



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:07 PM UTC

PDB ID : 6QTI / pdb_00006qti
EMDB ID : EMD-4635
Title : Structure of ovine transhydrogenase in the presence of NADP⁺ in a "double face-down" conformation
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2019-02-25
Resolution : 2.90 Å(reported)
Based on initial model : 1D4O

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

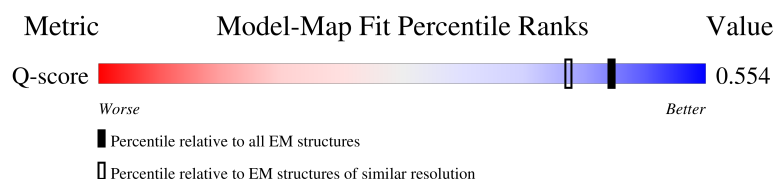
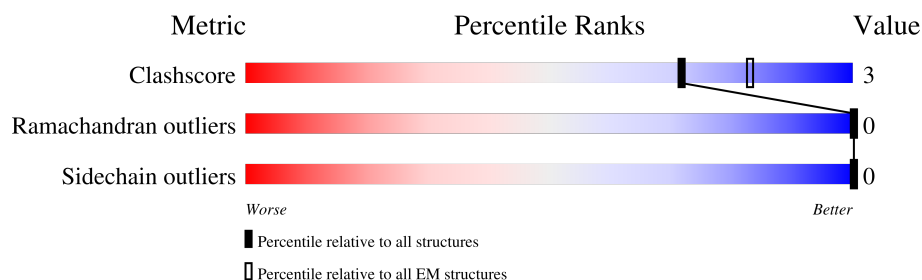
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1086	 6% 87% 9% .
1	B	1086	 6% 87% 8% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15996 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 Nicotinamide nucleotide transhydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0
			7620	4880	1264	1431	45		
1	B	1038	Total	C	N	O	S	0	0
			7620	4880	1264	1431	45		

There are 10 discrepancies between the modelled and reference sequences:

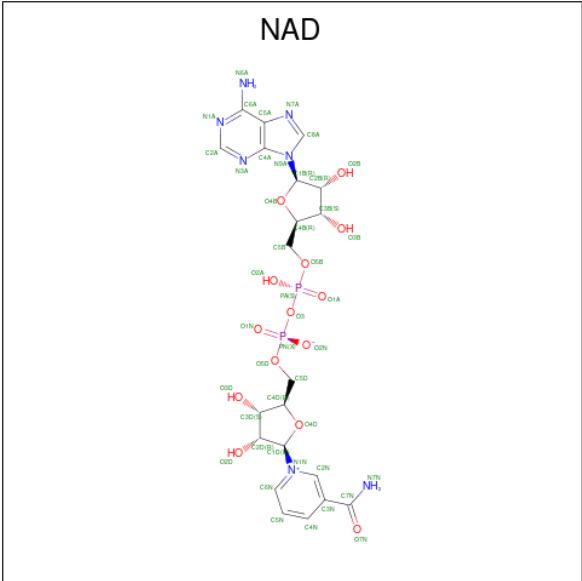
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	THR	ALA	conflict	UNP W5PFI3
A	822	ILE	-	insertion	UNP W5PFI3
A	823	GLY	-	insertion	UNP W5PFI3
A	824	SER	-	insertion	UNP W5PFI3
A	825	SER	-	insertion	UNP W5PFI3
B	-8	THR	ALA	conflict	UNP W5PFI3
B	822	ILE	-	insertion	UNP W5PFI3
B	823	GLY	-	insertion	UNP W5PFI3
B	824	SER	-	insertion	UNP W5PFI3
B	825	SER	-	insertion	UNP W5PFI3

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



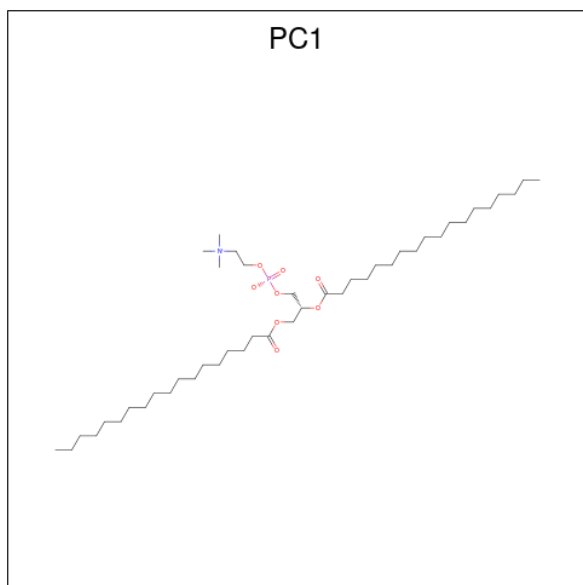
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



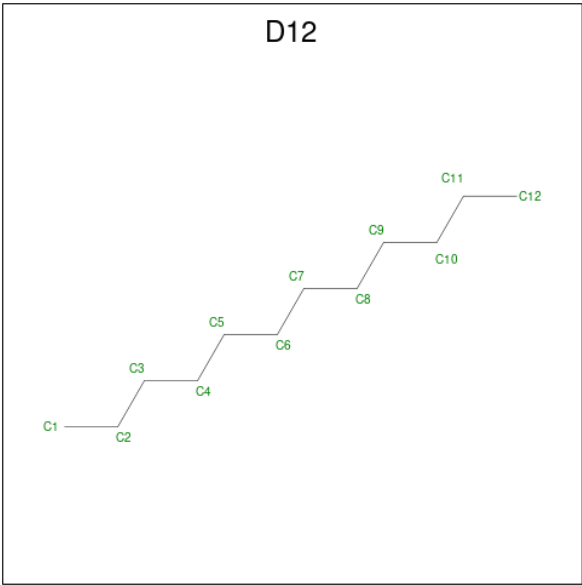
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	B	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 5 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).

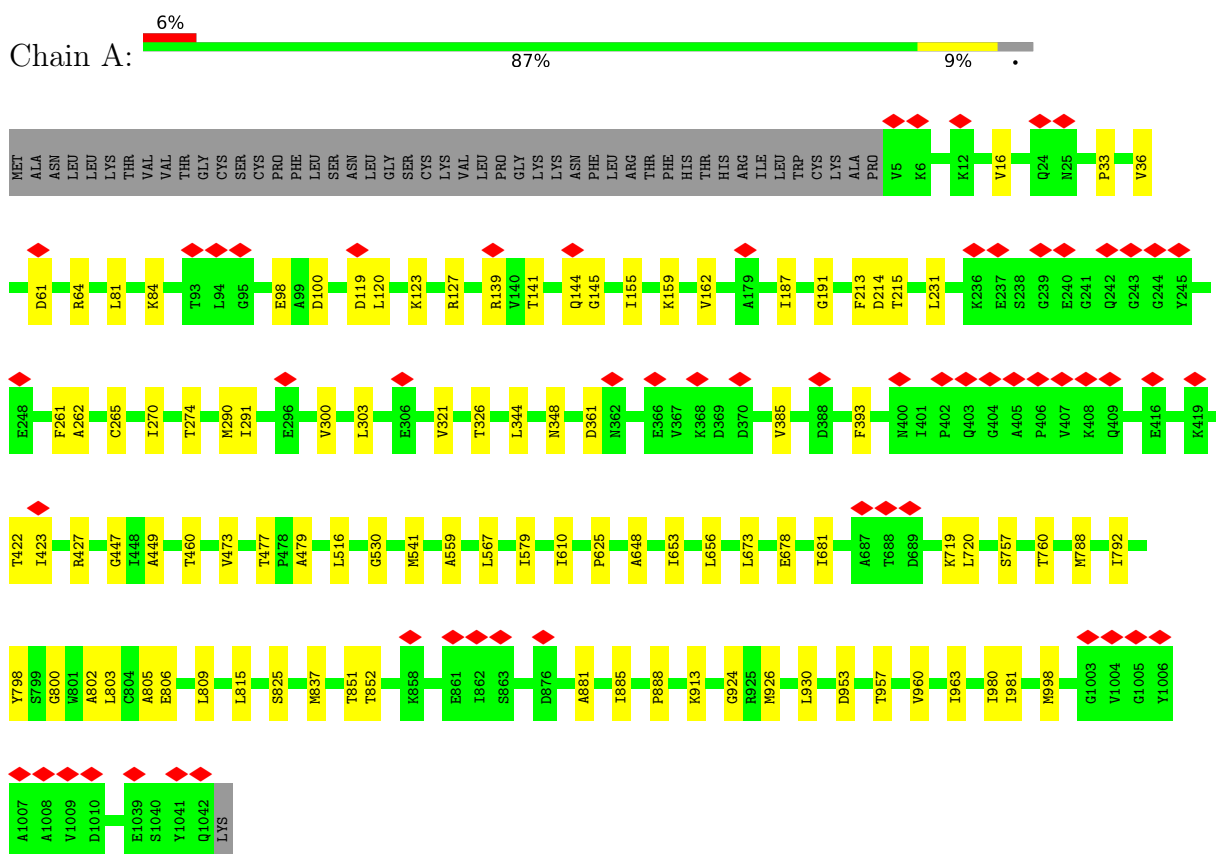


Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			12	12	
5	B	1	Total	C	0
			12	12	
5	B	1	Total	C	0
			12	12	

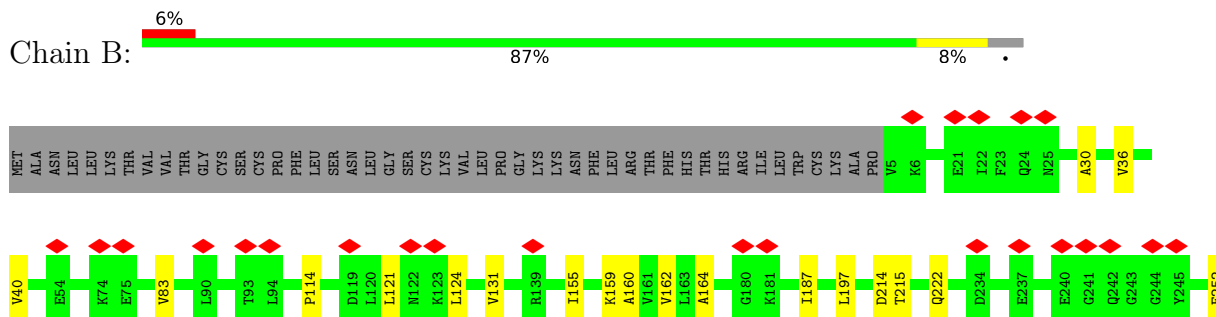
3 Residue-property plots

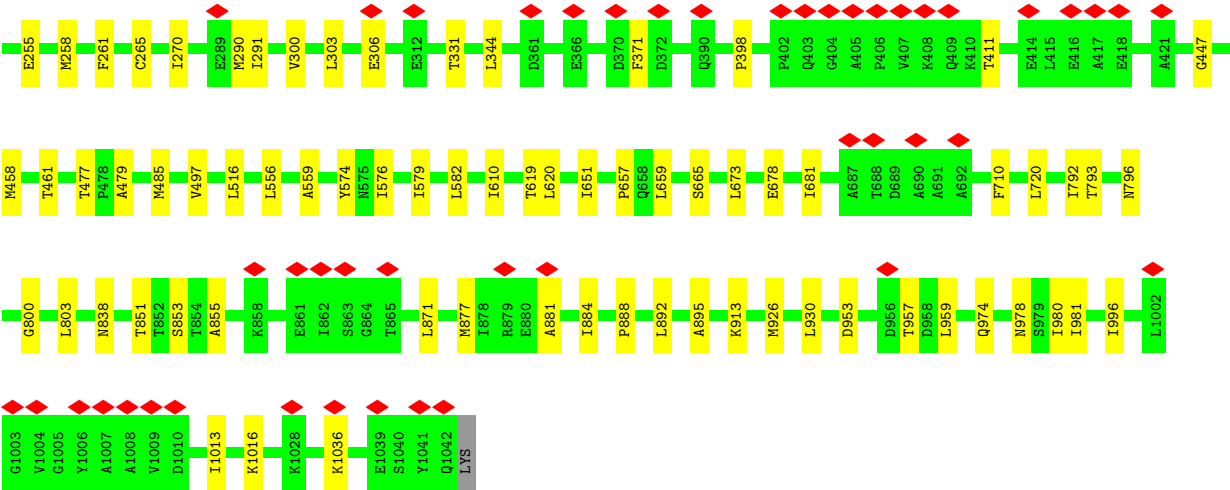
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Nicotinamide nucleotide transhydrogenase



- Molecule 1: Nicotinamide nucleotide transhydrogenase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	136.32, 126.73501, 124.605	wwPDB
Map dimensions	117, 119, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: D12, NAP, NAD, PC1

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	0/7759	0.52	0/10538
1	B	0.26	0/7759	0.55	2/10538 (0.0%)
All	All	0.25	0/15518	0.53	2/21076 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	VAL	N-CA-C	-7.46	105.50	112.96
1	B	36	VAL	N-CA-C	-5.92	107.04	112.96

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	7620	0	7827	57	0
1	B	7620	0	7827	49	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
4	A	258	0	366	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	278	0	412	7	0
5	A	12	0	26	0	0
5	B	24	0	52	0	0
All	All	15996	0	16612	110	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 3.

