



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 02:49 pm BST

PDB ID : 9TAO / pdb_00009tao
EMDB ID : EMD-55753
Title : Local refinement of E. coli Complex I D79N NuoA mutant membrane domain in LMNG
Authors : Beghiah, A.; Kovalova, T.; Kaila, V.R.I.
Deposited on : 2025-11-18
Resolution : 2.61 Å(reported)

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

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

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:

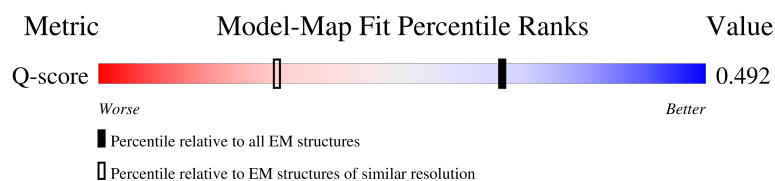
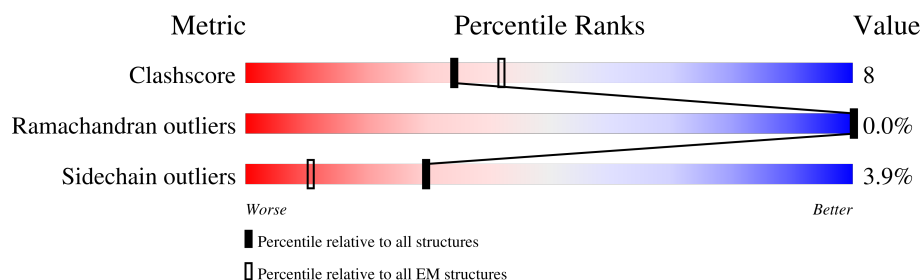
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.61 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	8735 (2.11 - 3.11)

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	H	325	
2	K	100	
3	L	613	
4	A	147	

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Mol	Chain	Length	Quality of chain
5	J	184	69% 19% • 11%
6	M	509	76% 22% ••
7	N	485	84% 16%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18764 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 NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	309	Total	C	N	O	S	0	0
			2421	1627	376	400	18		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	613	Total	C	N	O	S	0	0
			4685	3113	753	787	32		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	107	Total	C	N	O	S	0	0
			850	577	139	130	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASN	ASP	engineered mutation	UNP P0AFC3

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	163	Total	C	N	O	S	0	0
			1237	830	192	208	7		

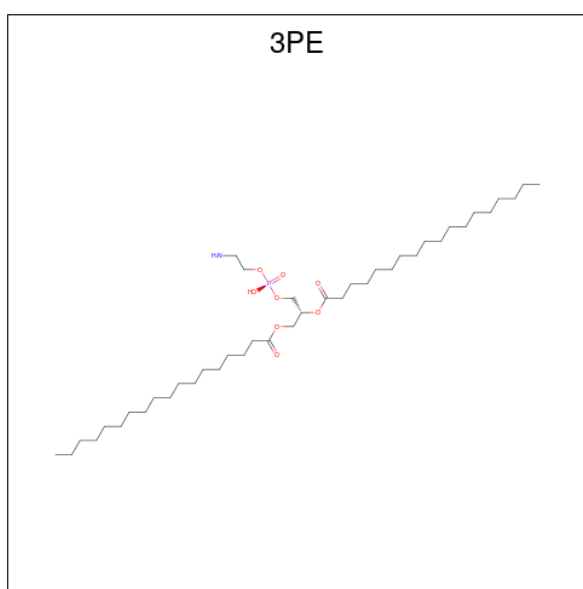
- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	504	Total	C	N	O	S	0	0
			3953	2661	617	646	29		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	485	Total	C	N	O	S	0	0
			3673	2448	582	623	20		

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



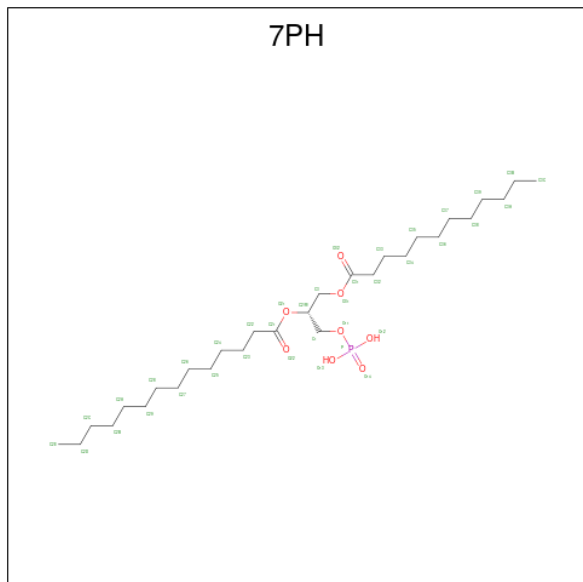
Mol	Chain	Residues	Atoms					AltConf
8	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	J	1	Total	C	N	O	P	0
			51	41	1	8	1	

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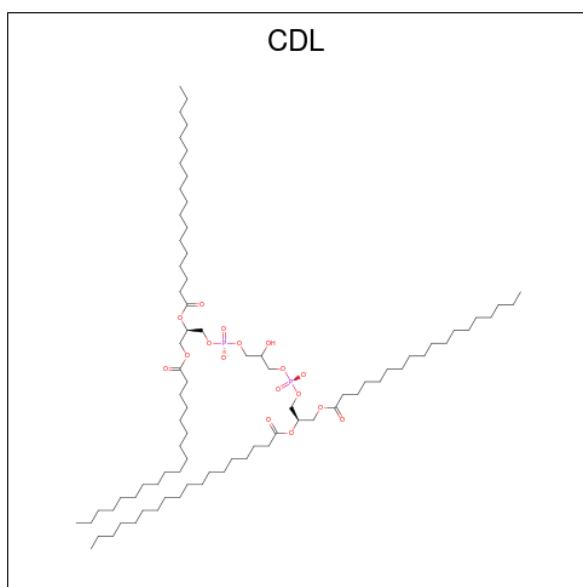
Mol	Chain	Residues	Atoms					AltConf
8	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 9 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



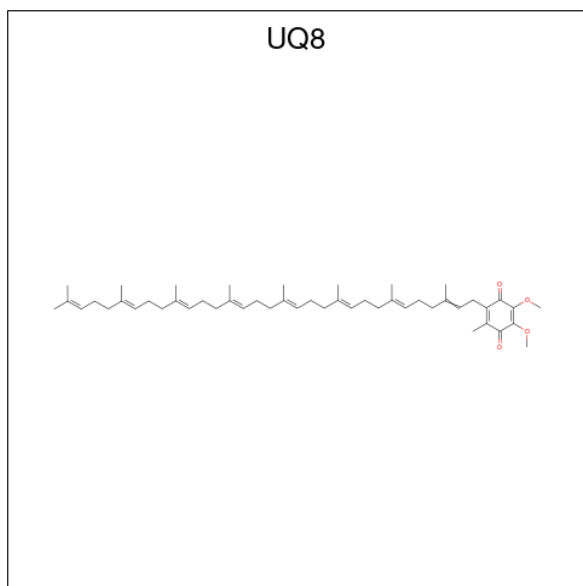
Mol	Chain	Residues	Atoms				AltConf
9	H	1	Total	C	O	P	0
			38	29	8	1	
9	J	1	Total	C	O	P	0
			38	29	8	1	
9	J	1	Total	C	O	P	0
			38	29	8	1	
9	M	1	Total	C	O	P	0
			38	29	8	1	
9	M	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	N	1	Total	C	O		0
			53	49	4		
11	N	1	Total	C	O		0
			53	49	4		

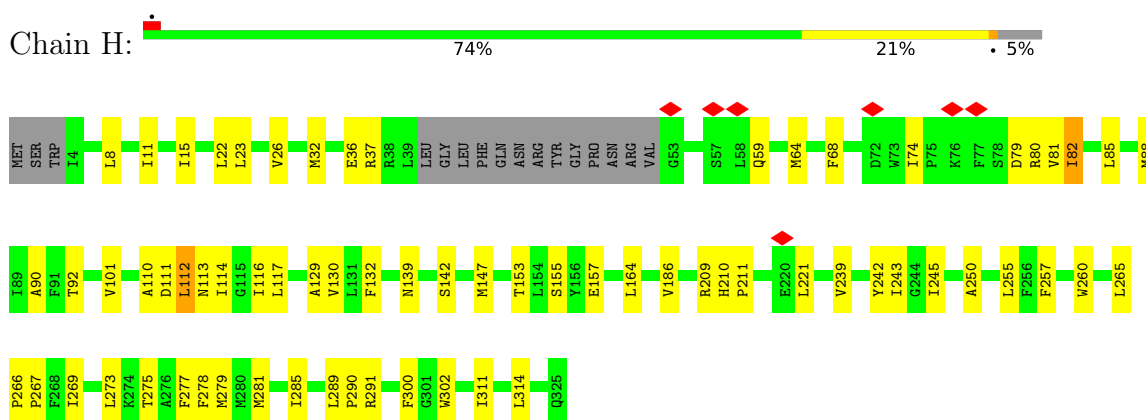
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	H	40	Total 40	O 40	0
12	K	15	Total 15	O 15	0
12	L	21	Total 21	O 21	0
12	A	9	Total 9	O 9	0
12	J	21	Total 21	O 21	0
12	M	12	Total 12	O 12	0
12	N	59	Total 59	O 59	0

