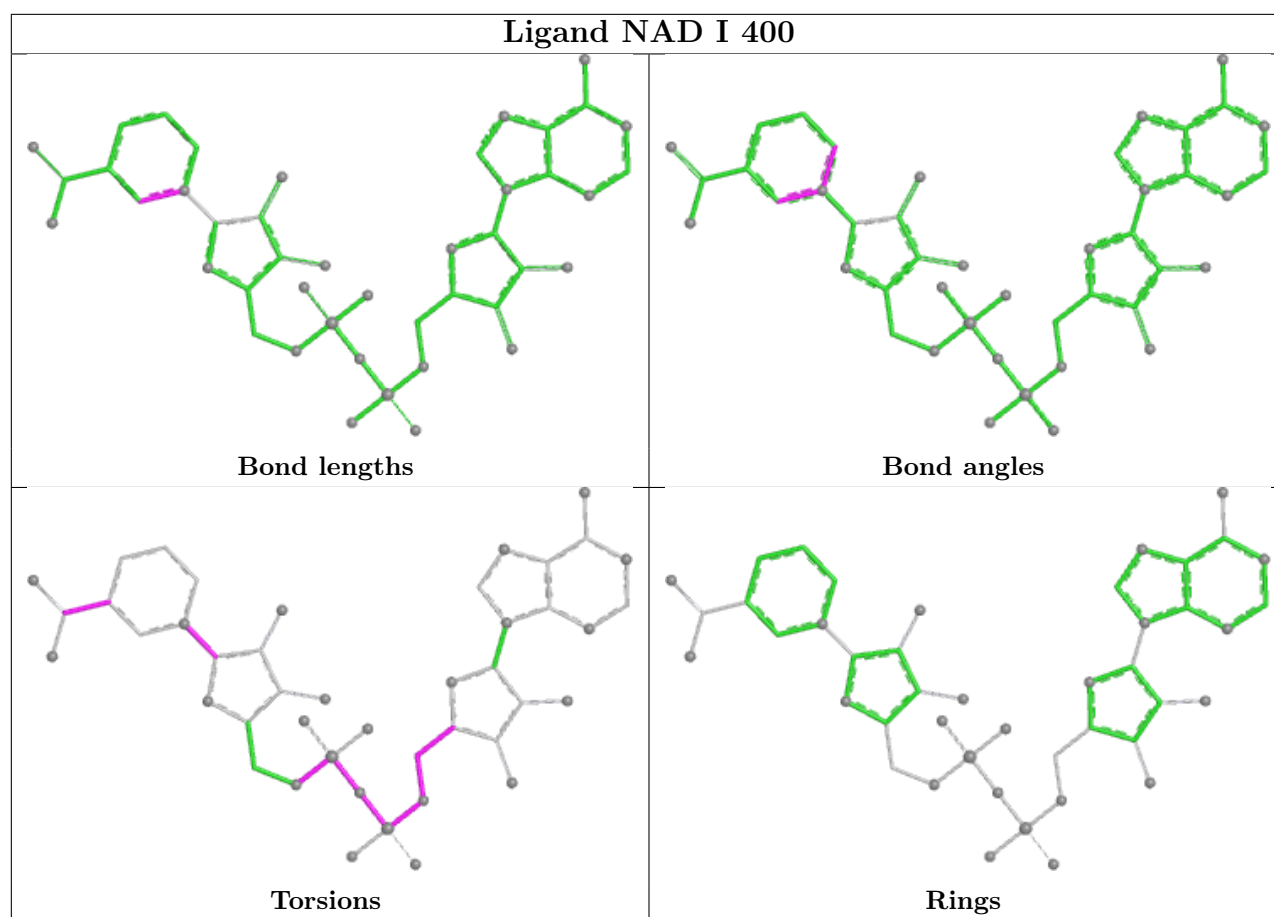












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

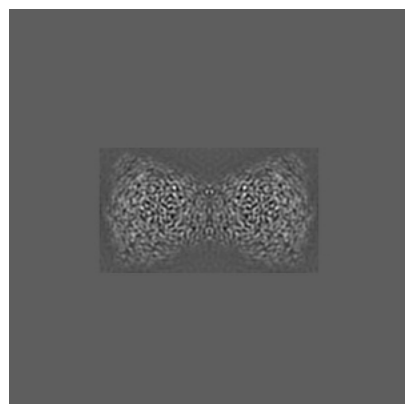
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52553. These allow visual inspection of the internal detail of the map and identification of artifacts.

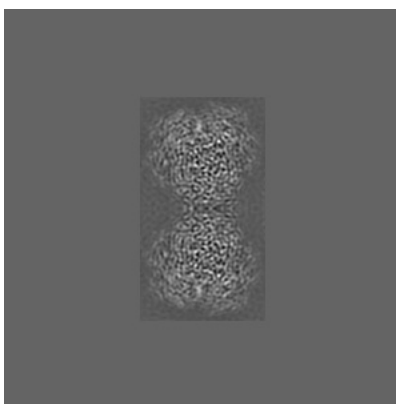
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