All (110) 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:261:PHE:O	1:B:265:CYS:HB2	1.93	0.68
1:A:261:PHE:O	1:A:265:CYS:HB2	1.95	0.67
1:A:119:ASP:OD2	1:A:123:LYS:NZ	2.32	0.63
1:B:155:ILE:HD11	1:B:344:LEU:HD12	1.82	0.61
1:A:477:THR:HG22	1:A:479:ALA:H	1.66	0.60
1:B:485:MET:SD	1:B:796:ASN:ND2	2.75	0.60
1:A:155:ILE:HD11	1:A:344:LEU:HD12	1.86	0.58
1:B:497:VAL:HG13	1:B:619:THR:HG21	1.86	0.57
1:B:855:ALA:O	1:B:978:ASN:ND2	2.37	0.57
1:A:924:GLY:O	2:A:1101:NAP:N7N	2.38	0.57
1:B:371:PHE:HB3	1:B:398:PRO:HA	1.87	0.57
1:A:141:THR:O	1:A:144:GLN:NE2	2.38	0.56
4:A:1109:PC1:H292	4:B:1104:PC1:H2C2	1.88	0.56
1:A:84:LYS:NZ	1:A:98:GLU:OE1	2.40	0.55
1:B:678:GLU:HA	1:B:681:ILE:HG22	1.88	0.54
1:B:559:ALA:HB2	1:B:610:ILE:HG12	1.88	0.54
1:B:197:LEU:HD21	1:B:222:GLN:HB3	1.88	0.54
1:B:124:LEU:HD13	1:B:131:VAL:HG21	1.89	0.54
4:A:1103:PC1:H351	4:A:1104:PC1:H242	1.89	0.54
1:A:321:VAL:HG22	1:A:326:THR:HG22	1.90	0.53
1:A:187:ILE:HG12	1:A:270:ILE:HB	1.90	0.53
1:A:16:VAL:HG12	1:A:81:LEU:HB3	1.89	0.53
1:A:720:LEU:HD11	1:A:792:ILE:HD11	1.90	0.53
1:A:881:ALA:O	1:A:913:LYS:NZ	2.40	0.52
1:A:963:ILE:HG12	1:A:998:MET:HE3	1.92	0.52
1:B:881:ALA:O	1:B:913:LYS:NZ	2.42	0.52
1:A:802:ALA:O	1:A:805:ALA:HB3	2.10	0.52
1:B:720:LEU:HD11	1:B:792:ILE:HD11	1.92	0.52
1:A:678:GLU:HA	1:A:681:ILE:HG22	1.93	0.51
1:A:719:LYS:HD2	1:A:788:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:GLU:HG3	1:A:815:LEU:HD13	1.93	0.51
1:B:187:ILE:HG12	1:B:270:ILE:HB	1.92	0.50
1:B:306:GLU:OE1	1:B:331:THR:OG1	2.29	0.50
1:A:851:THR:OG1	1:A:852:THR:N	2.45	0.49
1:B:258:MET:HB3	1:B:290:MET:HE1	1.94	0.49
1:B:291:ILE:HD11	1:B:300:VAL:HG11	1.94	0.49
4:B:1105:PC1:H3A1	4:B:1105:PC1:H2F2	1.94	0.49
1:A:656:LEU:HD23	1:A:926:MET:HE1	1.94	0.49
1:A:145:GLY:O	1:A:348:ASN:ND2	2.43	0.49
1:A:274:THR:HG22	1:A:303:LEU:HD12	1.92	0.49
1:A:473:VAL:HG11	1:A:825:SER:HA	1.95	0.49
1:A:579:ILE:HG13	1:B:447:GLY:HA2	1.94	0.49
1:A:625:PRO:HD2	4:A:1108:PC1:H322	1.94	0.49
1:A:159:LYS:HA	1:A:162:VAL:HG12	1.94	0.49
1:A:100:ASP:O	1:A:127:ARG:NH1	2.45	0.49
1:B:30:ALA:HB1	1:B:83:VAL:HG12	1.94	0.49
1:B:159:LYS:HA	1:B:162:VAL:HG12	1.95	0.48
1:A:139:ARG:NH1	3:A:1102:NAD:O2N	2.43	0.48
1:A:460:THR:HG22	1:B:582:LEU:HB2	1.96	0.48
1:A:422:THR:O	1:A:427:ARG:NH2	2.47	0.48
1:A:262:ALA:HB2	1:A:290:MET:HE2	1.96	0.48
1:B:164:ALA:HB1	1:B:270:ILE:HD13	1.96	0.47
1:B:516:LEU:HD22	1:B:673:LEU:HD22	1.96	0.47
1:A:516:LEU:HD22	1:A:673:LEU:HD22	1.96	0.47
1:B:114:PRO:HB3	1:B:121:LEU:HD11	1.95	0.47
1:A:980:ILE:HG23	1:A:981:ILE:HG23	1.96	0.47
1:B:838:ASN:HB3	1:B:851:THR:HG23	1.96	0.47
1:B:620:LEU:HD23	4:B:1110:PC1:H272	1.97	0.47
1:A:385:VAL:HG13	1:A:393:PHE:HB2	1.97	0.47
1:B:871:LEU:HB3	1:B:1036:LYS:HE3	1.96	0.46
1:B:665:SER:HA	1:B:710:PHE:HA	1.98	0.46
1:A:798:TYR:HE1	4:A:1105:PC1:H2B2	1.81	0.46
1:A:447:GLY:HA2	1:B:579:ILE:HG13	1.97	0.46
1:B:953:ASP:O	1:B:957:THR:OG1	2.30	0.46
1:A:567:LEU:HB3	4:A:1108:PC1:H252	1.98	0.45
1:A:800:GLY:O	1:A:803:LEU:HB2	2.16	0.45
1:A:530:GLY:HA2	1:A:648:ALA:HB2	1.98	0.45
1:B:851:THR:HG22	1:B:853:SER:H	1.82	0.45
1:B:877:MET:HE3	1:B:996:ILE:HD11	1.98	0.45
1:A:541:MET:HE1	1:A:653:ILE:HG13	1.98	0.45
1:B:895:ALA:HB2	2:B:1102:NAP:H62A	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLY:O	1:A:274:THR:OG1	2.35	0.44
1:A:61:ASP:OD1	1:A:64:ARG:NH1	2.50	0.44
1:B:160:ALA:HB2	1:B:303:LEU:HD21	1.99	0.44
1:A:953:ASP:O	1:A:957:THR:OG1	2.35	0.44
1:B:888:PRO:HG2	1:B:930:LEU:HD21	1.99	0.44
1:A:559:ALA:HB2	1:A:610:ILE:HG12	1.99	0.44
1:A:888:PRO:HG2	1:A:930:LEU:HD21	2.00	0.44
1:B:252:GLU:HA	1:B:255:GLU:HG2	1.99	0.44
1:B:477:THR:HG22	1:B:479:ALA:H	1.82	0.44
1:B:574:TYR:HB3	1:B:576:ILE:HD11	2.00	0.44
1:A:361:ASP:OD1	1:A:361:ASP:N	2.50	0.43
1:A:120:LEU:HA	1:A:123:LYS:HE2	2.00	0.43
1:B:793:THR:O	1:B:796:ASN:HB3	2.18	0.43
1:B:411:THR:OG1	1:B:974:GLN:O	2.30	0.43
1:B:800:GLY:O	1:B:803:LEU:HB2	2.17	0.43
4:B:1101:PC1:H372	4:B:1101:PC1:H3A1	1.90	0.43
4:B:1101:PC1:H133	4:B:1101:PC1:H112	1.87	0.43
1:A:291:ILE:HD11	1:A:300:VAL:HG11	2.01	0.43
1:A:449:ALA:HB2	4:B:1101:PC1:H262	2.00	0.43
1:A:885:ILE:O	1:A:960:VAL:HA	2.18	0.43
4:A:1104:PC1:H271	4:A:1104:PC1:H3A1	2.00	0.42
1:B:556:LEU:HD23	4:B:1109:PC1:H362	2.02	0.42
1:B:214:ASP:OD1	1:B:215:THR:N	2.52	0.42
1:A:837:MET:HE2	1:A:837:MET:HB3	1.96	0.42
1:B:458:MET:HA	1:B:461:THR:HG22	2.02	0.42
1:B:888:PRO:HB3	1:B:892:LEU:HD13	2.02	0.42
4:A:1104:PC1:H222	4:A:1104:PC1:H251	1.88	0.42
1:B:980:ILE:HG23	1:B:981:ILE:HG23	2.02	0.42
1:A:213:PHE:HB2	1:A:231:LEU:HB2	2.01	0.42
1:B:651:ILE:HD13	1:B:659:LEU:HD22	2.02	0.42
1:A:806:GLU:HA	1:A:809:LEU:HB3	2.03	0.41
1:B:1013:ILE:HA	1:B:1016:LYS:HE2	2.01	0.41
1:A:33:PRO:HA	1:A:36:VAL:HG22	2.03	0.41
1:A:214:ASP:OD1	1:A:215:THR:N	2.53	0.41
1:B:884:ILE:HG12	1:B:959:LEU:HB3	2.01	0.41
1:B:657:PRO:HG3	1:B:926:MET:HB2	2.02	0.41
1:A:757:SER:HB3	1:A:760:THR:HG22	2.03	0.41
1:A:423:ILE:HD13	1:A:427:ARG:HH21	1.85	0.41
1:A:926:MET:HB3	1:A:926:MET:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1036/1086 (95%)	974 (94%)	62 (6%)	0	100	100
1	B	1036/1086 (95%)	962 (93%)	74 (7%)	0	100	100
All	All	2072/2172 (95%)	1936 (93%)	136 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	801/844 (95%)	801 (100%)	0	100	100
1	B	801/844 (95%)	801 (100%)	0	100	100
All	All	1602/1688 (95%)	1602 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	71	GLN
1	A	122	ASN
1	A	263	GLN
1	A	310	ASN
1	A	348	ASN

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Mol	Chain	Res	Type
1	A	632	GLN
1	A	966	ASN
1	A	994	GLN
1	B	71	GLN
1	B	136	GLN
1	B	222	GLN
1	B	287	ASN
1	B	327	HIS
1	B	362	ASN
1	B	409	GLN
1	B	489	ASN
1	B	632	GLN
1	B	664	HIS
1	B	738	ASN
1	B	813	ASN
1	B	994	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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
2	NAP	A	1101	-	50,52,52	0.41	0	71,80,80	0.53	0
4	PC1	B	1104	-	45,45,53	0.30	0	51,53,61	0.34	0
4	PC1	A	1103	-	39,39,53	0.33	0	45,47,61	0.36	0
3	NAD	B	1103	-	46,48,48	0.35	0	64,73,73	0.40	0
5	D12	B	1107	-	11,11,11	0.08	0	10,10,10	0.12	0
5	D12	A	1106	-	11,11,11	0.09	0	10,10,10	0.15	0
4	PC1	B	1105	-	53,53,53	0.27	0	59,61,61	0.31	0
4	PC1	A	1104	-	44,44,53	0.31	0	50,52,61	0.31	0
4	PC1	A	1108	-	34,34,53	0.36	0	40,42,61	0.35	0
3	NAD	A	1102	-	46,48,48	0.35	0	64,73,73	0.39	0
2	NAP	B	1102	-	50,52,52	0.42	0	71,80,80	0.53	1 (1%)
4	PC1	A	1105	-	49,49,53	0.29	0	55,57,61	0.32	0
5	D12	B	1108	-	11,11,11	0.10	0	10,10,10	0.12	0
4	PC1	A	1109	-	36,36,53	0.36	0	42,44,61	0.52	1 (2%)
4	PC1	B	1101	-	44,44,53	0.31	0	50,52,61	0.37	0
4	PC1	A	1107	-	50,50,53	0.28	0	56,58,61	0.30	0
4	PC1	B	1110	-	34,34,53	0.34	0	40,42,61	0.36	0
4	PC1	B	1109	-	53,53,53	0.27	0	59,61,61	0.28	0
4	PC1	B	1106	-	43,43,53	0.33	0	49,51,61	0.33	0