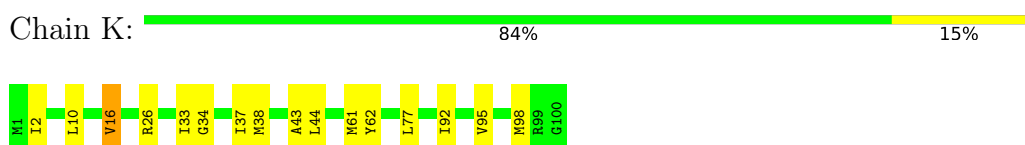
3 Residue-property plots

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

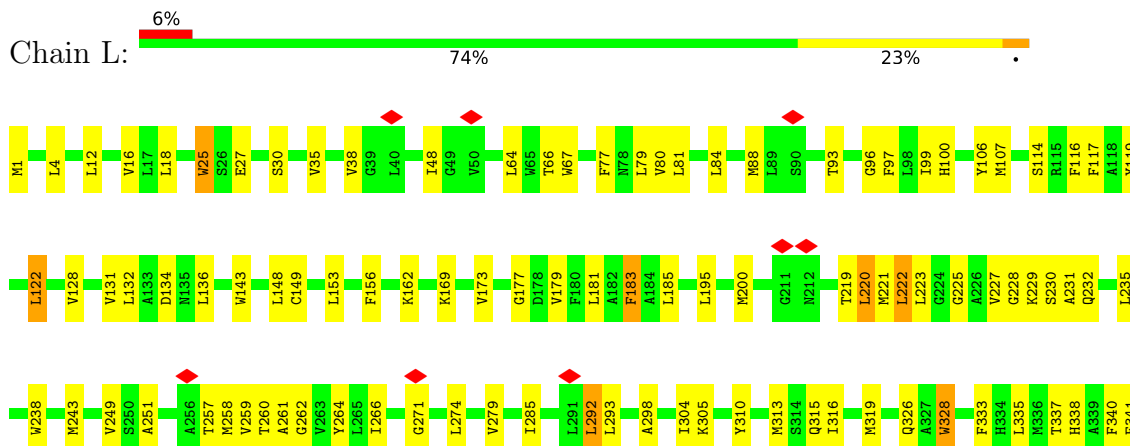
- Molecule 1: NADH-quinone oxidoreductase subunit H

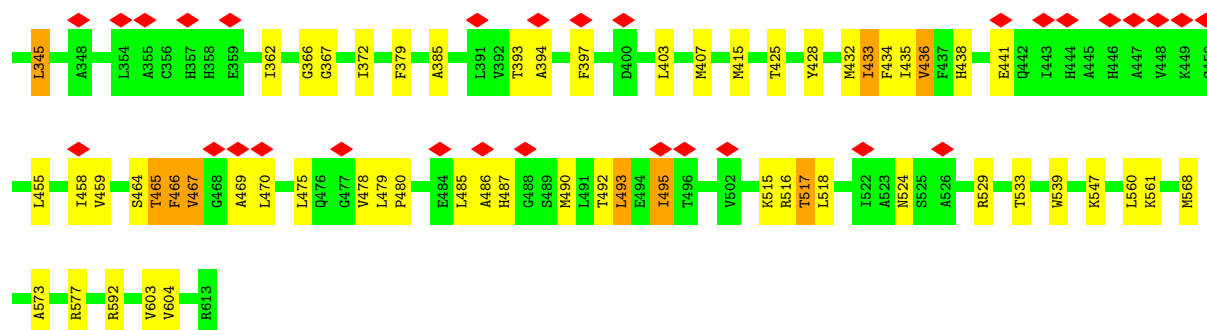


- Molecule 2: NADH-quinone oxidoreductase subunit K

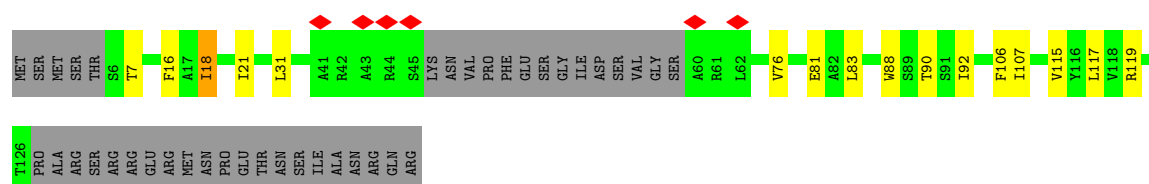


- Molecule 3: NADH-quinone oxidoreductase subunit L

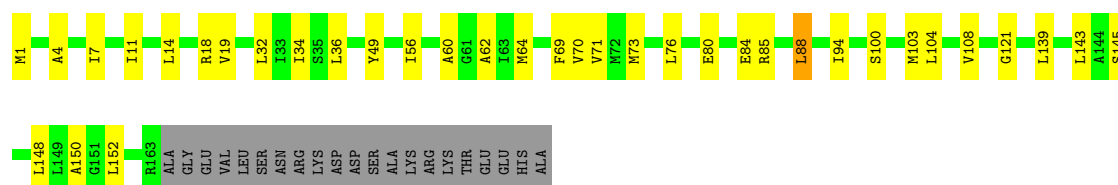




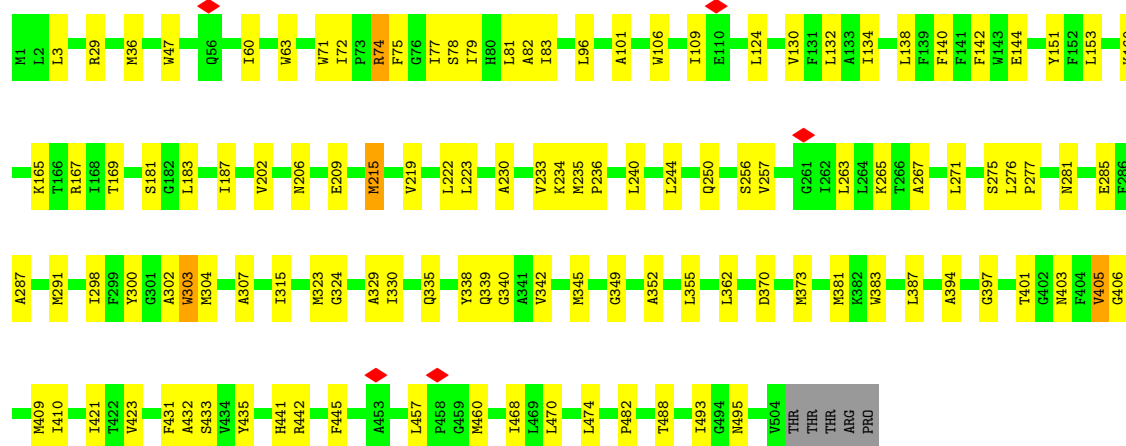
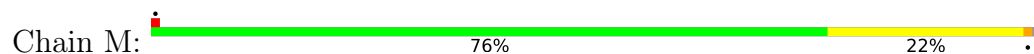
• Molecule 4: NADH-quinone oxidoreductase subunit A



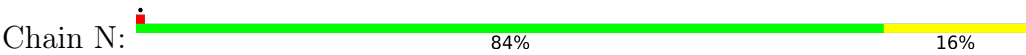
• Molecule 5: NADH-quinone oxidoreductase subunit J



• Molecule 6: NADH-quinone oxidoreductase subunit M



• Molecule 7: NADH-quinone oxidoreductase subunit N



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86927	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)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.925	Depositor
Minimum map value	-1.249	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	585.75, 585.75, 585.75	wwPDB
Map dimensions	710, 710, 710	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: UQ8, 7PH, CDL, 3PE