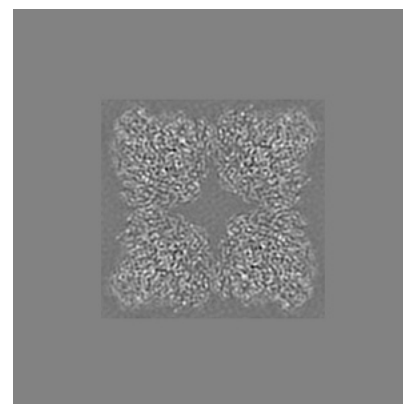
#### 6.1.1 Primary map



X

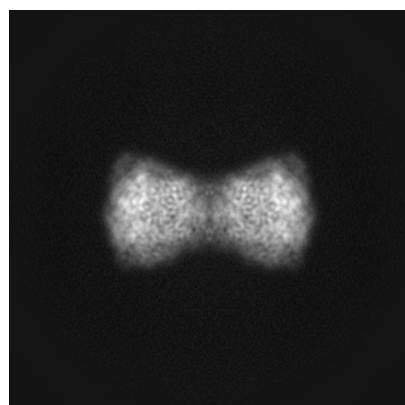


Y

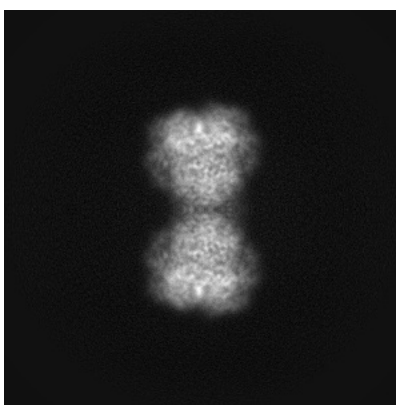


Z

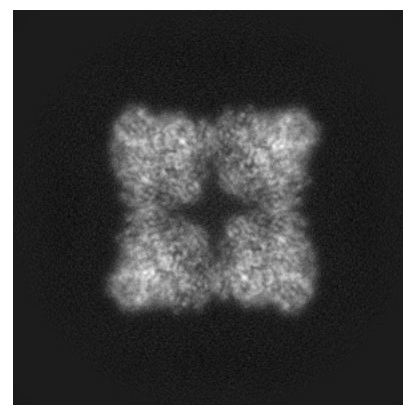
#### 6.1.2 Raw map



X



Y

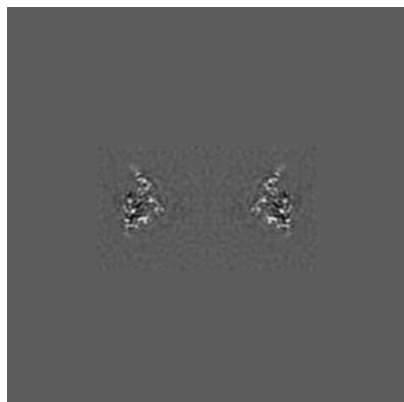


Z

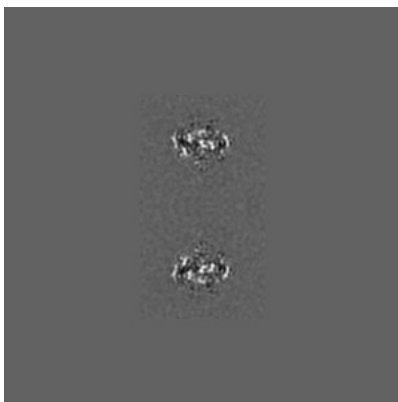
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