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	NAP	A	1101	-	-	11/35/67/67	0/5/5/5
4	PC1	B	1104	-	-	12/49/49/57	-
4	PC1	A	1103	-	-	10/43/43/57	-
3	NAD	B	1103	-	-	8/30/62/62	0/5/5/5
5	D12	B	1107	-	-	0/9/9/9	-
5	D12	A	1106	-	-	3/9/9/9	-
4	PC1	B	1105	-	-	11/57/57/57	-
4	PC1	A	1104	-	-	7/48/48/57	-
4	PC1	A	1108	-	-	12/38/38/57	-
3	NAD	A	1102	-	-	10/30/62/62	0/5/5/5
2	NAP	B	1102	-	-	6/35/67/67	0/5/5/5
4	PC1	A	1105	-	-	17/53/53/57	-
5	D12	B	1108	-	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PC1	A	1109	-	-	12/40/40/57	-
4	PC1	B	1101	-	-	8/48/48/57	-
4	PC1	A	1107	-	-	15/54/54/57	-
4	PC1	B	1110	-	-	12/38/38/57	-
4	PC1	B	1109	-	-	13/57/57/57	-
4	PC1	B	1106	-	-	13/47/47/57	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1102	NAP	C4D-O4D-C1D	-3.33	106.88	109.92
4	A	1109	PC1	O31-C3-C2	2.06	114.33	108.40

There are no chirality outliers.

All (181) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	NAP	C5B-O5B-PA-O2A
2	A	1101	NAP	C5D-O5D-PN-O2N
2	A	1101	NAP	O4D-C1D-N1N-C6N
3	A	1102	NAD	C5B-O5B-PA-O3
3	A	1102	NAD	C5D-O5D-PN-O3
3	B	1103	NAD	C5B-O5B-PA-O1A
3	B	1103	NAD	C5D-O5D-PN-O3
3	B	1103	NAD	C5D-O5D-PN-O1N
3	B	1103	NAD	C5D-O5D-PN-O2N
4	A	1103	PC1	C11-O13-P-O12
4	A	1104	PC1	C11-O13-P-O14
4	A	1104	PC1	O13-C11-C12-N
4	A	1105	PC1	C11-O13-P-O12
4	A	1105	PC1	C11-O13-P-O14
4	A	1105	PC1	C11-O13-P-O11
4	A	1105	PC1	C1-O11-P-O14
4	A	1107	PC1	C11-O13-P-O12
4	A	1107	PC1	C11-O13-P-O14
4	A	1107	PC1	C11-O13-P-O11
4	A	1107	PC1	O13-C11-C12-N
4	A	1108	PC1	C11-O13-P-O14
4	A	1108	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
4	A	1108	PC1	C1-O11-P-O12
4	A	1108	PC1	C1-O11-P-O14
4	A	1108	PC1	C1-O11-P-O13
4	A	1109	PC1	C1-O11-P-O13
4	B	1101	PC1	C11-O13-P-O12
4	B	1104	PC1	C11-O13-P-O14
4	B	1104	PC1	C11-O13-P-O11
4	B	1105	PC1	C11-O13-P-O14
4	B	1105	PC1	C11-O13-P-O11
4	B	1106	PC1	C11-O13-P-O12
4	B	1106	PC1	C1-O11-P-O12
4	B	1106	PC1	C1-O11-P-O14
4	B	1106	PC1	C1-O11-P-O13
4	B	1109	PC1	C1-O11-P-O12
4	B	1109	PC1	C1-O11-P-O14
4	B	1109	PC1	C1-O11-P-O13
4	B	1110	PC1	C11-O13-P-O12
4	B	1110	PC1	C11-O13-P-O14
4	B	1110	PC1	C11-O13-P-O11
4	B	1110	PC1	C1-O11-P-O14
4	B	1110	PC1	C1-O11-P-O13
4	B	1110	PC1	O13-C11-C12-N
4	A	1108	PC1	C11-C12-N-C13
2	B	1102	NAP	C3B-C4B-C5B-O5B
4	A	1108	PC1	C11-C12-N-C15
2	B	1102	NAP	O4B-C4B-C5B-O5B
4	A	1105	PC1	C31-C32-C33-C34
4	A	1104	PC1	C2-C1-O11-P
4	A	1109	PC1	C11-C12-N-C14
4	A	1109	PC1	C11-C12-N-C15
4	B	1109	PC1	C29-C2A-C2B-C2C
4	B	1106	PC1	C35-C36-C37-C38
2	A	1101	NAP	C1B-C2B-O2B-P2B
2	A	1101	NAP	C3B-C2B-O2B-P2B
4	B	1110	PC1	C33-C34-C35-C36
4	A	1108	PC1	C11-C12-N-C14
4	A	1109	PC1	C11-C12-N-C13
4	B	1109	PC1	C37-C38-C39-C3A
4	B	1101	PC1	C24-C25-C26-C27
3	B	1103	NAD	C3D-C4D-C5D-O5D
4	B	1110	PC1	C31-C32-C33-C34
4	A	1105	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
4	B	1104	PC1	C26-C27-C28-C29
4	A	1105	PC1	C3E-C3F-C3G-C3H
4	B	1104	PC1	C35-C36-C37-C38
4	A	1107	PC1	C2A-C2B-C2C-C2D
4	B	1109	PC1	C35-C36-C37-C38
3	A	1102	NAD	O4D-C4D-C5D-O5D
3	B	1103	NAD	O4D-C4D-C5D-O5D
4	B	1109	PC1	C2D-C2E-C2F-C2G
4	A	1108	PC1	C24-C25-C26-C27
4	B	1104	PC1	C36-C37-C38-C39
4	A	1109	PC1	C21-C22-C23-C24
4	B	1101	PC1	O11-C1-C2-O21
3	A	1102	NAD	C3D-C4D-C5D-O5D
4	A	1109	PC1	C32-C31-O31-C3
4	B	1106	PC1	C11-C12-N-C14
4	A	1104	PC1	C21-C22-C23-C24
4	A	1107	PC1	O11-C1-C2-C3
4	B	1105	PC1	C37-C38-C39-C3A
5	A	1106	D12	C6-C7-C8-C9
4	A	1107	PC1	C24-C25-C26-C27
4	B	1109	PC1	C1-C2-C3-O31
4	A	1105	PC1	C21-C22-C23-C24
4	B	1106	PC1	C11-C12-N-C13
4	A	1109	PC1	C2-C1-O11-P
4	A	1107	PC1	C25-C26-C27-C28
4	B	1101	PC1	C38-C39-C3A-C3B
2	A	1101	NAP	PA-O3-PN-O5D
4	B	1109	PC1	C3B-C3C-C3D-C3E
4	A	1105	PC1	C26-C27-C28-C29
4	B	1104	PC1	C27-C28-C29-C2A
4	B	1104	PC1	C22-C23-C24-C25
4	A	1103	PC1	C26-C27-C28-C29
4	A	1107	PC1	O11-C1-C2-O21
4	B	1101	PC1	C22-C23-C24-C25
4	B	1106	PC1	C12-C11-O13-P
4	B	1109	PC1	O21-C2-C3-O31
4	A	1109	PC1	O32-C31-O31-C3
3	A	1102	NAD	C2B-C1B-N9A-C8A
4	A	1103	PC1	O13-C11-C12-N
4	A	1105	PC1	O13-C11-C12-N
4	B	1104	PC1	O13-C11-C12-N
4	B	1105	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
4	B	1109	PC1	O13-C11-C12-N
4	A	1107	PC1	C37-C38-C39-C3A
4	B	1101	PC1	C37-C38-C39-C3A
4	B	1106	PC1	C11-C12-N-C15
4	B	1105	PC1	C2-C1-O11-P
4	A	1105	PC1	O11-C1-C2-O21
2	A	1101	NAP	C5B-O5B-PA-O1A
2	A	1101	NAP	C5B-O5B-PA-O3
2	A	1101	NAP	C5D-O5D-PN-O3
2	A	1101	NAP	C5D-O5D-PN-O1N
3	A	1102	NAD	C5B-O5B-PA-O1A
3	A	1102	NAD	C5D-O5D-PN-O1N
3	B	1103	NAD	C5B-O5B-PA-O3
4	A	1103	PC1	C11-O13-P-O11
4	A	1104	PC1	C1-O11-P-O14
4	A	1105	PC1	C1-O11-P-O13
4	A	1109	PC1	C1-O11-P-O14
4	B	1104	PC1	C11-O13-P-O12
4	B	1105	PC1	C11-O13-P-O12
4	B	1106	PC1	C11-O13-P-O14
4	B	1106	PC1	C11-O13-P-O11
4	A	1107	PC1	C29-C2A-C2B-C2C
4	A	1105	PC1	C2-C1-O11-P
4	A	1107	PC1	C2-C1-O11-P
4	B	1105	PC1	C23-C24-C25-C26
4	A	1103	PC1	C32-C33-C34-C35
4	A	1103	PC1	O21-C2-C3-O31
4	A	1109	PC1	C1-C2-C3-O31
4	B	1109	PC1	C3E-C3F-C3G-C3H
4	B	1101	PC1	C33-C34-C35-C36
4	B	1105	PC1	C2B-C2C-C2D-C2E
4	A	1104	PC1	O21-C2-C3-O31
4	A	1108	PC1	O21-C2-C3-O31
4	A	1109	PC1	O21-C2-C3-O31
5	B	1108	D12	C5-C6-C7-C8
4	A	1103	PC1	C1-C2-C3-O31
3	A	1102	NAD	C4D-C5D-O5D-PN
4	B	1104	PC1	C2A-C2B-C2C-C2D
2	B	1102	NAP	C2B-O2B-P2B-O1X
4	B	1106	PC1	O11-C1-C2-C3
4	B	1110	PC1	O11-C1-C2-C3
4	B	1110	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
4	B	1105	PC1	C29-C2A-C2B-C2C
4	A	1105	PC1	O11-C1-C2-C3
4	B	1101	PC1	O11-C1-C2-C3
4	A	1103	PC1	C33-C34-C35-C36
4	A	1104	PC1	C35-C36-C37-C38
2	B	1102	NAP	PN-O3-PA-O2A
4	A	1103	PC1	O31-C31-C32-C33
4	A	1108	PC1	O31-C31-C32-C33
3	A	1102	NAD	O4B-C4B-C5B-O5B
2	B	1102	NAP	C2B-O2B-P2B-O2X
4	B	1104	PC1	O31-C31-C32-C33
4	B	1105	PC1	O21-C21-C22-C23
4	B	1106	PC1	C27-C28-C29-C2A
4	A	1107	PC1	C2B-C2C-C2D-C2E
4	A	1107	PC1	C35-C36-C37-C38
3	A	1102	NAD	O4B-C1B-N9A-C8A
4	B	1110	PC1	O31-C31-C32-C33
4	A	1109	PC1	C22-C21-O21-C2
5	A	1106	D12	C4-C5-C6-C7
4	A	1108	PC1	O32-C31-C32-C33
4	A	1107	PC1	C34-C35-C36-C37
4	B	1104	PC1	O32-C31-C32-C33
4	A	1105	PC1	C28-C29-C2A-C2B
4	B	1105	PC1	O22-C21-C22-C23
4	A	1105	PC1	O21-C21-C22-C23
4	A	1103	PC1	O32-C31-C32-C33
4	B	1110	PC1	O32-C31-C32-C33
4	A	1105	PC1	C22-C23-C24-C25
4	B	1109	PC1	C28-C29-C2A-C2B
2	B	1102	NAP	PA-O3-PN-O2N
3	B	1103	NAD	PA-O3-PN-O2N
2	A	1101	NAP	O4D-C4D-C5D-O5D
5	A	1106	D12	C5-C6-C7-C8

There are no ring outliers.