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	H	0.23	0/2491	0.37	0/3389
2	K	0.09	0/769	0.21	0/1040
3	L	0.31	0/4806	0.49	0/6549
4	A	0.14	0/874	0.25	0/1186
5	J	0.13	0/1263	0.26	0/1722
6	M	0.18	0/4074	0.34	0/5546
7	N	0.23	0/3764	0.41	0/5138
All	All	0.23	0/18041	0.39	0/24570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2421	0	2472	48	0
2	K	760	0	817	13	0
3	L	4685	0	4831	95	0
4	A	850	0	870	14	0
5	J	1237	0	1310	31	0
6	M	3953	0	4053	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	3673	0	3836	48	0
8	A	51	0	82	2	0
8	H	102	0	164	6	0
8	J	51	0	82	7	0
8	L	153	0	246	7	0
8	M	51	0	82	2	0
8	N	204	0	328	3	0
9	H	38	0	55	1	0
9	J	76	0	110	3	0
9	M	76	0	110	6	0
10	A	100	0	156	10	0
11	N	106	0	148	6	0
12	A	9	0	0	0	0
12	H	40	0	0	0	0
12	J	21	0	0	0	0
12	K	15	0	0	0	0
12	L	21	0	0	0	0
12	M	12	0	0	0	0
12	N	59	0	0	1	0
All	All	18764	0	19752	311	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 (311) 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)
3:L:219:THR:HA	3:L:222:LEU:HD23	1.59	0.84
3:L:230:SER:HB3	3:L:232:GLN:HE21	1.42	0.82
3:L:153:LEU:HB3	3:L:249:VAL:HG21	1.62	0.82
6:M:329:ALA:HB2	6:M:410:ILE:HG23	1.65	0.78
6:M:370:ASP:HB3	6:M:373:MET:HG2	1.63	0.77
3:L:229:LYS:HB3	3:L:261:ALA:HB3	1.66	0.76
6:M:36:MET:HE2	6:M:124:LEU:HD13	1.67	0.76
3:L:434:PHE:HA	3:L:438:HIS:HB2	1.69	0.75
3:L:293:LEU:HG	3:L:539:TRP:CD1	2.21	0.75
7:N:217:LYS:HB3	7:N:250:ILE:HD13	1.69	0.75
6:M:47:TRP:HE1	6:M:488:THR:HG21	1.52	0.74
1:H:15:ILE:HG23	4:A:18:ILE:HG21	1.68	0.73
1:H:37:ARG:HH22	1:H:59:GLN:HE21	1.38	0.72
3:L:394:ALA:HB2	3:L:466:PHE:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:403:LEU:HB3	3:L:493:LEU:HD11	1.74	0.69
2:K:16:VAL:HG13	5:J:100:SER:HB3	1.74	0.68
7:N:248:ILE:HG12	7:N:330:LEU:HD22	1.73	0.68
3:L:220:LEU:HA	3:L:223:LEU:HD12	1.76	0.67
6:M:315:ILE:HG12	6:M:355:LEU:HD12	1.78	0.66
6:M:72:ILE:HB	6:M:77:ILE:HB	1.76	0.66
1:H:113:ASN:HD22	5:J:49:TYR:HE2	1.44	0.66
1:H:289:LEU:HD12	1:H:290:PRO:HD2	1.78	0.66
1:H:275:THR:HG22	1:H:279:MET:HE3	1.76	0.65
6:M:432:ALA:HA	6:M:435:TYR:CE2	2.30	0.65
6:M:181:SER:HB3	6:M:230:ALA:HA	1.78	0.65
7:N:180:GLN:HG3	7:N:200:GLU:HG2	1.78	0.65
6:M:441:HIS:HA	6:M:445:PHE:HB2	1.79	0.64
3:L:337:THR:HG23	3:L:338:HIS:HD2	1.63	0.64
5:J:143:LEU:HD13	7:N:118:LEU:HD22	1.78	0.64
3:L:435:ILE:HG23	3:L:516:ARG:HH21	1.62	0.64
2:K:34:GLY:O	2:K:38:MET:HG3	1.97	0.64
5:J:150:ALA:HB2	7:N:111:ILE:HG21	1.81	0.63
2:K:16:VAL:HG21	5:J:104:LEU:HB2	1.81	0.63
6:M:387:LEU:HD13	6:M:468:ILE:HG21	1.81	0.62
4:A:21:ILE:HD11	8:A:202:3PE:H2E1	1.81	0.62
3:L:64:LEU:HB2	3:L:77:PHE:HB3	1.82	0.62
3:L:362:ILE:HG21	3:L:432:MET:HG3	1.81	0.62
1:H:210:HIS:CG	1:H:211:PRO:HA	2.34	0.62
5:J:34:ILE:HD11	9:J:203:7PH:H28A	1.81	0.62
6:M:236:PRO:HG3	6:M:244:LEU:HD22	1.82	0.62
3:L:183:PHE:HB3	3:L:221:MET:SD	2.40	0.61
3:L:106:TYR:HE2	3:L:107:MET:HE2	1.65	0.61
5:J:4:ALA:HB2	8:J:201:3PE:H352	1.82	0.61
3:L:84:LEU:HD13	3:L:475:LEU:HD21	1.82	0.61
3:L:328:TRP:HB3	3:L:479:LEU:HD11	1.83	0.60
3:L:84:LEU:O	3:L:88:MET:HG2	2.01	0.60
3:L:333:PHE:HZ	3:L:469:ALA:HA	1.66	0.60
1:H:314:LEU:HD13	4:A:107:ILE:HD12	1.83	0.59
3:L:259:VAL:HG22	3:L:316:ILE:HD13	1.83	0.59
3:L:367:GLY:HA3	3:L:441:GLU:HA	1.83	0.59
5:J:85:ARG:HB3	5:J:88:LEU:HD23	1.84	0.59
6:M:281:ASN:O	6:M:285:GLU:HG2	2.02	0.59
6:M:339:GLN:HG2	6:M:493:ILE:HG21	1.84	0.59
7:N:89:THR:HG21	7:N:456:VAL:HG21	1.84	0.59
7:N:124:HIS:HD2	7:N:126:ALA:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:298:ALA:HB2	3:L:310:TYR:HB3	1.86	0.58
3:L:492:THR:HA	3:L:495:ILE:HB	1.86	0.58
6:M:29:ARG:NH1	6:M:106:TRP:O	2.37	0.58
7:N:248:ILE:HD11	7:N:334:LEU:HB2	1.86	0.58
6:M:406:GLY:O	6:M:410:ILE:HG13	2.03	0.58
7:N:421:GLY:HA2	7:N:424:TYR:CE2	2.39	0.57
6:M:291:MET:HB3	6:M:421:ILE:HG21	1.85	0.57
6:M:381:MET:HE3	6:M:457:LEU:HD13	1.85	0.57
1:H:155:SER:HG	1:H:302:TRP:CD1	2.23	0.57
6:M:79:ILE:HA	6:M:138:LEU:HD22	1.86	0.57
5:J:56:ILE:HA	5:J:60:ALA:HB3	1.86	0.57
7:N:77:THR:HG23	7:N:117:ILE:HG12	1.87	0.57
7:N:9:ILE:HD12	7:N:9:ILE:H	1.69	0.57
3:L:604:VAL:HG21	8:L:703:3PE:H2H2	1.86	0.56
3:L:219:THR:HG21	3:L:279:VAL:HG21	1.86	0.56
3:L:524:ASN:O	3:L:529:ARG:NH2	2.38	0.56
4:A:115:VAL:HG22	10:A:201:CDL:H511	1.87	0.56
6:M:263:LEU:HD21	6:M:352:ALA:HB3	1.88	0.56
3:L:455:LEU:O	3:L:459:VAL:HG13	2.05	0.56
3:L:366:GLY:HA2	3:L:436:VAL:HA	1.87	0.56
8:L:703:3PE:H2H1	8:N:504:3PE:H3A1	1.86	0.56
6:M:74:ARG:HG3	7:N:475:ILE:HG21	1.88	0.55
3:L:385:ALA:HA	3:L:393:THR:HG21	1.87	0.55
6:M:187:ILE:HD11	7:N:415:VAL:HG21	1.88	0.55
6:M:215:MET:HE1	6:M:223:LEU:HD12	1.88	0.55
3:L:136:LEU:HD12	3:L:185:LEU:HD11	1.89	0.55
1:H:82:ILE:HG23	1:H:132:PHE:HB3	1.89	0.55
6:M:234:LYS:HB3	6:M:267:ALA:HB2	1.88	0.55
7:N:47:ALA:HB2	11:N:505:UQ8:H20B	1.88	0.54
1:H:36:GLU:OE2	1:H:209:ARG:NH1	2.32	0.54
7:N:70:ASP:OD1	7:N:256:ARG:NH2	2.41	0.54
1:H:111:ASP:HB2	8:H:401:3PE:H112	1.88	0.54
1:H:265:LEU:HD12	1:H:266:PRO:HD2	1.89	0.54
3:L:96:GLY:O	3:L:99:ILE:HG22	2.07	0.54
6:M:151:TYR:CE2	7:N:426:LEU:HD12	2.43	0.54
5:J:150:ALA:HB2	7:N:111:ILE:HD13	1.89	0.53
1:H:32:MET:HG2	1:H:242:TYR:HD2	1.71	0.53