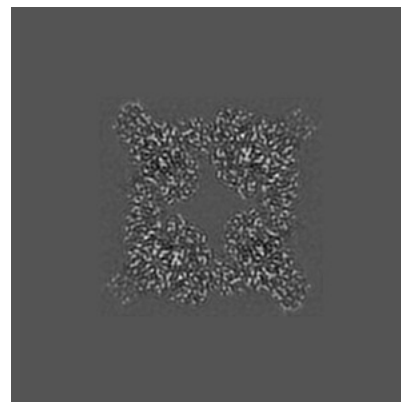
### 6.2.1 Primary map



X Index: 206

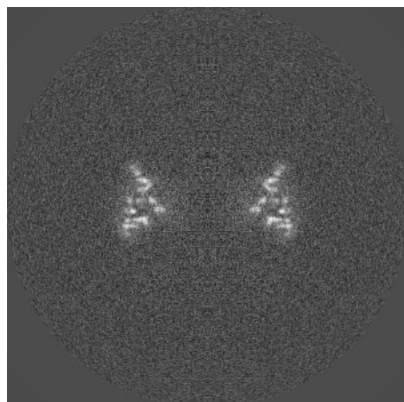


Y Index: 206

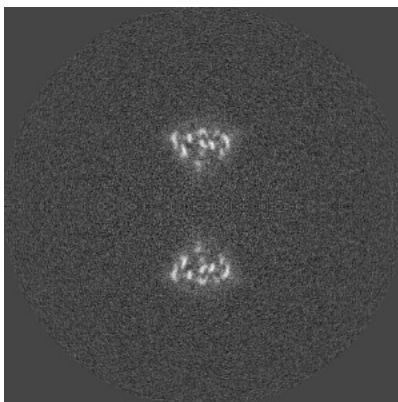


Z Index: 206

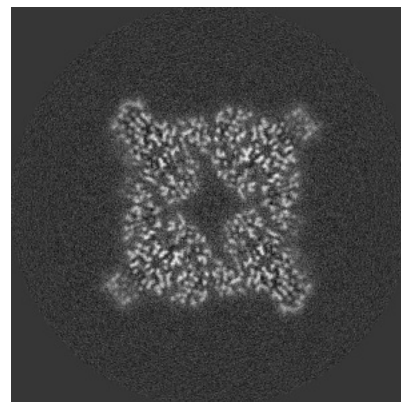
### 6.2.2 Raw map



X Index: 206



Y Index: 206



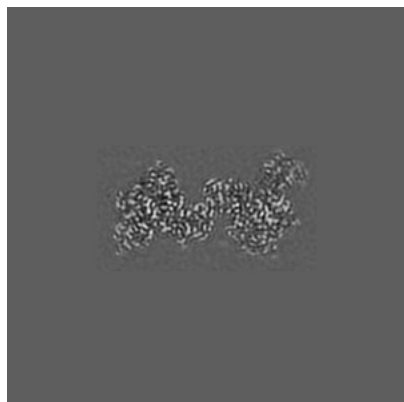
Z Index: 206

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

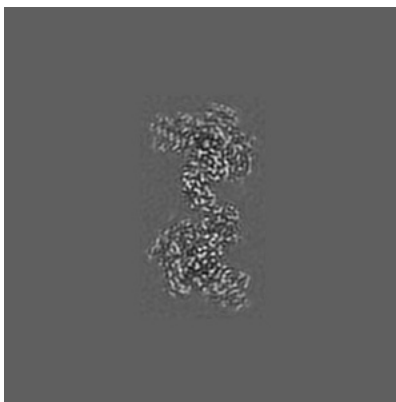


## 6.3 Largest variance slices [i](#)

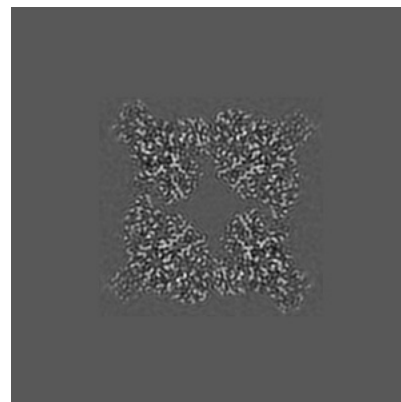