13 monomers are involved in 16 short contacts:

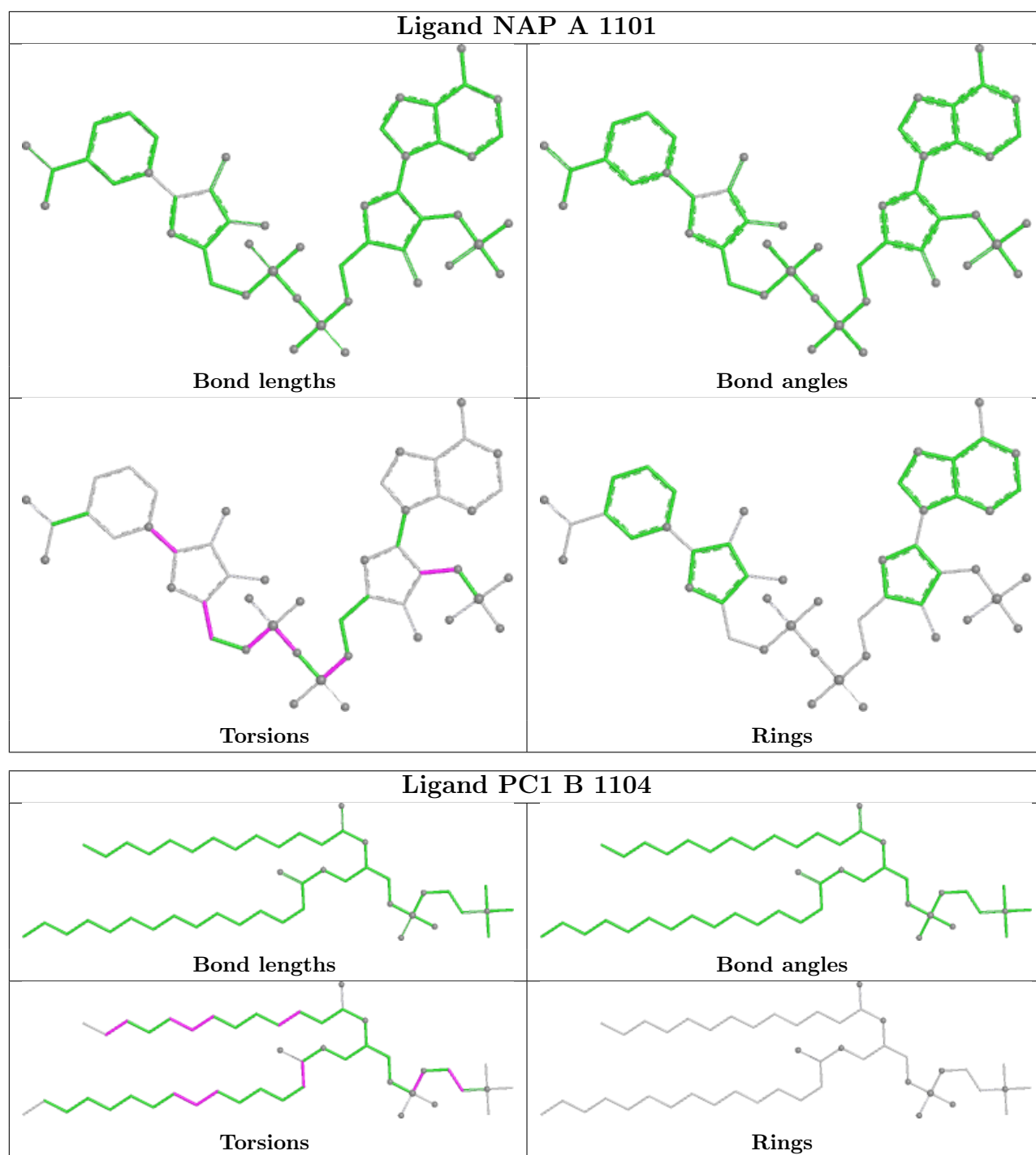
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	NAP	1	0
4	B	1104	PC1	1	0
4	A	1103	PC1	1	0
4	B	1105	PC1	1	0

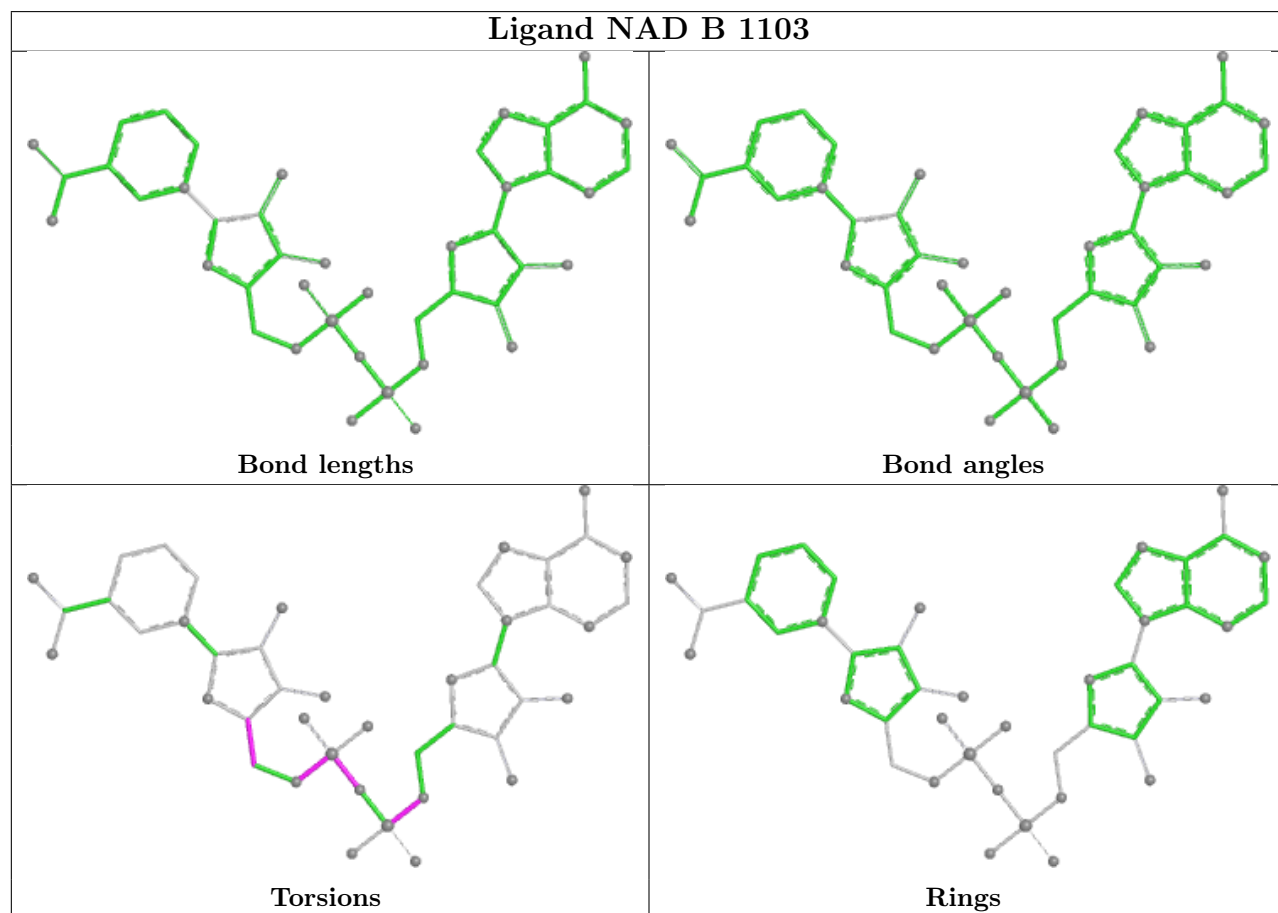
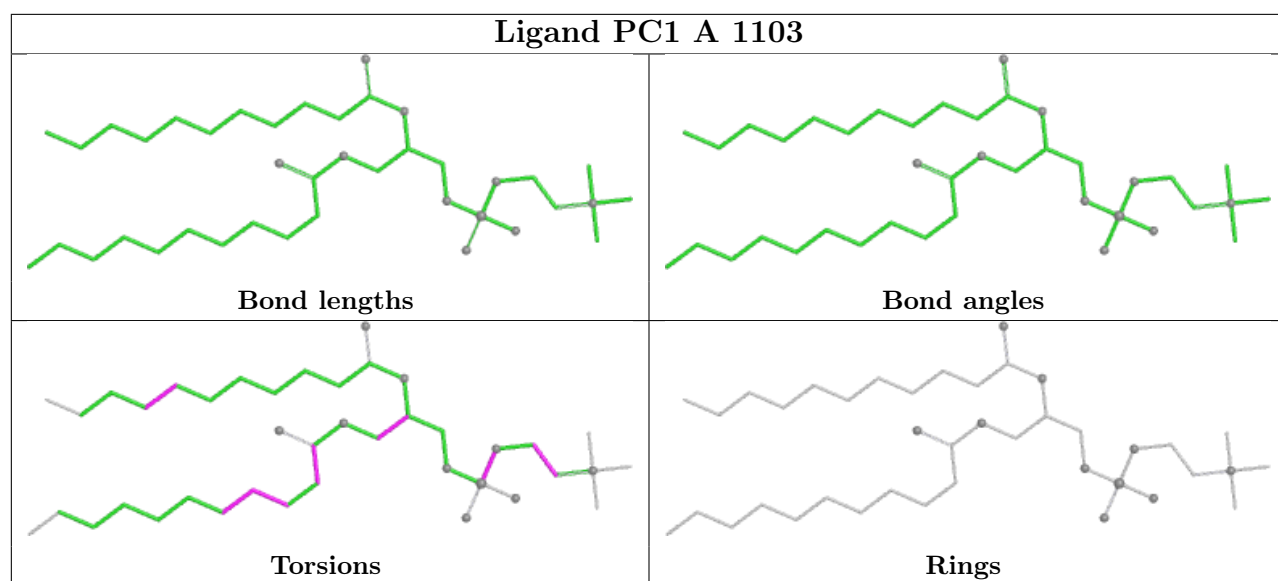
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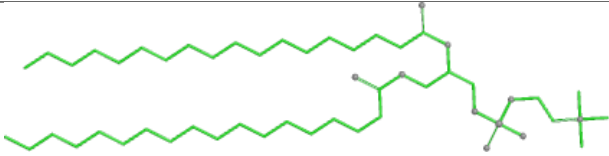
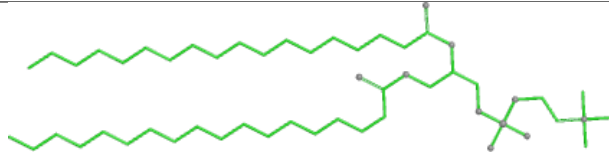
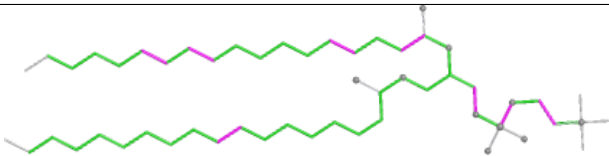
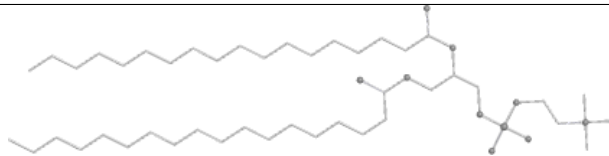
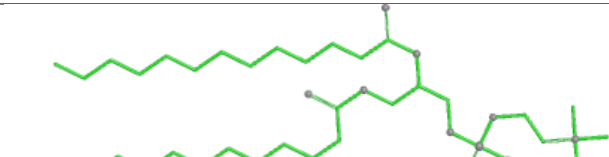
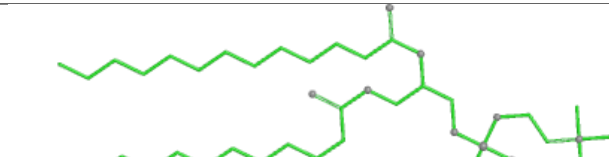
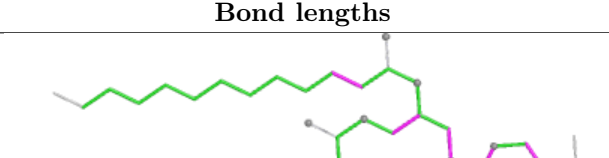
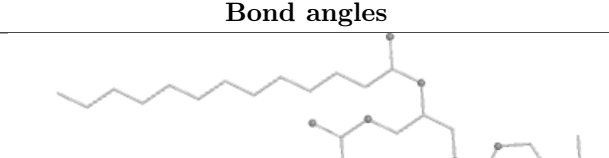
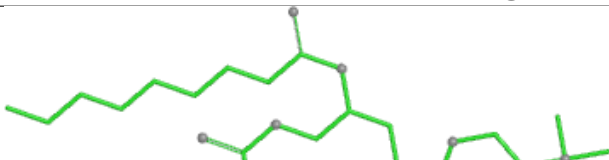
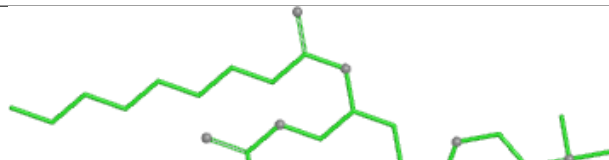
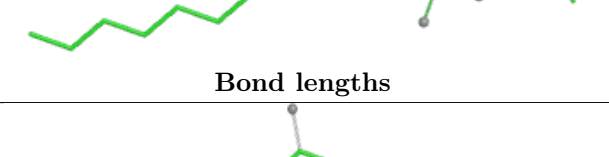
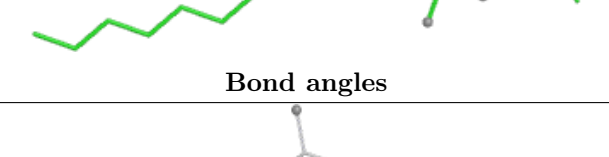
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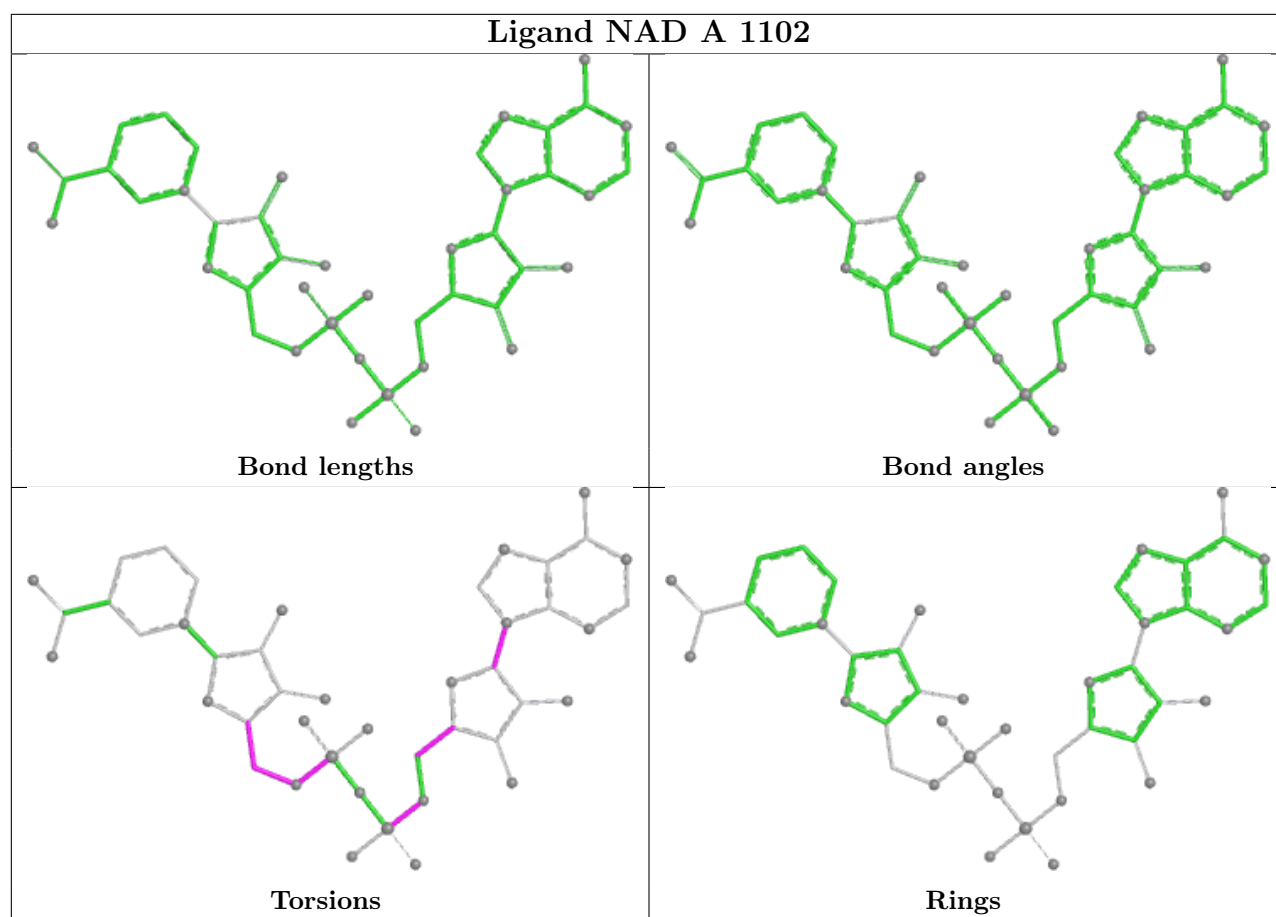
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1104	PC1	3	0
4	A	1108	PC1	2	0
3	A	1102	NAD	1	0
2	B	1102	NAP	1	0
4	A	1105	PC1	1	0
4	A	1109	PC1	1	0
4	B	1101	PC1	3	0
4	B	1110	PC1	1	0
4	B	1109	PC1	1	0