3:L:119:TYR:HB3	3:L:153:LEU:HG	1.91	0.53
3:L:561:LYS:HD2	6:M:307:ALA:HB1	1.90	0.53
1:H:74:ILE:HD12	1:H:80:ARG:HG2	1.91	0.52
7:N:170:LEU:HD12	7:N:210:MET:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:ARG:HH22	1:H:59:GLN:NE2	2.06	0.52
1:H:110:ALA:HB2	4:A:16:PHE:HB2	1.91	0.52
1:H:164:LEU:HD22	1:H:255:LEU:HD13	1.92	0.52
6:M:144:GLU:HB2	7:N:387:PRO:HG2	1.91	0.52
3:L:425:THR:HA	3:L:428:TYR:CE2	2.44	0.52
3:L:466:PHE:O	3:L:470:LEU:HG	2.10	0.52
3:L:18:LEU:HD21	3:L:117:PHE:HB3	1.91	0.51
1:H:139:ASN:HB3	1:H:142:SER:HB2	1.93	0.51
4:A:76:VAL:HG22	5:J:62:ALA:HB1	1.92	0.51
3:L:603:VAL:HG22	5:J:103:MET:HB2	1.93	0.51
7:N:1:MET:HE3	7:N:65:PRO:HG3	1.91	0.51
3:L:4:LEU:HD21	3:L:81:LEU:HD22	1.93	0.51
3:L:333:PHE:CZ	3:L:469:ALA:HA	2.45	0.51
7:N:446:SER:O	11:N:506:UQ8:H43	2.10	0.51
3:L:407:MET:HE2	3:L:407:MET:HA	1.92	0.51
3:L:407:MET:HE3	3:L:415:MET:HB2	1.93	0.51
2:K:77:LEU:HD22	5:J:70:VAL:HG11	1.92	0.51
6:M:187:ILE:HD11	7:N:415:VAL:CG2	2.41	0.51
1:H:112:LEU:HD11	8:H:401:3PE:H322	1.91	0.51
1:H:311:ILE:HG12	10:A:201:CDL:H621	1.93	0.51
7:N:482:MET:HE2	7:N:482:MET:HA	1.94	0.50
3:L:529:ARG:O	3:L:533:THR:HG22	2.12	0.50
6:M:340:GLY:HA3	6:M:409:MET:HB2	1.94	0.50
2:K:2:ILE:HD12	5:J:1:MET:HE3	1.93	0.50
6:M:235:MET:HG2	6:M:323:MET:HG3	1.93	0.50
6:M:470:LEU:O	6:M:474:LEU:HG	2.12	0.50
7:N:98:TYR:CE2	7:N:100:ASP:HB3	2.46	0.50
7:N:339:GLY:HA3	7:N:379:MET:HE2	1.94	0.50
3:L:271:GLY:HA2	3:L:274:LEU:HB2	1.93	0.50
6:M:3:LEU:HD11	6:M:83:ILE:HG13	1.94	0.50
1:H:269:ILE:O	1:H:273:LEU:HG	2.12	0.49
3:L:466:PHE:O	3:L:467:VAL:C	2.54	0.49
3:L:235:LEU:HD21	8:M:601:3PE:H2C2	1.94	0.49
8:L:701:3PE:H222	7:N:423:TYR:CE1	2.47	0.49
4:A:88:TRP:O	4:A:92:ILE:HG13	2.12	0.49
6:M:206:ASN:HB3	6:M:209:GLU:HG2	1.94	0.49
5:J:80:GLU:O	5:J:84:GLU:HG3	2.12	0.49
3:L:515:LYS:HG3	3:L:517:THR:HG23	1.94	0.49
2:K:33:ILE:HG23	5:J:32:LEU:HD22	1.93	0.49
3:L:313:MET:O	3:L:316:ILE:HG22	2.13	0.49
1:H:36:GLU:OE2	1:H:242:TYR:OH	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:THR:O	1:H:157:GLU:HB2	2.13	0.49
1:H:311:ILE:HD13	10:A:201:CDL:H221	1.95	0.49
3:L:169:LYS:O	3:L:173:VAL:HG23	2.13	0.49
6:M:287:ALA:O	6:M:291:MET:HG3	2.12	0.48
3:L:560:LEU:HD22	6:M:303:TRP:HB3	1.95	0.48
4:A:88:TRP:CE2	4:A:92:ILE:HG12	2.48	0.48
7:N:277:ALA:HB2	7:N:310:LEU:HD23	1.95	0.48
1:H:101:VAL:HG11	1:H:250:ALA:HB1	1.94	0.48
6:M:342:VAL:O	6:M:345:MET:HG2	2.14	0.48
3:L:337:THR:HA	3:L:340:PHE:CZ	2.49	0.48
3:L:433:ILE:C	3:L:435:ILE:H	2.21	0.48
8:L:703:3PE:H3F1	7:N:412:GLY:HA3	1.96	0.48
1:H:85:LEU:HD12	1:H:88:MET:HE3	1.95	0.48
6:M:276:LEU:HB2	6:M:277:PRO:HD3	1.95	0.48
5:J:1:MET:HE1	5:J:121:GLY:HA3	1.95	0.47
6:M:101:ALA:HB1	6:M:256:SER:HB3	1.95	0.47
3:L:177:GLY:O	3:L:225:GLY:HA2	2.14	0.47
6:M:72:ILE:HD12	6:M:77:ILE:HG21	1.96	0.47
6:M:300:TYR:O	6:M:304:MET:HG2	2.13	0.47
3:L:292:LEU:HD13	3:L:292:LEU:HA	1.72	0.47
6:M:302:ALA:HB1	6:M:431:PHE:HB3	1.96	0.47
3:L:455:LEU:O	3:L:458:ILE:HG13	2.13	0.47
3:L:128:VAL:HA	3:L:131:VAL:HG22	1.96	0.47
3:L:243:MET:HE2	3:L:243:MET:HA	1.95	0.47
5:J:11:ILE:HG21	8:J:201:3PE:H2F2	1.96	0.47
6:M:263:LEU:HD22	6:M:349:GLY:HA2	1.97	0.47
11:N:506:UQ8:H7	11:N:506:UQ8:H10	1.42	0.47
6:M:338:TYR:HB3	6:M:493:ILE:HD12	1.97	0.47
1:H:147:MET:HE2	5:J:73:MET:HG3	1.96	0.47
6:M:130:VAL:HG23	6:M:142:PHE:HB3	1.97	0.47
8:H:401:3PE:H352	8:J:201:3PE:H2A2	1.97	0.47
3:L:1:MET:HA	3:L:48:ILE:HG23	1.97	0.47
3:L:136:LEU:HB2	3:L:195:LEU:HB3	1.96	0.47
3:L:326:GLN:HE22	3:L:480:PRO:HB2	1.79	0.47
1:H:74:ILE:HG21	1:H:80:ARG:HE	1.80	0.47
3:L:122:LEU:HB3	3:L:149:CYS:SG	2.55	0.47
5:J:34:ILE:HG12	8:J:201:3PE:H2I2	1.97	0.47
7:N:82:LEU:HD22	11:N:506:UQ8:H10A	1.96	0.47
5:J:104:LEU:O	5:J:108:VAL:HG13	2.15	0.47
5:J:139:LEU:HD13	7:N:67:MET:SD	2.54	0.47
3:L:573:ALA:HB2	8:L:701:3PE:H381	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:160:LYS:HE2	6:M:160:LYS:HB2	1.56	0.46
6:M:394:ALA:HB2	6:M:401:THR:HG21	1.98	0.46
8:N:502:3PE:H362	8:N:502:3PE:H3C1	1.97	0.46
6:M:63:TRP:CD2	6:M:82:ALA:HB1	2.51	0.46
3:L:106:TYR:CE2	3:L:107:MET:HE2	2.48	0.46
4:A:106:PHE:CE1	5:J:145:SER:HB3	2.51	0.46
2:K:37:ILE:HD11	5:J:19:VAL:HG11	1.98	0.46
3:L:143:TRP:CZ2	3:L:229:LYS:HB2	2.51	0.46
1:H:11:ILE:O	1:H:15:ILE:HG13	2.15	0.46
1:H:22:LEU:O	1:H:26:VAL:HG23	2.15	0.46
6:M:219:VAL:HG22	9:M:603:7PH:C21	2.46	0.46
1:H:210:HIS:CD2	1:H:211:PRO:HA	2.51	0.46
4:A:117:LEU:HD11	5:J:152:LEU:HD11	1.98	0.46
1:H:32:MET:SD	1:H:279:MET:HG2	2.56	0.45
1:H:114:ILE:HB	1:H:117:LEU:HB2	1.96	0.45
6:M:183:LEU:O	6:M:187:ILE:HG13	2.16	0.45
9:M:602:7PH:H26	9:M:602:7PH:H23A	1.56	0.45
6:M:383:TRP:HB2	6:M:460:MET:SD	2.56	0.45
7:N:73:ALA:HB1	7:N:121:ASN:OD1	2.17	0.45
1:H:64:MET:HE2	1:H:68:PHE:HE2	1.82	0.45
6:M:222:LEU:HB3	9:M:603:7PH:H25A	1.98	0.45
6:M:298:ILE:HG13	6:M:324:GLY:HA3	1.99	0.45
3:L:333:PHE:HZ	3:L:469:ALA:CA	2.30	0.45
4:A:81:GLU:HG3	5:J:148:LEU:HD13	1.98	0.45
4:A:119:ARG:NH1	10:A:201:CDL:OB4	2.50	0.45
9:M:603:7PH:H23	7:N:408:TRP:CZ2	2.52	0.45
1:H:15:ILE:HD13	4:A:18:ILE:HG12	1.97	0.44
3:L:162:LYS:HE3	3:L:162:LYS:HB2	1.55	0.44
10:A:201:CDL:H191	10:A:201:CDL:H241	1.99	0.44