### 6.3.1 Primary map



X Index: 270

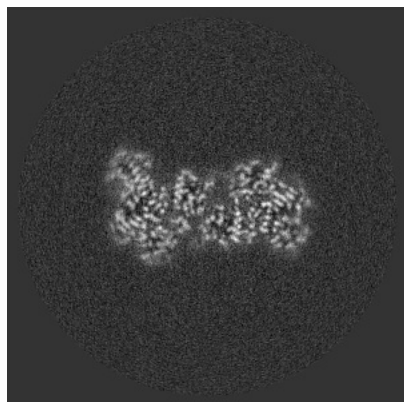


Y Index: 274

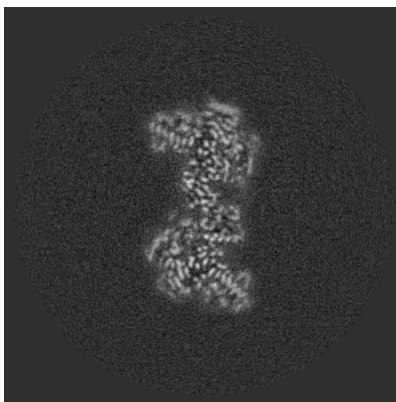


Z Index: 208

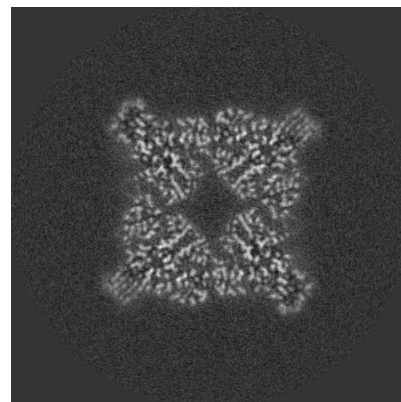
### 6.3.2 Raw map



X Index: 136



Y Index: 275

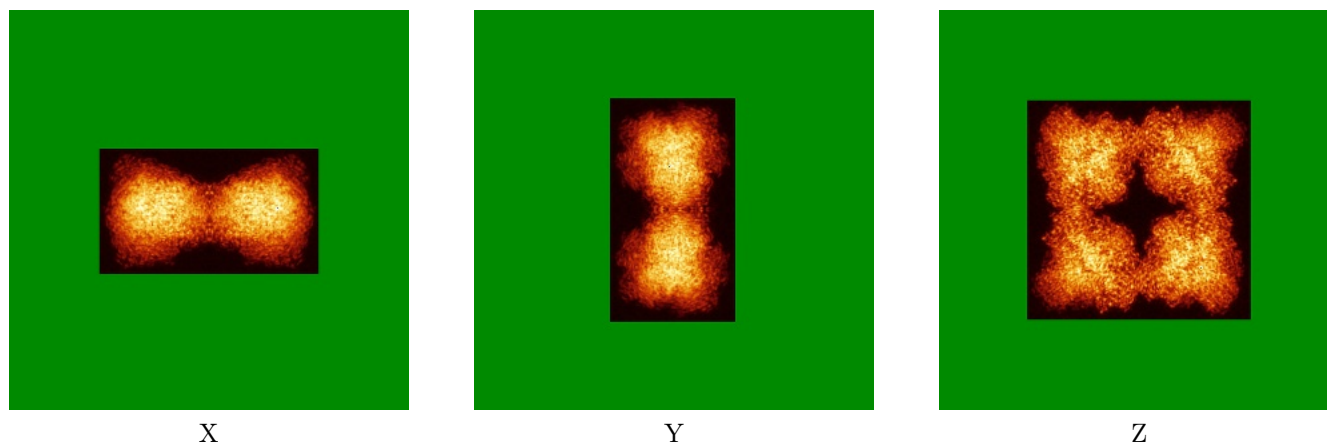


Z Index: 208

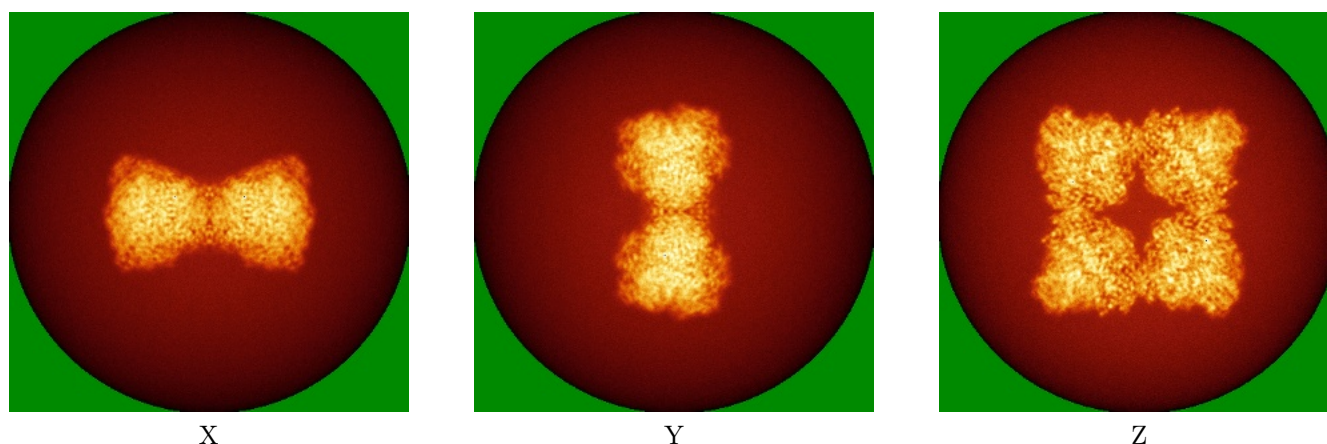
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

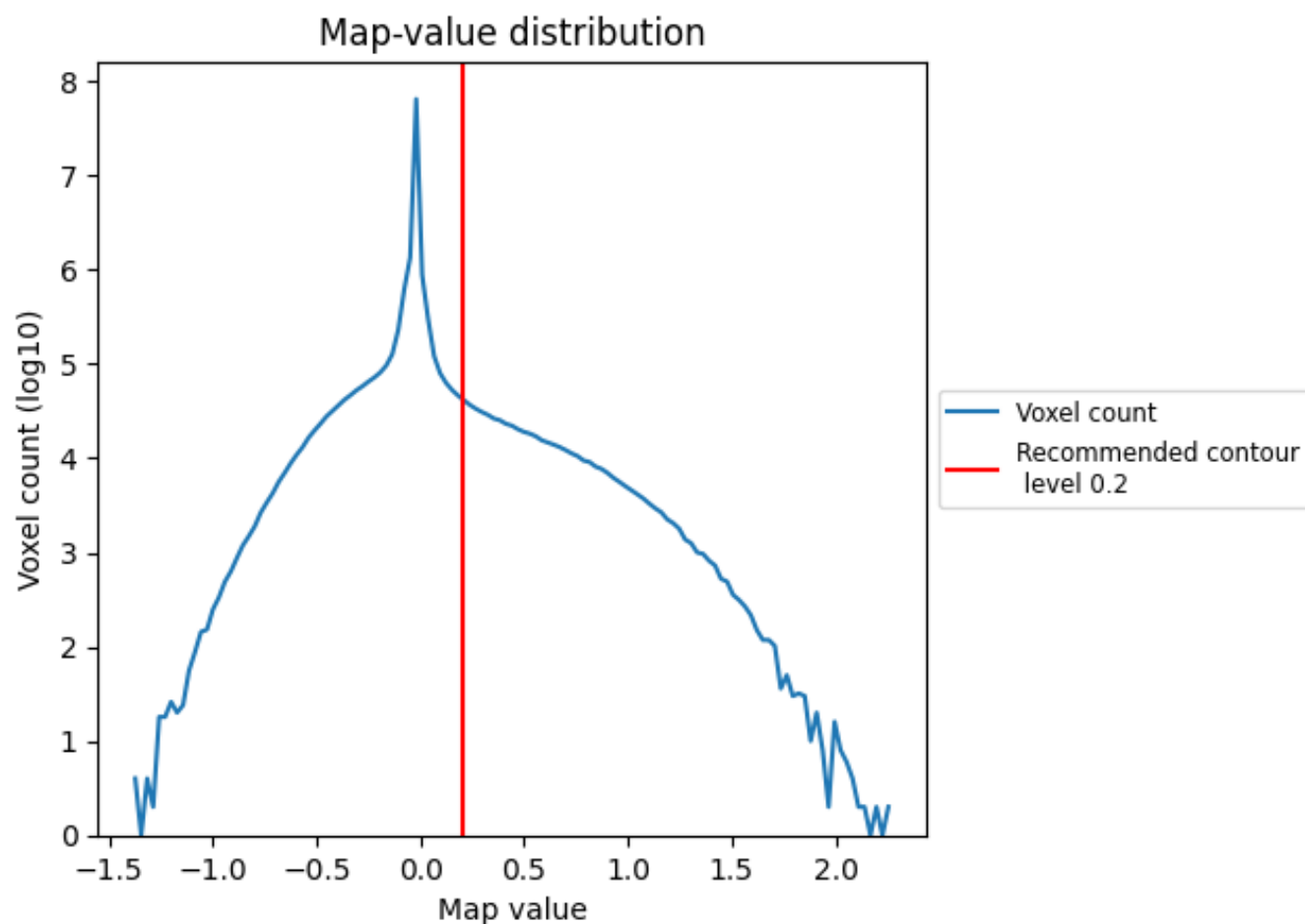
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