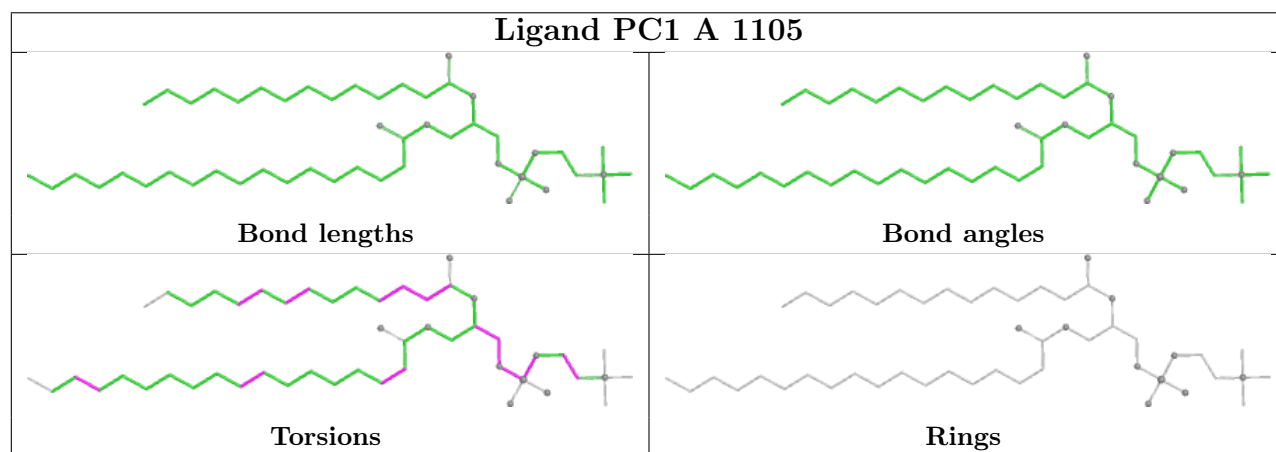
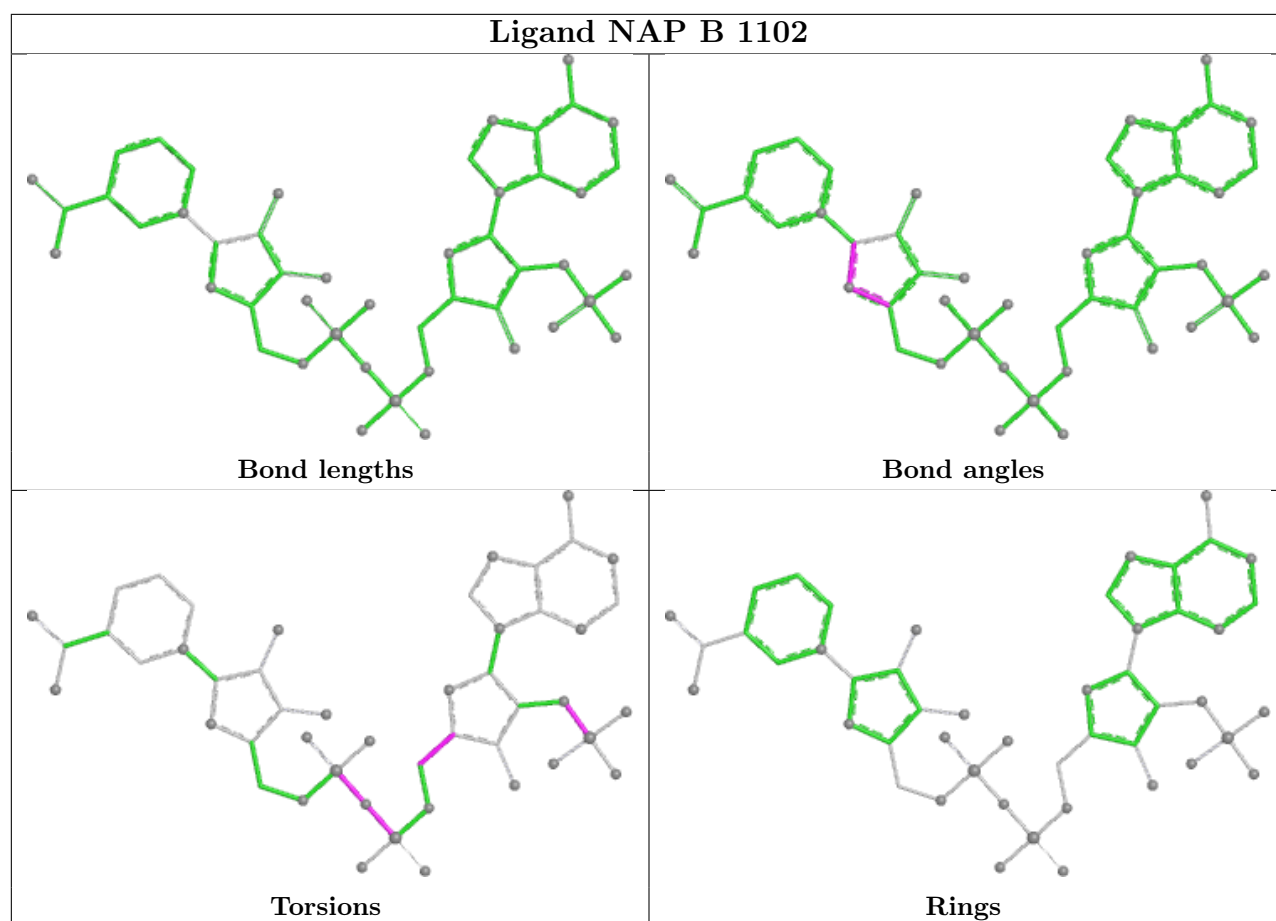
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