6:M:165:LYS:HA	6:M:165:LYS:HD3	1.63	0.44
6:M:167:ARG:HA	6:M:250:GLN:HG3	1.99	0.44
7:N:68:ARG:HD3	7:N:484:LEU:HB3	1.98	0.44
1:H:210:HIS:NE2	1:H:291:ARG:HB3	2.33	0.44
8:H:401:3PE:H262	8:J:201:3PE:H252	1.98	0.44
3:L:231:ALA:HB2	3:L:238:TRP:NE1	2.32	0.44
7:N:251:PHE:CZ	7:N:309:LEU:HB3	2.53	0.44
8:N:501:3PE:H2H1	8:N:501:3PE:H3C2	1.98	0.44
3:L:38:VAL:HG21	3:L:100:HIS:CD2	2.52	0.44
3:L:181:LEU:HB2	3:L:225:GLY:HA3	1.98	0.44
7:N:321:MET:HG2	7:N:404:GLN:HE22	1.83	0.44
11:N:505:UQ8:H10	11:N:505:UQ8:H7A	1.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:TRP:HB2	1:H:267:PRO:HB2	1.99	0.44
3:L:116:PHE:HB2	3:L:156:PHE:CE1	2.53	0.44
3:L:177:GLY:HA3	3:L:228:GLY:HA3	1.99	0.44
7:N:162:LEU:HB3	7:N:216:PHE:CE1	2.53	0.44
3:L:88:MET:HE1	3:L:264:TYR:CE1	2.53	0.44
9:J:202:7PH:H39	9:J:202:7PH:H36	1.77	0.44
6:M:234:LYS:HB2	6:M:234:LYS:HE3	1.75	0.44
6:M:235:MET:HB3	6:M:267:ALA:HB3	2.00	0.44
2:K:77:LEU:HB3	5:J:70:VAL:HG21	1.99	0.44
7:N:61:MET:HE2	7:N:61:MET:HB3	1.90	0.44
6:M:397:GLY:HA2	6:M:403:ASN:HB2	2.00	0.44
3:L:183:PHE:CZ	6:M:423:VAL:HA	2.53	0.43
10:A:201:CDL:H771	10:A:201:CDL:H742	1.52	0.43
3:L:80:VAL:HB	3:L:134:ASP:HB3	2.00	0.43
10:A:201:CDL:H202	10:A:201:CDL:H171	1.57	0.43
6:M:60:ILE:HG13	6:M:495:ASN:HB3	2.00	0.43
6:M:71:TRP:H	6:M:78:SER:HA	1.83	0.43
6:M:140:PHE:HE2	7:N:392:PHE:CZ	2.36	0.43
9:M:603:7PH:H32	9:M:603:7PH:H3	1.73	0.43
1:H:242:TYR:HA	1:H:245:ILE:HG22	1.99	0.43
8:H:401:3PE:H2B2	8:J:201:3PE:H3D2	2.00	0.43
6:M:3:LEU:HG	6:M:83:ILE:HD11	2.00	0.43
6:M:271:LEU:HD22	6:M:330:ILE:HG21	1.99	0.43
9:M:602:7PH:H27A	9:M:602:7PH:H2A	1.76	0.43
6:M:81:LEU:HD13	6:M:132:LEU:HD23	2.01	0.43
4:A:31:LEU:HD23	4:A:31:LEU:HA	1.82	0.43
3:L:285:ILE:HD12	3:L:285:ILE:HA	1.85	0.43
1:H:257:PHE:CE1	1:H:278:PHE:HZ	2.37	0.43
2:K:98:MET:HB3	7:N:296:ARG:HH12	1.84	0.43
10:A:201:CDL:H772	10:A:201:CDL:H801	1.50	0.43
6:M:153:LEU:HD13	6:M:257:VAL:HG22	2.01	0.43
6:M:362:LEU:HD12	6:M:381:MET:HE1	1.99	0.43
6:M:442:ARG:HE	8:M:601:3PE:H111	1.83	0.43
8:A:202:3PE:H3B1	5:J:7:ILE:HG21	2.01	0.42
7:N:200:GLU:HG3	7:N:203:LEU:H	1.84	0.42
1:H:80:ARG:O	1:H:81:VAL:C	2.62	0.42
6:M:470:LEU:HD12	6:M:470:LEU:HA	1.89	0.42
3:L:262:GLY:O	3:L:266:ILE:HG12	2.19	0.42
6:M:271:LEU:HA	6:M:275:SER:HB3	2.01	0.42
6:M:405:VAL:HG21	6:M:482:PRO:HG3	2.01	0.42
7:N:33:ASN:O	7:N:34:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:465:THR:C	3:L:467:VAL:H	2.28	0.42
9:J:202:7PH:H39A	9:J:202:7PH:H2CA	2.01	0.42
7:N:217:LYS:HA	7:N:217:LYS:HD3	1.91	0.42
2:K:92:ILE:HD12	2:K:92:ILE:HA	1.88	0.42
9:H:403:7PH:H22	9:H:403:7PH:H2	1.76	0.42
3:L:99:ILE:HD11	3:L:251:ALA:HB3	2.02	0.42
3:L:305:LYS:HA	3:L:305:LYS:HD3	1.73	0.42
5:J:71:VAL:O	5:J:76:LEU:HB2	2.20	0.42
7:N:308:TYR:CD1	7:N:414:VAL:HG22	2.55	0.42
1:H:300:PHE:HB2	10:A:201:CDL:H332	2.02	0.41
3:L:35:VAL:HG13	3:L:97:PHE:HE1	1.84	0.41
8:L:701:3PE:H322	8:L:701:3PE:H352	1.86	0.41
6:M:338:TYR:HB2	6:M:493:ILE:HG23	2.02	0.41
2:K:43:ALA:HB1	2:K:62:TYR:CD1	2.55	0.41
7:N:444:ALA:N	7:N:445:PRO:HD3	2.35	0.41
3:L:67:TRP:HB2	3:L:77:PHE:HD1	1.85	0.41
2:K:26:ARG:HA	3:L:592:ARG:HD3	2.01	0.41
3:L:341:PHE:O	3:L:345:LEU:HD12	2.20	0.41
3:L:568:MET:HE3	3:L:568:MET:HB2	1.90	0.41
7:N:100:ASP:CG	7:N:101:ASN:H	2.28	0.41
7:N:267:GLU:HG3	12:N:652:HOH:O	2.20	0.41
3:L:257:THR:O	3:L:258:MET:HB3	2.20	0.41
3:L:397:PHE:HB2	3:L:469:ALA:HB2	2.03	0.41
5:J:14:LEU:O	5:J:18:ARG:HG2	2.21	0.41
11:N:505:UQ8:H17	11:N:505:UQ8:H20	1.67	0.41
3:L:487:HIS:O	3:L:490:MET:HG3	2.20	0.41
2:K:61:MET:HE3	2:K:61:MET:HB3	1.91	0.41
3:L:25:TRP:CD1	3:L:30:SER:HG	2.39	0.41
3:L:316:ILE:HD12	3:L:319:MET:HE1	2.02	0.41
1:H:79:ASP:OD1	1:H:81:VAL:HB	2.21	0.41
3:L:260:THR:HB	3:L:335:LEU:HD11	2.01	0.41
3:L:577:ARG:HD3	8:L:701:3PE:C21	2.50	0.41
6:M:335:GLN:HG2	6:M:493:ILE:HG22	2.02	0.41
3:L:394:ALA:CB	3:L:466:PHE:HA	2.43	0.41
10:A:201:CDL:H121	10:A:201:CDL:HB32	2.02	0.41
7:N:142:LEU:O	7:N:238:VAL:HG21	2.21	0.41
1:H:90:ALA:HB2	1:H:129:ALA:HB1	2.03	0.40
1:H:281:MET:O	1:H:285:ILE:HG23	2.20	0.40
6:M:233:VAL:HG23	6:M:240:LEU:HD13	2.03	0.40
3:L:485:LEU:HD23	3:L:486:ALA:N	2.36	0.40
8:J:201:3PE:H262	8:J:201:3PE:H291	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ILE:HD12	1:H:116:ILE:HA	1.96	0.40
1:H:277:PHE:O	1:H:281:MET:HG2	2.21	0.40
3:L:12:LEU:O	3:L:16:VAL:HG13	2.21	0.40
5:J:32:LEU:O	5:J:36:LEU:HG	2.22	0.40
6:M:134:ILE:HD12	6:M:134:ILE:HA	1.93	0.40
1:H:239:VAL:O	1:H:243:ILE:HG13	2.22	0.40
3:L:79:LEU:HG	3:L:132:LEU:HB3	2.02	0.40
1:H:92:THR:HB	8:H:401:3PE:H3G1	2.03	0.40
3:L:475:LEU:HD23	3:L:478:VAL:HG23	2.02	0.40
7:N:130:LEU:HD12	7:N:130:LEU:HA	1.95	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	H	305/325 (94%)	294 (96%)	11 (4%)	0	100	100
2	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	L	611/613 (100%)	569 (93%)	42 (7%)	0	100	100
4	A	103/147 (70%)	102 (99%)	1 (1%)	0	100	100
5	J	161/184 (88%)	159 (99%)	2 (1%)	0	100	100
6	M	502/509 (99%)	485 (97%)	17 (3%)	0	100	100
7	N	483/485 (100%)	472 (98%)	10 (2%)	1 (0%)	43	64
All	All	2263/2363 (96%)	2177 (96%)	85 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	349	SER