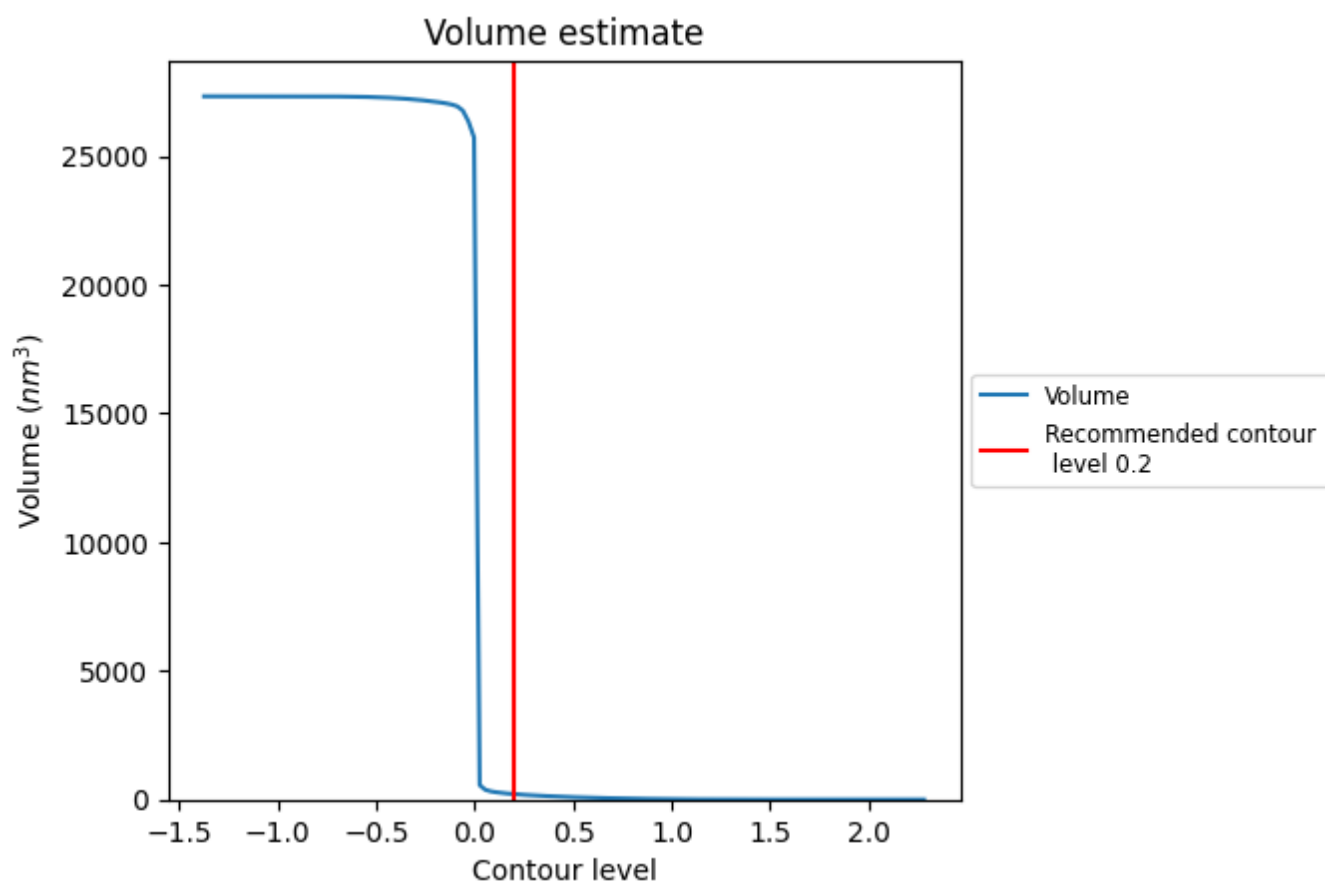
This section contains the results of statistical analysis of the map.