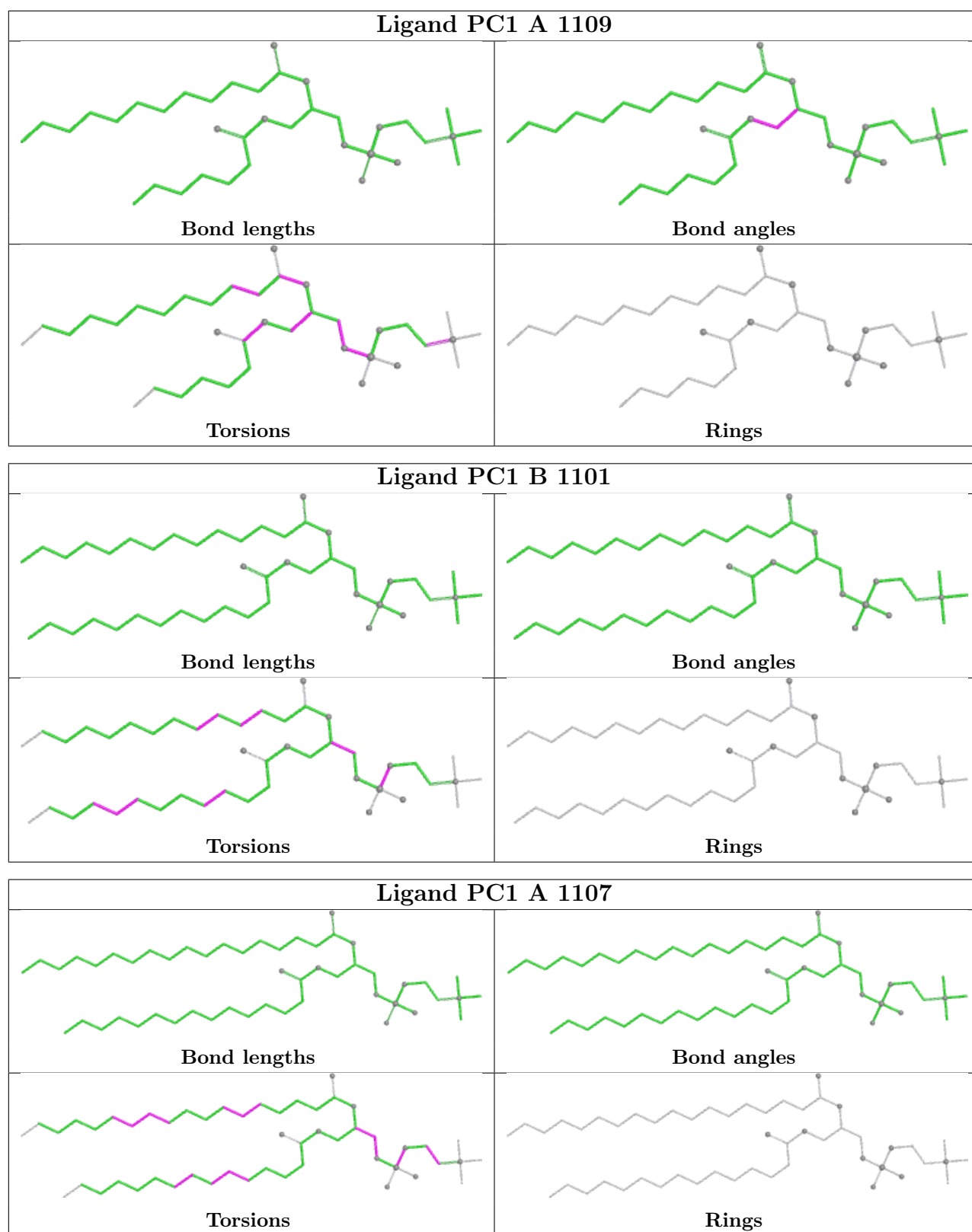


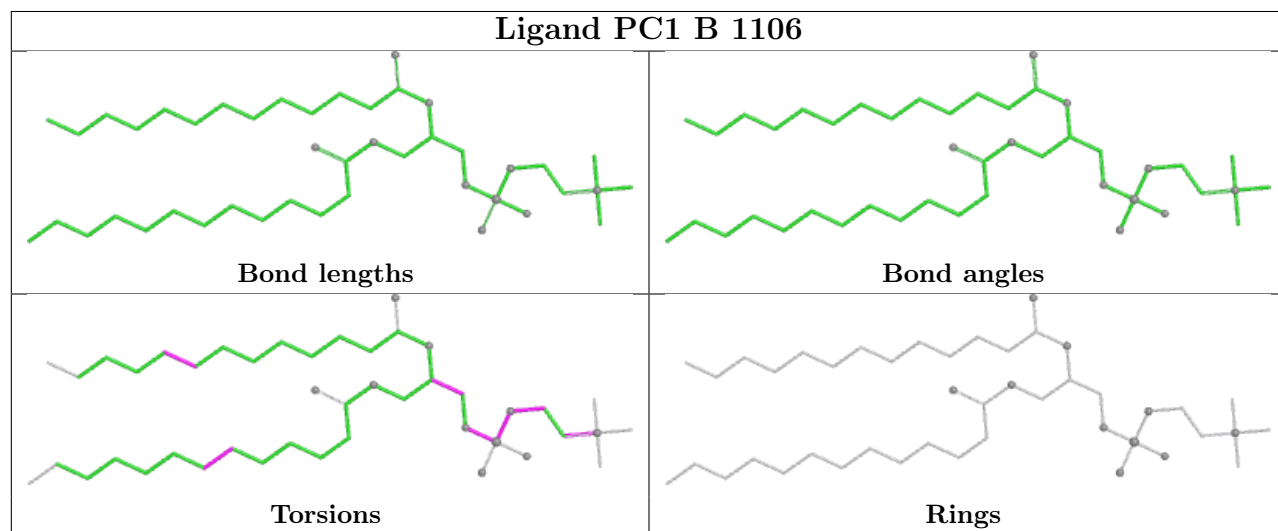
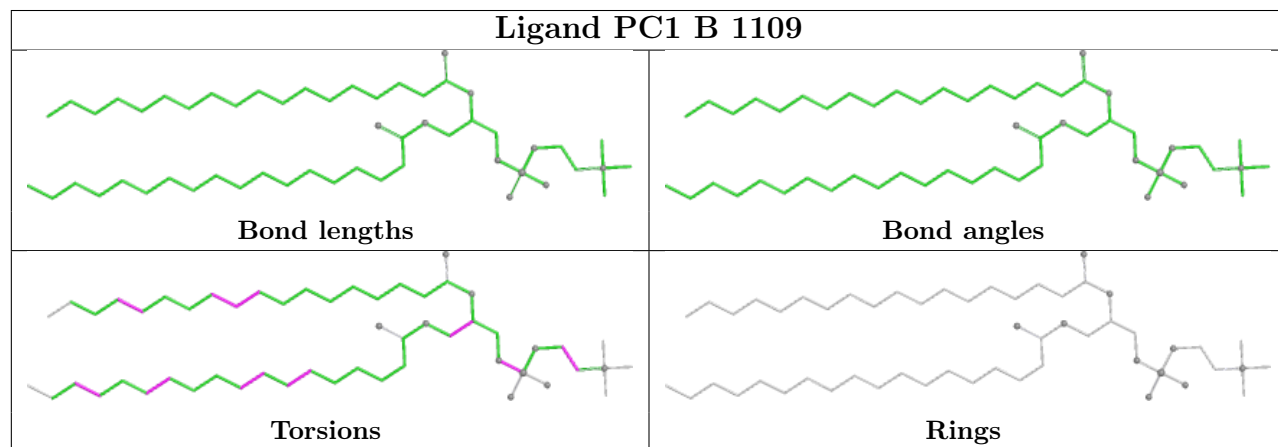
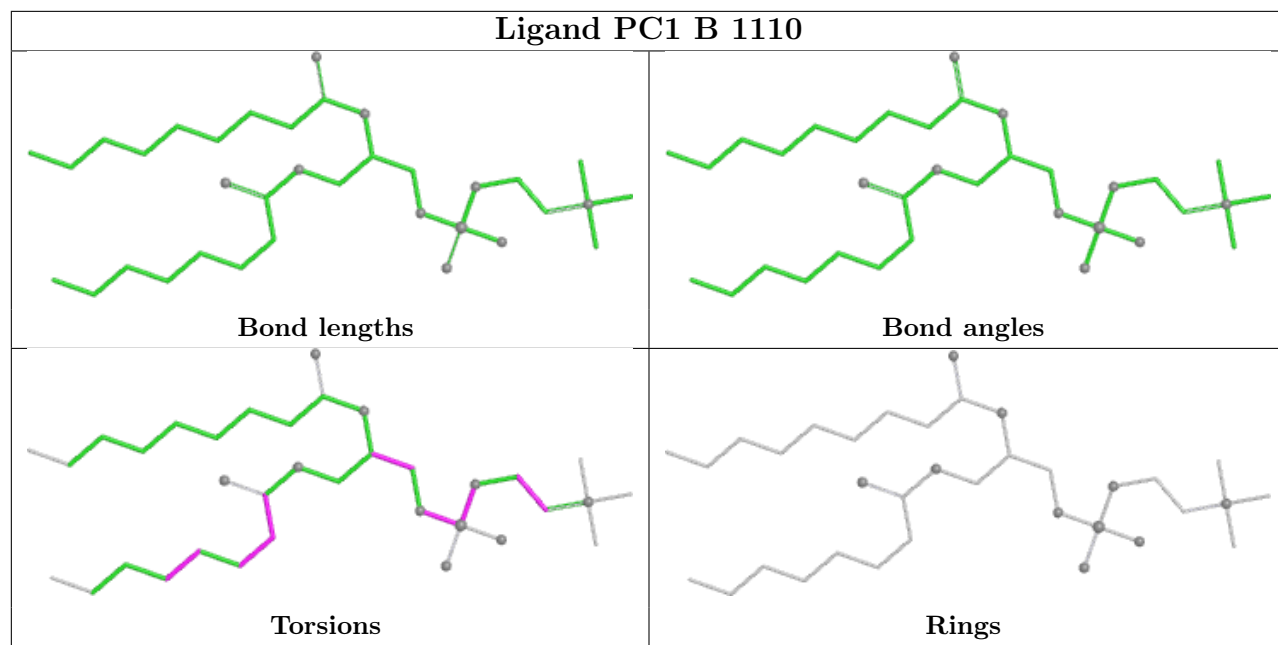


Ligand PC1 B 1105	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1108	
 Bond lengths	 Bond angles
 Torsions	 Rings









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.

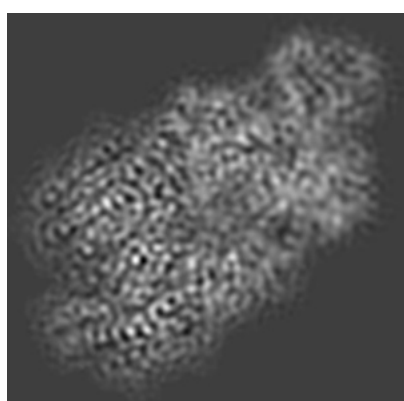
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4635. These allow visual inspection of the internal detail of the map and identification of artifacts.