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	H	255/269 (95%)	248 (97%)	7 (3%)	39	65
2	K	79/79 (100%)	75 (95%)	4 (5%)	21	43
3	L	485/485 (100%)	454 (94%)	31 (6%)	16	33
4	A	83/119 (70%)	79 (95%)	4 (5%)	23	45
5	J	129/146 (88%)	125 (97%)	4 (3%)	35	61
6	M	413/418 (99%)	402 (97%)	11 (3%)	39	65
7	N	385/385 (100%)	374 (97%)	11 (3%)	37	63
All	All	1829/1901 (96%)	1757 (96%)	72 (4%)	30	53

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	8	LEU
1	H	23	LEU
1	H	82	ILE
1	H	112	LEU
1	H	130	VAL
1	H	186	VAL
1	H	221	LEU
2	K	10	LEU
2	K	16	VAL
2	K	44	LEU
2	K	95	VAL
3	L	25	TRP
3	L	27	GLU
3	L	66	THR
3	L	93	THR
3	L	114	SER
3	L	122	LEU
3	L	148	LEU
3	L	179	VAL
3	L	183	PHE

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Mol	Chain	Res	Type
3	L	200	MET
3	L	220	LEU
3	L	222	LEU
3	L	227	VAL
3	L	292	LEU
3	L	304	ILE
3	L	315	GLN
3	L	328	TRP
3	L	345	LEU
3	L	372	ILE
3	L	379	PHE
3	L	433	ILE
3	L	436	VAL
3	L	464	SER
3	L	465	THR
3	L	466	PHE
3	L	467	VAL
3	L	493	LEU
3	L	495	ILE
3	L	517	THR
3	L	518	LEU
3	L	547	LYS
4	A	7	THR
4	A	18	ILE
4	A	83	LEU
4	A	90	THR
5	J	64	MET
5	J	69	PHE
5	J	88	LEU
5	J	94	ILE
6	M	74	ARG
6	M	75	PHE
6	M	96	LEU
6	M	109	ILE
6	M	169	THR
6	M	202	VAL
6	M	215	MET
6	M	265	LYS
6	M	303	TRP
6	M	405	VAL
6	M	433	SER
7	N	4	THR

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Mol	Chain	Res	Type
7	N	62	ASP
7	N	103	ASP
7	N	193	LEU
7	N	195	ASP
7	N	324	GLU
7	N	358	SER
7	N	369	ARG
7	N	430	VAL
7	N	457	VAL
7	N	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	59	GLN
1	H	113	ASN
1	H	152	GLN
1	H	208	HIS
3	L	78	ASN
3	L	212	ASN
3	L	281	HIS
3	L	315	GLN
3	L	326	GLN
3	L	361	ASN
3	L	409	ASN
3	L	411	HIS
4	A	13	HIS
6	M	281	ASN
6	M	403	ASN
7	N	149	GLN
7	N	291	GLN
7	N	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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$
8	3PE	N	504	-	50,50,50	0.51	0	53,55,55	0.52	1 (1%)
10	CDL	A	201	-	99,99,99	0.29	0	105,111,111	0.19	0
8	3PE	L	701	-	50,50,50	0.51	0	53,55,55	0.52	1 (1%)
9	7PH	J	203	-	37,37,37	1.39	3 (8%)	41,42,42	1.20	4 (9%)
9	7PH	M	603	-	37,37,37	1.39	3 (8%)	41,42,42	1.20	3 (7%)
8	3PE	M	601	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
8	3PE	J	201	-	50,50,50	0.51	0	53,55,55	0.52	1 (1%)
9	7PH	J	202	-	37,37,37	1.39	3 (8%)	41,42,42	1.22	3 (7%)
8	3PE	A	202	-	50,50,50	0.51	0	53,55,55	0.51	1 (1%)
9	7PH	H	403	-	37,37,37	1.40	3 (8%)	41,42,42	1.20	3 (7%)
8	3PE	N	503	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
8	3PE	L	702	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
8	3PE	H	401	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
8	3PE	N	502	-	50,50,50	0.52	0	53,55,55	0.51	1 (1%)
11	UQ8	N	506	-	53,53,53	0.68	0	64,67,67	1.63	12 (18%)
11	UQ8	N	505	-	53,53,53	0.68	0	64,67,67	1.64	11 (17%)
8	3PE	H	402	-	50,50,50	0.51	0	53,55,55	0.52	1 (1%)
8	3PE	N	501	-	50,50,50	0.51	0	53,55,55	0.57	2 (3%)
9	7PH	M	602	-	37,37,37	1.39	3 (8%)	41,42,42	1.21	4 (9%)
8	3PE	L	703	-	50,50,50	0.52	0	53,55,55	0.50	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
8	3PE	N	504	-	-	5/54/54/54	-
10	CDL	A	201	-	-	72/110/110/110	-
8	3PE	L	701	-	-	12/54/54/54	-
9	7PH	J	203	-	-	22/39/39/39	-
9	7PH	M	603	-	-	20/39/39/39	-
8	3PE	M	601	-	-	8/54/54/54	-
8	3PE	J	201	-	-	17/54/54/54	-
9	7PH	J	202	-	-	22/39/39/39	-
8	3PE	A	202	-	-	8/54/54/54	-
9	7PH	H	403	-	-	22/39/39/39	-
8	3PE	N	503	-	-	7/54/54/54	-
8	3PE	L	702	-	-	9/54/54/54	-
8	3PE	H	401	-	-	20/54/54/54	-
8	3PE	N	502	-	-	16/54/54/54	-
11	UQ8	N	506	-	-	9/51/75/75	0/1/1/1
11	UQ8	N	505	-	-	14/51/75/75	0/1/1/1
8	3PE	H	402	-	-	10/54/54/54	-
8	3PE	N	501	-	-	14/54/54/54	-
9	7PH	M	602	-	-	22/39/39/39	-
8	3PE	L	703	-	-	10/54/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	403	7PH	P-O11	7.14	1.83	1.60
9	J	203	7PH	P-O11	7.12	1.83	1.60
9	J	202	7PH	P-O11	7.11	1.83	1.60
9	M	603	7PH	P-O11	7.09	1.83	1.60
9	M	602	7PH	P-O11	7.08	1.83	1.60
9	M	602	7PH	O11-C1	-2.66	1.34	1.44
9	H	403	7PH	O11-C1	-2.66	1.34	1.44
9	J	202	7PH	O11-C1	-2.65	1.34	1.44
9	J	203	7PH	O11-C1	-2.65	1.34	1.44
9	M	603	7PH	O11-C1	-2.64	1.34	1.44
9	J	202	7PH	C1-C2	2.11	1.57	1.50
9	J	203	7PH	C1-C2	2.06	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	403	7PH	C1-C2	2.06	1.57	1.50
9	M	602	7PH	C1-C2	2.04	1.56	1.50
9	M	603	7PH	C1-C2	2.02	1.56	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	505	UQ8	C7-C8-C9	-6.28	116.33	126.79
11	N	506	UQ8	C7-C8-C9	-6.18	116.51	126.79
11	N	505	UQ8	C6-C1-C2	4.64	122.85	119.18
11	N	506	UQ8	C6-C1-C2	4.44	122.69	119.18
11	N	505	UQ8	C17-C18-C19	-3.16	120.06	127.66
11	N	505	UQ8	C1-C6-C5	3.13	122.54	119.58
11	N	505	UQ8	C40-C39-C41	3.12	120.52	115.27
9	M	603	7PH	O11-P-O14	-3.06	97.88	106.47
11	N	506	UQ8	C40-C39-C41	3.06	120.42	115.27
9	J	202	7PH	O11-P-O14	-3.05	97.91	106.47
9	M	602	7PH	O11-P-O14	-3.05	97.91	106.47
9	H	403	7PH	O11-P-O14	-3.05	97.92	106.47
9	J	203	7PH	O11-P-O14	-3.01	98.04	106.47
11	N	506	UQ8	C1-C6-C5	2.96	122.38	119.58
11	N	506	UQ8	C17-C18-C19	-2.87	120.74	127.66
9	H	403	7PH	O13-P-O11	-2.76	99.38	106.73
9	J	203	7PH	O13-P-O11	-2.76	99.39	106.73
9	J	202	7PH	O13-P-O11	-2.76	99.40	106.73
9	M	602	7PH	O13-P-O11	-2.75	99.41	106.73
9	M	603	7PH	O13-P-O11	-2.75	99.42	106.73
11	N	506	UQ8	C7-C6-C5	-2.61	115.34	118.48
11	N	505	UQ8	C12-C13-C14	-2.54	121.55	127.66
11	N	506	UQ8	C12-C13-C14	-2.49	121.65	127.66
9	M	603	7PH	O13-P-O12	2.49	117.14	107.64
9	H	403	7PH	O13-P-O12	2.48	117.12	107.64
9	J	202	7PH	O13-P-O12	2.48	117.10	107.64
9	M	602	7PH	O13-P-O12	2.47	117.07	107.64
9	J	203	7PH	O13-P-O12	2.46	117.02	107.64
11	N	506	UQ8	C10-C9-C11	2.40	119.31	115.27
8	H	402	3PE	O12-P-O14	2.39	124.05	112.24
8	L	701	3PE	O12-P-O14	2.39	124.05	112.24
8	M	601	3PE	O12-P-O14	2.35	123.84	112.24
8	H	401	3PE	O12-P-O14	2.34	123.80	112.24
8	N	503	3PE	O12-P-O14	2.31	123.65	112.24
8	N	504	3PE	O12-P-O14	2.29	123.58	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	703	3PE	O12-P-O14	2.29	123.57	112.24
11	N	505	UQ8	C37-C38-C39	-2.28	122.16	127.66
11	N	505	UQ8	C10-C9-C11	2.28	119.10	115.27
8	A	202	3PE	O12-P-O14	2.27	123.46	112.24
8	N	502	3PE	O12-P-O14	2.26	123.41	112.24
8	J	201	3PE	O12-P-O14	2.26	123.39	112.24
8	L	702	3PE	O12-P-O14	2.25	123.38	112.24
8	N	501	3PE	O12-P-O14	2.25	123.36	112.24
11	N	505	UQ8	C41-C39-C38	-2.25	116.57	121.12
8	N	501	3PE	C2-O21-C21	2.18	123.16	117.79
11	N	505	UQ8	C8-C7-C6	2.18	117.92	112.05
9	J	203	7PH	O31-C3-C2	-2.10	102.33	108.43
9	M	602	7PH	O31-C3-C2	-2.08	102.37	108.43
11	N	506	UQ8	C41-C39-C38	-2.08	116.91	121.12
11	N	506	UQ8	C37-C38-C39	-2.07	122.68	127.66
11	N	506	UQ8	C3M-O3-C3	-2.06	109.17	116.47
11	N	506	UQ8	C8-C7-C6	2.05	117.56	112.05
11	N	505	UQ8	C3M-O3-C3	-2.02	109.32	116.47