### 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.

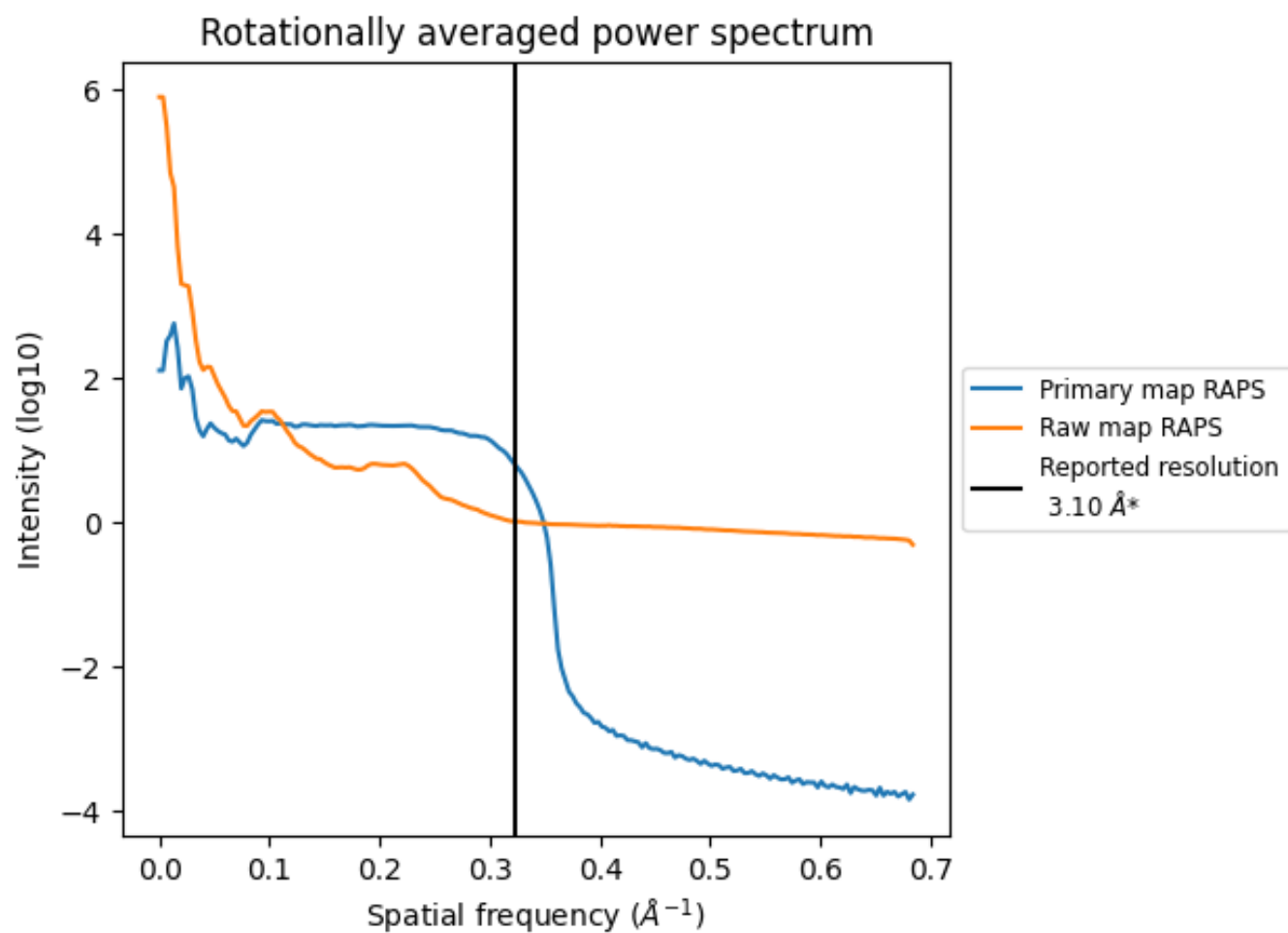
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213  $\text{nm}^3$ ; this corresponds to an approximate mass of 192 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 ⓘ