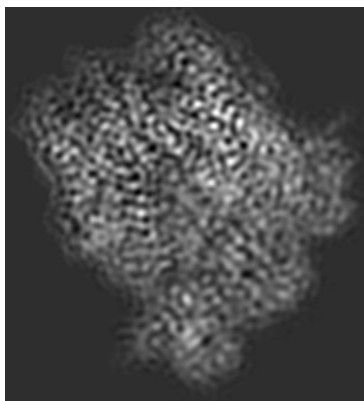
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

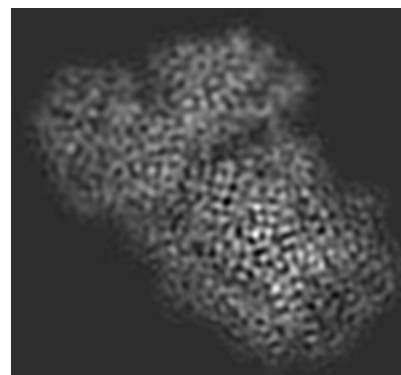
6.1.1 Primary map



X



Y

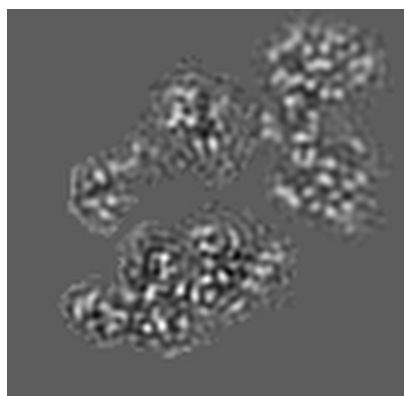


Z

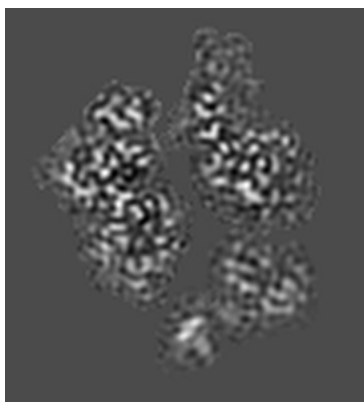
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

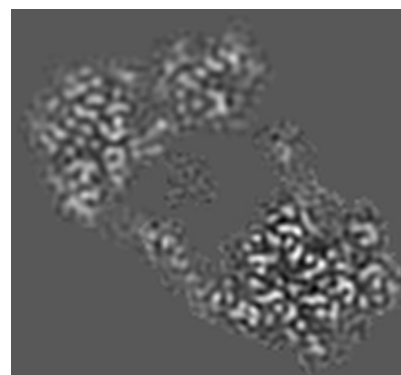
6.2.1 Primary map



X Index: 64



Y Index: 59

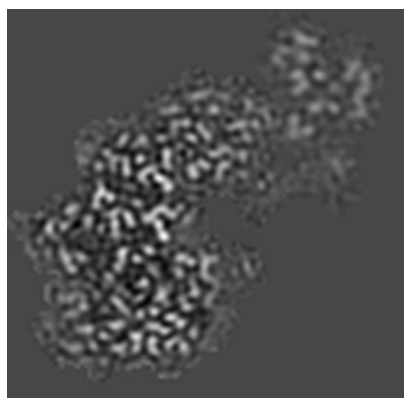


Z Index: 58

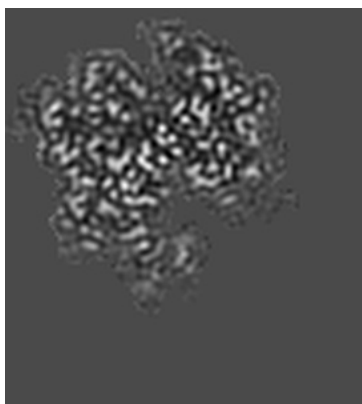
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

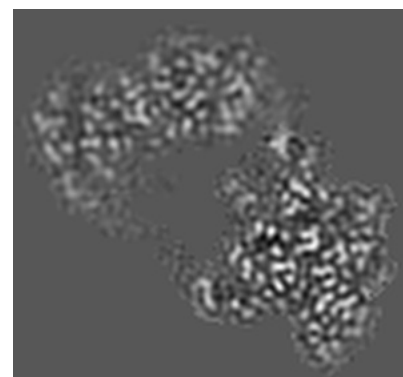
6.3.1 Primary map



X Index: 82



Y Index: 42



Z Index: 64

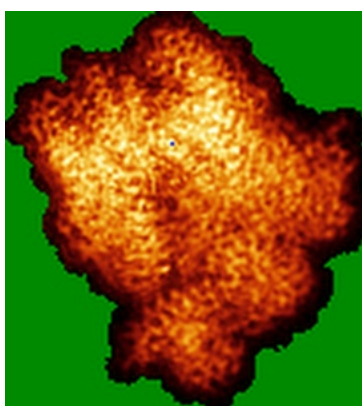
The images above show the largest variance slices of the map in three orthogonal directions.

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

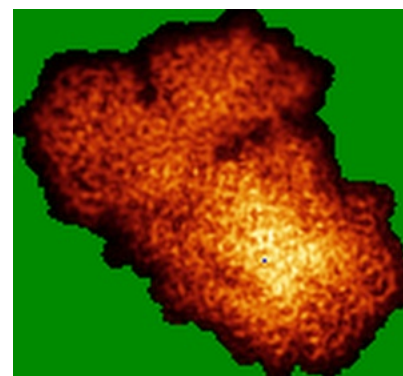
6.4.1 Primary map



X



Y

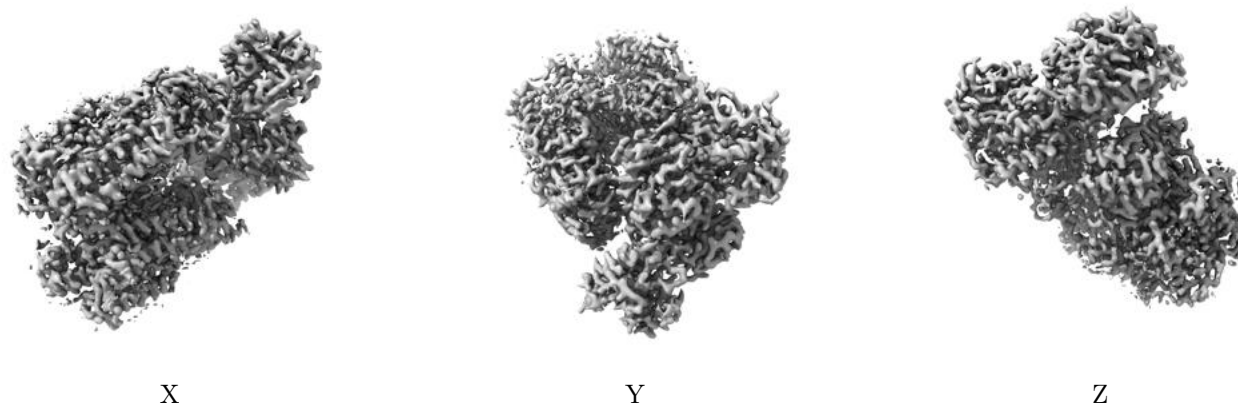


Z

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

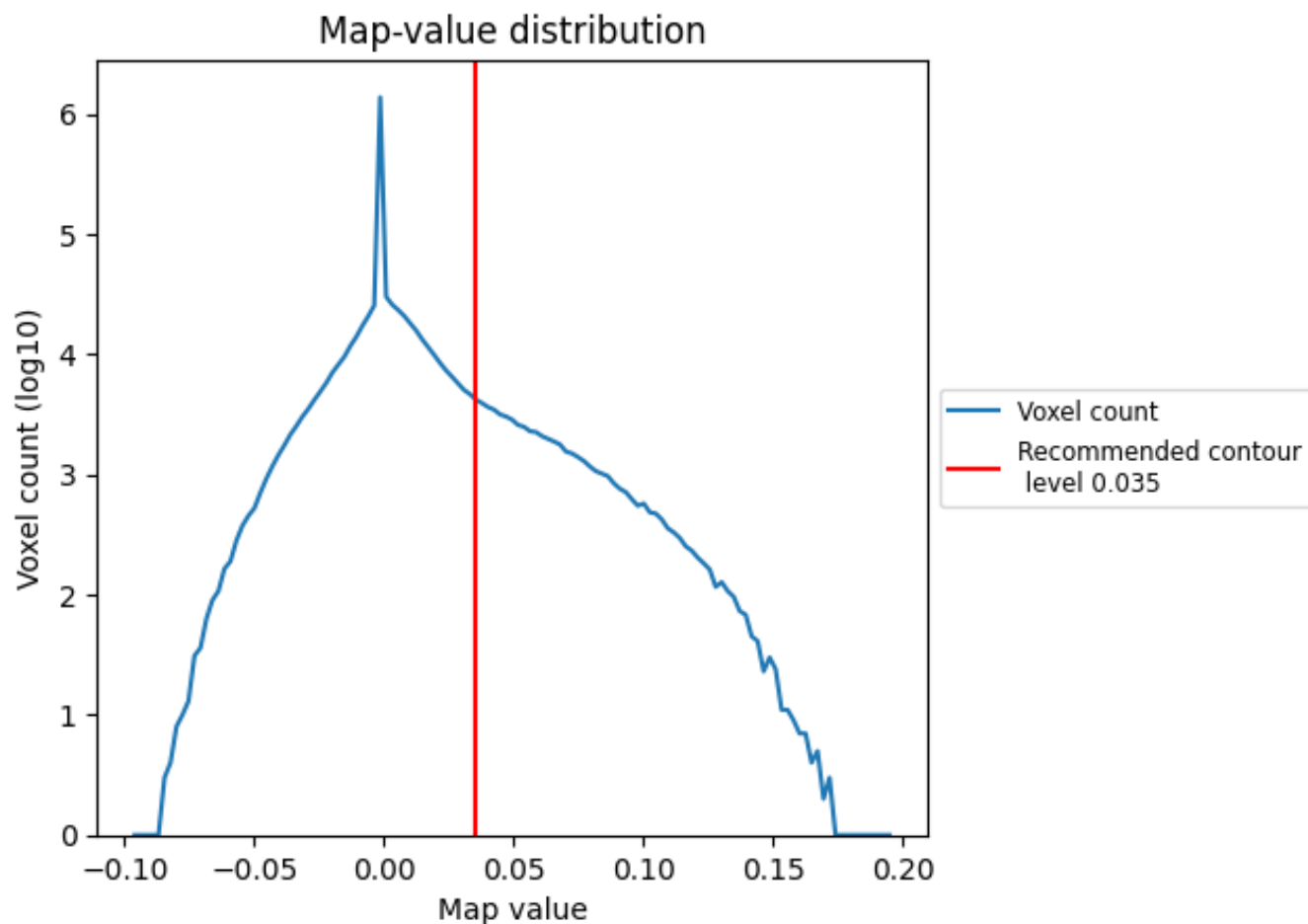
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

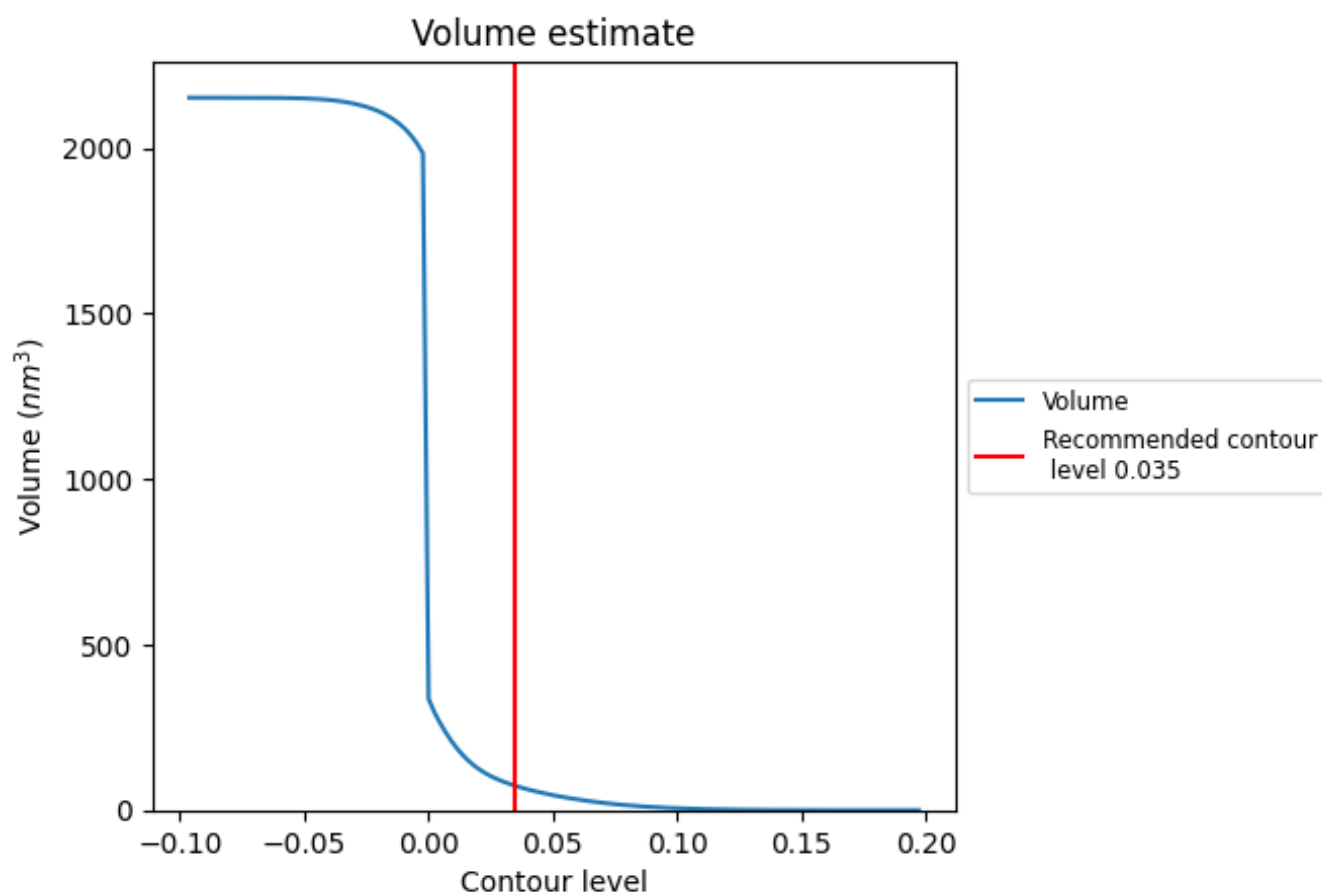
This section contains the results of statistical analysis of the map.