There are no chirality outliers.

All (339) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	401	3PE	C11-O13-P-O12
8	H	401	3PE	C12-C11-O13-P
8	H	401	3PE	O13-C11-C12-N
8	H	402	3PE	C11-O13-P-O14
8	H	402	3PE	O13-C11-C12-N
8	H	402	3PE	C22-C21-O21-C2
8	L	701	3PE	C11-O13-P-O14
8	L	701	3PE	O13-C11-C12-N
8	L	702	3PE	O13-C11-C12-N
8	A	202	3PE	C22-C21-O21-C2
8	J	201	3PE	C11-O13-P-O12
8	J	201	3PE	C12-C11-O13-P
8	J	201	3PE	O13-C11-C12-N
8	M	601	3PE	C11-O13-P-O12
8	M	601	3PE	C22-C21-O21-C2
8	N	501	3PE	C11-O13-P-O12
8	N	501	3PE	O13-C11-C12-N
8	N	502	3PE	C11-O13-P-O12
8	N	502	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
8	N	502	3PE	O13-C11-C12-N
8	N	503	3PE	O13-C11-C12-N
8	N	504	3PE	C11-O13-P-O12
9	H	403	7PH	C1-O11-P-O12
9	H	403	7PH	C1-O11-P-O13
9	H	403	7PH	C1-O11-P-O14
9	H	403	7PH	O22-C21-O21-C2
9	J	202	7PH	C1-O11-P-O12
9	J	202	7PH	C1-O11-P-O13
9	J	202	7PH	C1-O11-P-O14
9	J	202	7PH	C22-C21-O21-C2
9	J	203	7PH	O22-C21-O21-C2
9	J	203	7PH	C22-C21-O21-C2
9	M	602	7PH	C1-O11-P-O12
9	M	602	7PH	C1-O11-P-O13
9	M	603	7PH	C1-O11-P-O12
9	M	603	7PH	C1-O11-P-O13
9	M	603	7PH	C1-O11-P-O14
9	M	603	7PH	O11-C1-C2-O21
10	A	201	CDL	CA2-OA2-PA1-OA3
10	A	201	CDL	CA3-OA5-PA1-OA4
10	A	201	CDL	CB2-OB2-PB2-OB3
10	A	201	CDL	CB2-OB2-PB2-OB4
10	A	201	CDL	CB3-OB5-PB2-OB4
10	A	201	CDL	OB6-CB4-CB6-OB8
11	N	506	UQ8	C30-C29-C31-C32
11	N	506	UQ8	C28-C29-C31-C32
9	M	603	7PH	O32-C31-O31-C3
9	M	603	7PH	C32-C31-O31-C3
8	H	402	3PE	O32-C31-O31-C3
8	A	202	3PE	O32-C31-O31-C3
10	A	201	CDL	OA9-CA7-OA8-CA6
8	H	402	3PE	O22-C21-O21-C2
8	A	202	3PE	O22-C21-O21-C2
8	M	601	3PE	O22-C21-O21-C2
9	J	202	7PH	O22-C21-O21-C2
8	H	402	3PE	C32-C31-O31-C3
8	A	202	3PE	C32-C31-O31-C3
10	A	201	CDL	C31-CA7-OA8-CA6
9	H	403	7PH	C22-C21-O21-C2
10	A	201	CDL	C74-C75-C76-C77
10	A	201	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
8	L	702	3PE	C32-C31-O31-C3
8	N	502	3PE	C22-C21-O21-C2
10	A	201	CDL	C77-C78-C79-C80
10	A	201	CDL	C37-C38-C39-C40
10	A	201	CDL	C51-C52-C53-C54
9	M	603	7PH	C27-C28-C29-C2A
11	N	505	UQ8	C24-C26-C27-C28
11	N	506	UQ8	C39-C41-C42-C43
11	N	506	UQ8	C14-C16-C17-C18
8	L	702	3PE	O32-C31-O31-C3
10	A	201	CDL	C11-CA5-OA6-CA4
10	A	201	CDL	CA2-C1-CB2-OB2
8	N	502	3PE	O22-C21-O21-C2
10	A	201	CDL	C71-C72-C73-C74
9	J	203	7PH	C31-C32-C33-C34
10	A	201	CDL	C17-C18-C19-C20
9	M	602	7PH	C27-C28-C29-C2A
9	H	403	7PH	C21-C22-C23-C24
9	M	602	7PH	C21-C22-C23-C24
10	A	201	CDL	CB7-C71-C72-C73
9	H	403	7PH	C31-C32-C33-C34
11	N	505	UQ8	C39-C41-C42-C43
11	N	506	UQ8	C29-C31-C32-C33
11	N	506	UQ8	C24-C26-C27-C28
10	A	201	CDL	OA7-CA5-OA6-CA4
8	H	401	3PE	C1-O11-P-O13
8	H	401	3PE	C11-O13-P-O11
8	J	201	3PE	C11-O13-P-O11
8	M	601	3PE	C1-O11-P-O13
8	M	601	3PE	C11-O13-P-O11
8	N	501	3PE	C11-O13-P-O11
8	N	502	3PE	C11-O13-P-O11
8	N	504	3PE	C11-O13-P-O11
10	A	201	CDL	CA2-OA2-PA1-OA5
10	A	201	CDL	CA3-OA5-PA1-OA2
10	A	201	CDL	CB2-OB2-PB2-OB5
9	M	602	7PH	C23-C24-C25-C26
9	J	202	7PH	C21-C22-C23-C24
9	H	403	7PH	C27-C28-C29-C2A
8	N	501	3PE	C22-C21-O21-C2
8	L	703	3PE	C26-C27-C28-C29
8	N	502	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
8	N	504	3PE	C24-C25-C26-C27
8	N	504	3PE	C2A-C2B-C2C-C2D
9	H	403	7PH	C22-C23-C24-C25
9	H	403	7PH	C25-C26-C27-C28
9	M	602	7PH	C38-C39-C3A-C3B
8	H	401	3PE	C3E-C3F-C3G-C3H
8	L	703	3PE	C2C-C2D-C2E-C2F
8	N	501	3PE	O22-C21-O21-C2
8	L	701	3PE	C33-C34-C35-C36
9	J	203	7PH	C37-C38-C39-C3A
10	A	201	CDL	C82-C83-C84-C85
8	H	401	3PE	C3C-C3D-C3E-C3F
8	N	501	3PE	C3D-C3E-C3F-C3G
8	N	503	3PE	C25-C26-C27-C28
10	A	201	CDL	C59-C60-C61-C62
8	M	601	3PE	C38-C39-C3A-C3B
8	J	201	3PE	C22-C23-C24-C25
9	J	203	7PH	C29-C2A-C2B-C2C
10	A	201	CDL	C12-C13-C14-C15
8	J	201	3PE	C2E-C2F-C2G-C2H
9	J	202	7PH	C25-C26-C27-C28