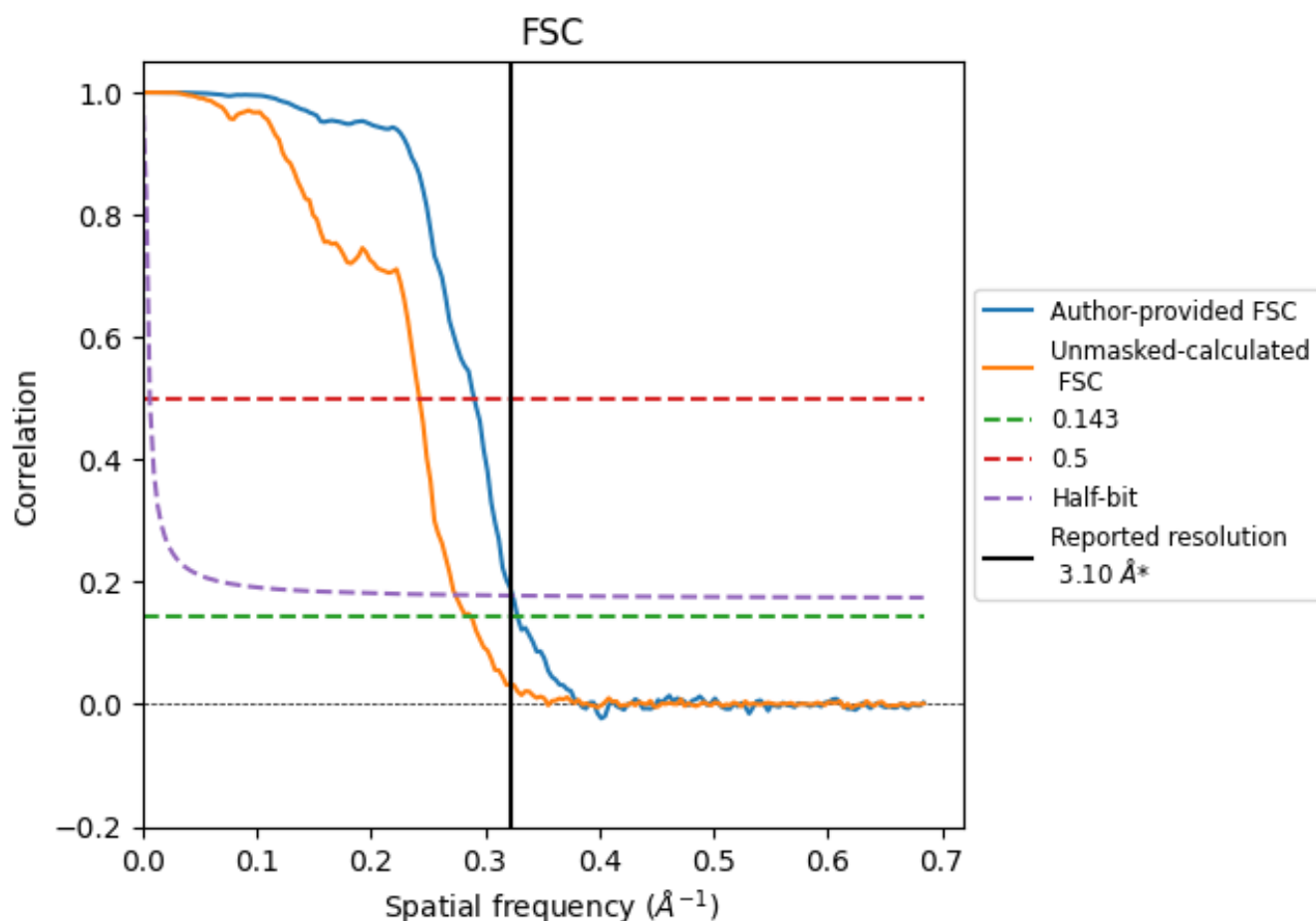


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

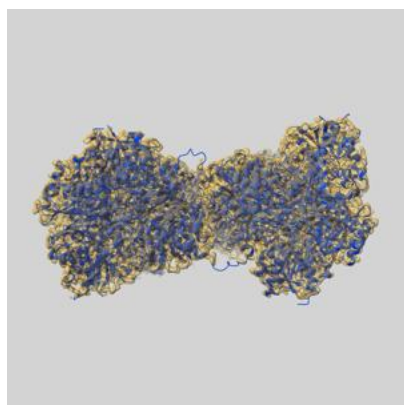
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.44	3.09
Unmasked-calculated*	3.48	4.12	3.65

\*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 3.48 differs from the reported value 3.1 by more than 10 %

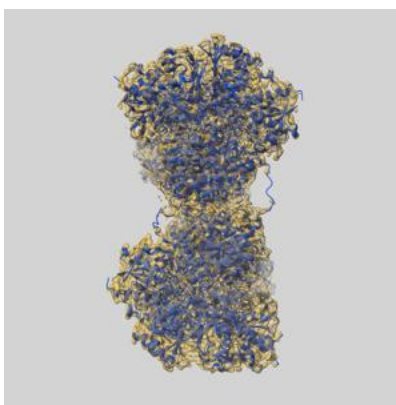
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52553 and PDB model 9I07. Per-residue inclusion information can be found in section [3](#) on page [7](#).

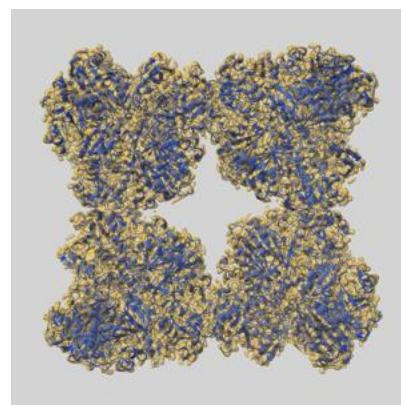
### 9.1 Map-model overlay [i](#)