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 73 nm³; this corresponds to an approximate mass of 66 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.

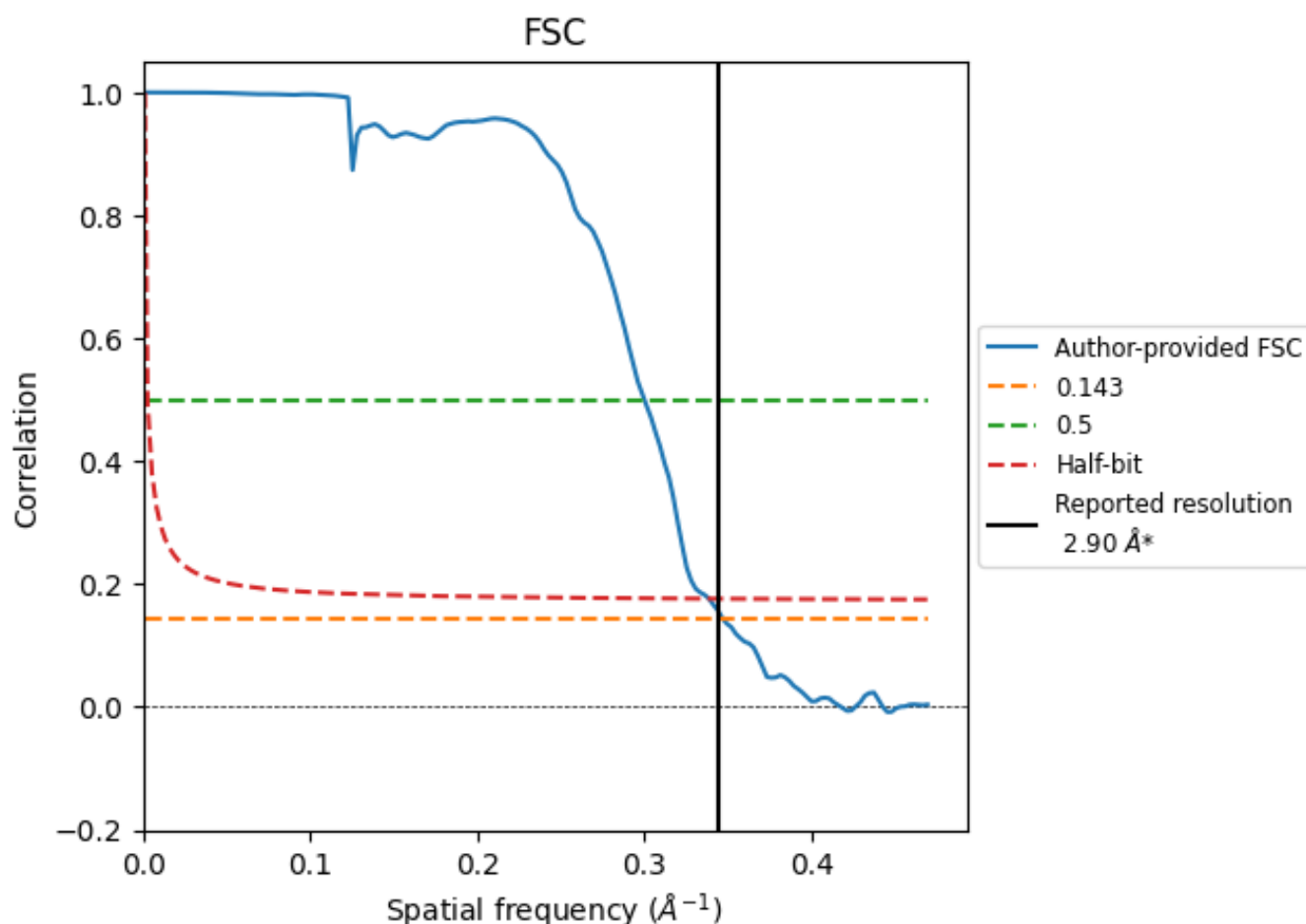
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

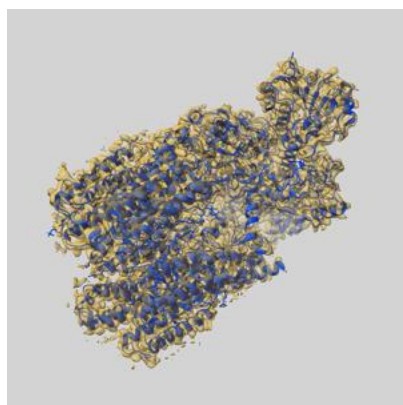
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.33	2.95
Unmasked-calculated*	-	-	-

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

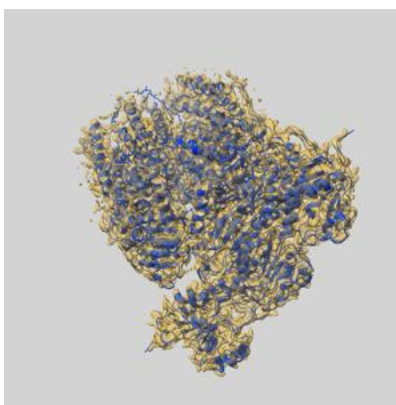
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4635 and PDB model 6QTI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

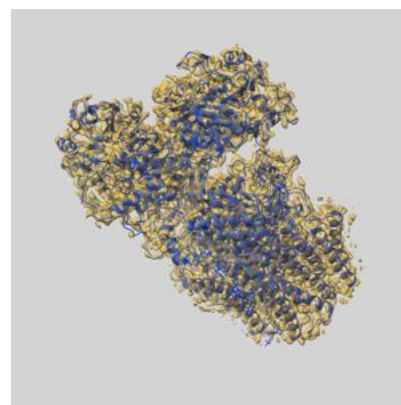
9.1 Map-model overlay [i](#)



X



Y



Z

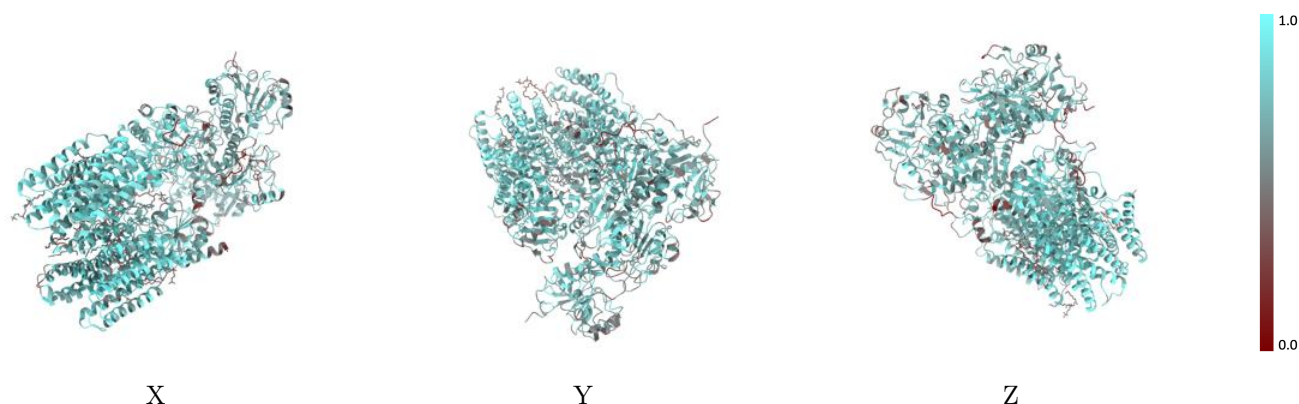
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



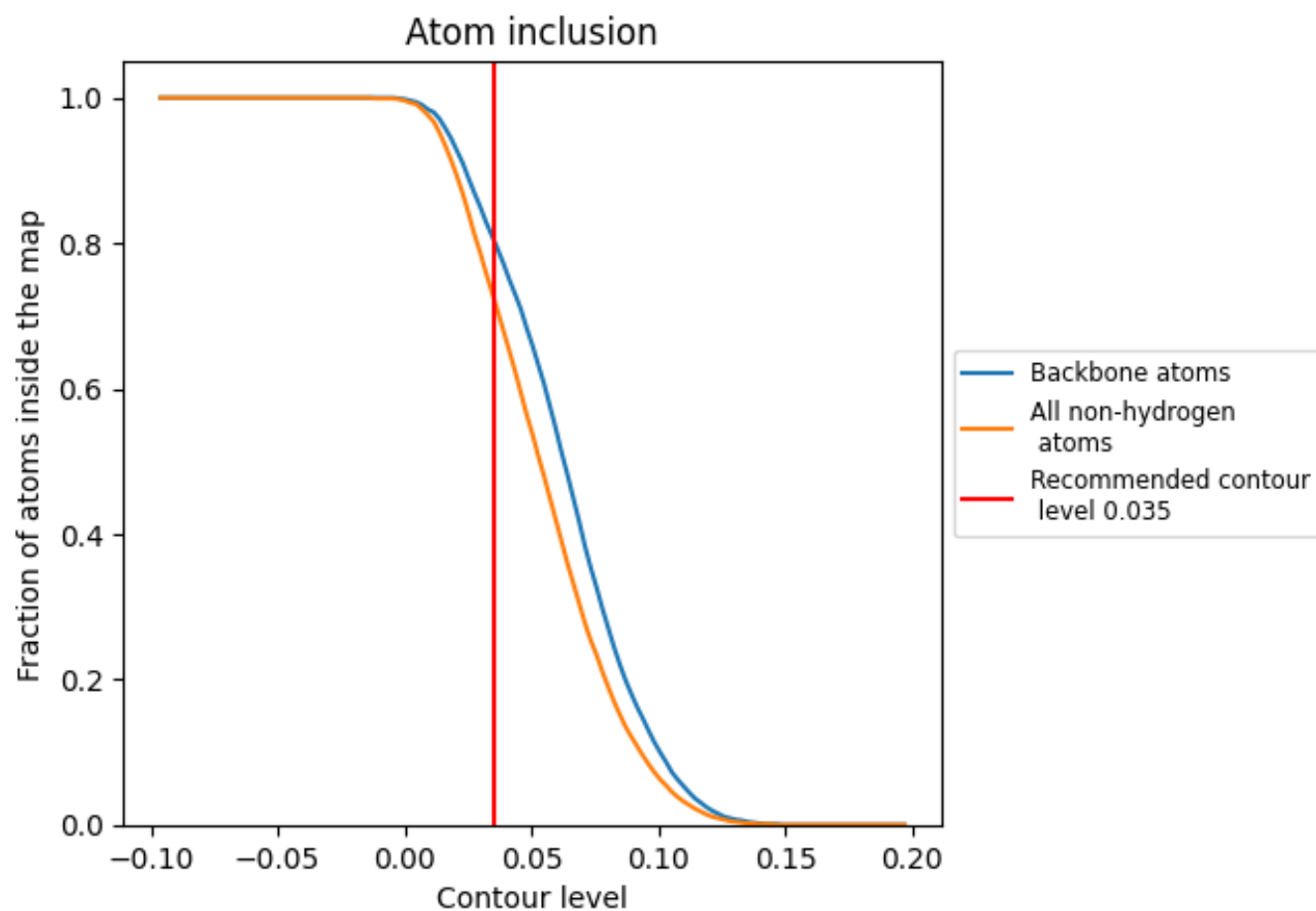
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.5540
A	0.7310	0.5560
B	0.7240	0.5520