X



Y

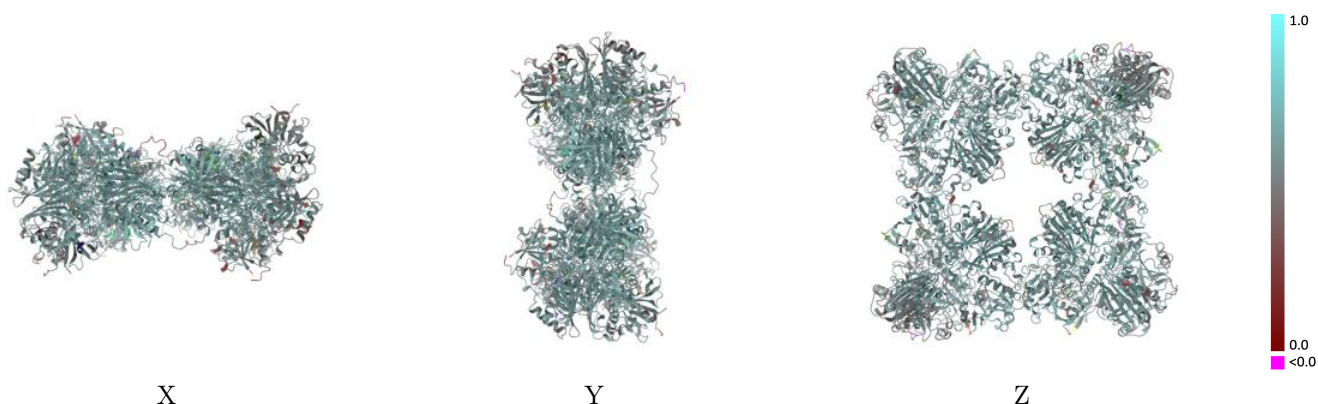


Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

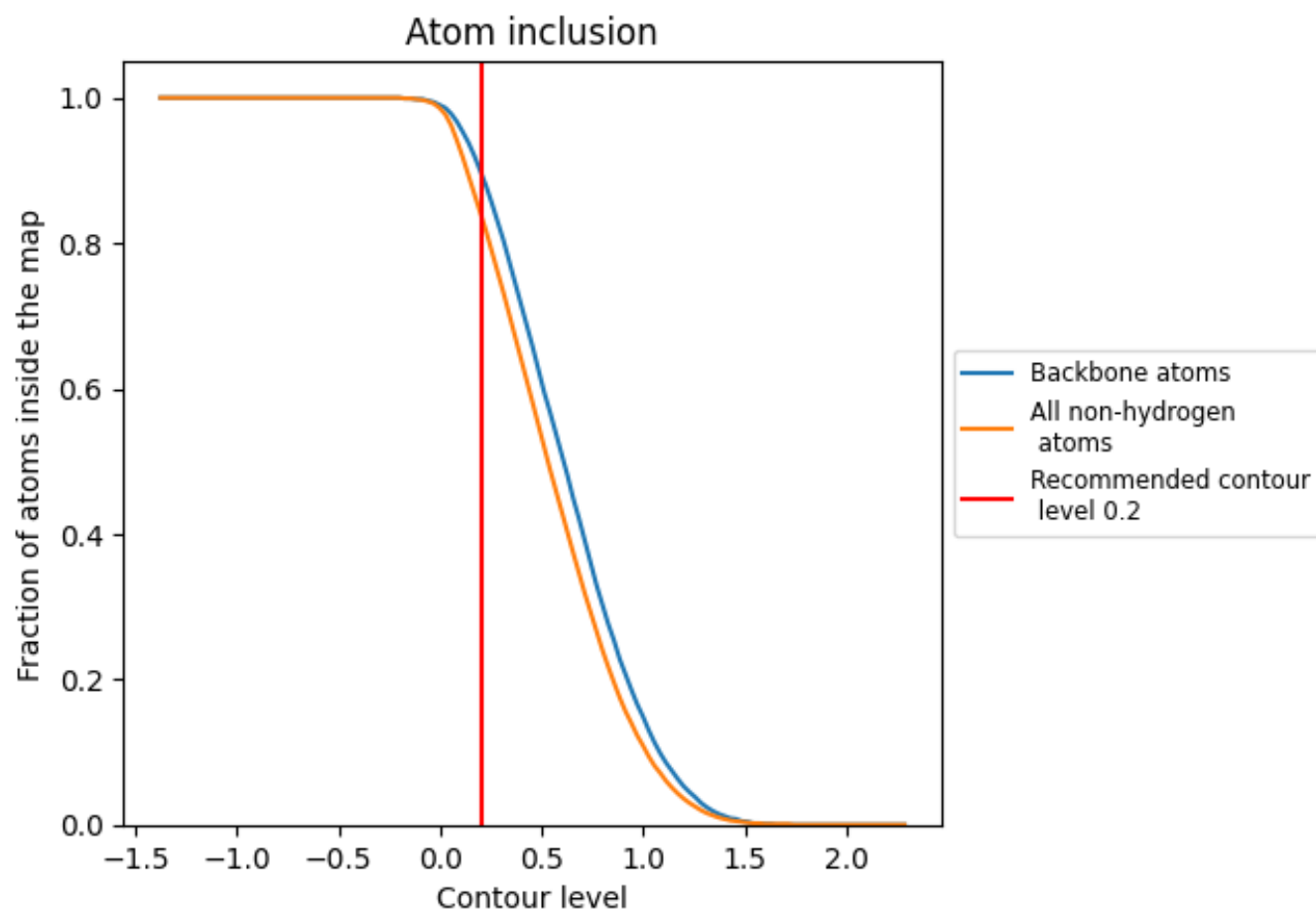


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8400</div>	<div><div></div>0.5840</div>
A	<div><div></div>0.8920</div>	<div><div></div>0.6090</div>
B	<div><div></div>0.8030</div>	<div><div></div>0.5720</div>
C	<div><div></div>0.8950</div>	<div><div></div>0.6090</div>
D	<div><div></div>0.8300</div>	<div><div></div>0.5800</div>
E	<div><div></div>0.8940</div>	<div><div></div>0.6050</div>
F	<div><div></div>0.7480</div>	<div><div></div>0.5430</div>
G	<div><div></div>0.8790</div>	<div><div></div>0.5990</div>
H	<div><div></div>0.7610</div>	<div><div></div>0.5490</div>
I	<div><div></div>0.8910</div>	<div><div></div>0.6110</div>
J	<div><div></div>0.8080</div>	<div><div></div>0.5700</div>
K	<div><div></div>0.8910</div>	<div><div></div>0.6080</div>
L	<div><div></div>0.8290</div>	<div><div></div>0.5820</div>
O	<div><div></div>0.8920</div>	<div><div></div>0.6070</div>
P	<div><div></div>0.7570</div>	<div><div></div>0.5440</div>
Q	<div><div></div>0.8790</div>	<div><div></div>0.5970</div>
R	<div><div></div>0.7580</div>	<div><div></div>0.5470</div>

1.0

0.0

<0.0