10	A	201	CDL	C11-C12-C13-C14
10	A	201	CDL	C34-C35-C36-C37
10	A	201	CDL	C72-C73-C74-C75
8	H	402	3PE	C2B-C2C-C2D-C2E
9	J	203	7PH	C25-C26-C27-C28
9	M	602	7PH	C32-C33-C34-C35
10	A	201	CDL	C20-C21-C22-C23
10	A	201	CDL	C61-C62-C63-C64
9	M	603	7PH	C25-C26-C27-C28
10	A	201	CDL	C16-C17-C18-C19
10	A	201	CDL	C60-C61-C62-C63
10	A	201	CDL	C80-C81-C82-C83
9	J	202	7PH	C37-C38-C39-C3A
9	J	203	7PH	C27-C28-C29-C2A
10	A	201	CDL	C32-C33-C34-C35
10	A	201	CDL	C76-C77-C78-C79
10	A	201	CDL	C23-C24-C25-C26
10	A	201	CDL	C73-C74-C75-C76
9	J	202	7PH	C27-C28-C29-C2A
9	M	603	7PH	C37-C38-C39-C3A
9	J	203	7PH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	H	401	3PE	C37-C38-C39-C3A
9	J	202	7PH	C32-C33-C34-C35
10	A	201	CDL	CA5-C11-C12-C13
9	M	602	7PH	C22-C23-C24-C25
10	A	201	CDL	C63-C64-C65-C66
8	H	401	3PE	C21-C22-C23-C24
8	N	502	3PE	C36-C37-C38-C39
9	J	202	7PH	C26-C27-C28-C29
9	J	203	7PH	C32-C31-O31-C3
10	A	201	CDL	C51-CB5-OB6-CB4
10	A	201	CDL	C44-C45-C46-C47
8	N	501	3PE	C24-C25-C26-C27
9	J	202	7PH	C32-C31-O31-C3
9	H	403	7PH	C32-C33-C34-C35
10	A	201	CDL	C14-C15-C16-C17
9	H	403	7PH	C37-C38-C39-C3A
9	H	403	7PH	C33-C34-C35-C36
9	J	203	7PH	C26-C27-C28-C29
10	A	201	CDL	C19-C20-C21-C22
9	M	602	7PH	C37-C38-C39-C3A
9	J	203	7PH	C33-C34-C35-C36
10	A	201	CDL	C78-C79-C80-C81
9	H	403	7PH	C2A-C2B-C2C-C2D
10	A	201	CDL	OB7-CB5-OB6-CB4
9	M	603	7PH	C33-C34-C35-C36
8	H	402	3PE	C11-O13-P-O11
8	L	701	3PE	C11-O13-P-O11
10	A	201	CDL	CB3-OB5-PB2-OB2
9	J	203	7PH	O32-C31-O31-C3
9	J	203	7PH	O11-C1-C2-C3
9	M	603	7PH	O11-C1-C2-C3
10	A	201	CDL	OB5-CB3-CB4-CB6
9	M	603	7PH	C26-C27-C28-C29
9	J	203	7PH	C32-C33-C34-C35
9	J	202	7PH	C34-C35-C36-C37
8	H	401	3PE	C1-C2-C3-O31
9	H	403	7PH	C1-C2-C3-O31
9	J	203	7PH	C1-C2-C3-O31
10	A	201	CDL	C18-C19-C20-C21
8	H	401	3PE	C38-C39-C3A-C3B
8	N	501	3PE	C2D-C2E-C2F-C2G
9	J	202	7PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
10	A	201	CDL	C38-C39-C40-C41
11	N	505	UQ8	C12-C11-C9-C10
9	M	603	7PH	C21-C22-C23-C24
9	J	203	7PH	C38-C39-C3A-C3B
10	A	201	CDL	C84-C85-C86-C87
9	M	602	7PH	C1-O11-P-O14
11	N	505	UQ8	C12-C11-C9-C8
8	N	501	3PE	C2C-C2D-C2E-C2F
9	H	403	7PH	C26-C27-C28-C29
9	H	403	7PH	C24-C25-C26-C27
9	J	203	7PH	C2A-C2B-C2C-C2D
9	H	403	7PH	O11-C1-C2-C3
9	M	602	7PH	C32-C31-O31-C3
8	L	701	3PE	C39-C3A-C3B-C3C
8	J	201	3PE	C1-C2-C3-O31
9	M	602	7PH	C1-C2-C3-O31
8	A	202	3PE	C27-C28-C29-C2A
8	J	201	3PE	C27-C28-C29-C2A
9	J	202	7PH	C33-C34-C35-C36
9	M	602	7PH	C34-C35-C36-C37
8	N	501	3PE	C3A-C3B-C3C-C3D
9	J	203	7PH	O11-C1-C2-O21
10	A	201	CDL	OA5-CA3-CA4-OA6
9	M	603	7PH	O21-C2-C3-O31
11	N	506	UQ8	C34-C36-C37-C38
8	N	502	3PE	C33-C34-C35-C36
8	N	502	3PE	C2-C1-O11-P
10	A	201	CDL	C1-CB2-OB2-PB2
8	L	703	3PE	C27-C28-C29-C2A
9	M	602	7PH	C2B-C2C-C2D-C2E
10	A	201	CDL	C13-C14-C15-C16
8	L	701	3PE	C32-C33-C34-C35
10	A	201	CDL	C39-C40-C41-C42
10	A	201	CDL	C40-C41-C42-C43
9	M	602	7PH	O11-C1-C2-C3
10	A	201	CDL	OA5-CA3-CA4-CA6
10	A	201	CDL	C56-C57-C58-C59
9	J	202	7PH	C22-C23-C24-C25
8	H	401	3PE	C22-C23-C24-C25
8	H	401	3PE	C33-C34-C35-C36
9	J	203	7PH	C23-C24-C25-C26
8	L	703	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
9	M	603	7PH	C1-C2-C3-O31
10	A	201	CDL	CA3-CA4-CA6-OA8
10	A	201	CDL	CB3-CB4-CB6-OB8
9	J	202	7PH	C2A-C2B-C2C-C2D
9	M	602	7PH	O32-C31-O31-C3
9	H	403	7PH	C29-C2A-C2B-C2C
8	H	401	3PE	O21-C2-C3-O31
9	H	403	7PH	O21-C2-C3-O31
8	A	202	3PE	C29-C2A-C2B-C2C
9	M	603	7PH	C34-C35-C36-C37
8	L	701	3PE	C34-C35-C36-C37
9	J	203	7PH	C39-C3A-C3B-C3C
10	A	201	CDL	C54-C55-C56-C57
9	M	603	7PH	C2B-C2C-C2D-C2E
10	A	201	CDL	C42-C43-C44-C45
8	L	701	3PE	C32-C31-O31-C3
8	L	702	3PE	C11-O13-P-O11
8	H	401	3PE	C1-O11-P-O14
8	M	601	3PE	C1-O11-P-O14
10	A	201	CDL	CA2-OA2-PA1-OA4
10	A	201	CDL	CB3-OB5-PB2-OB3
8	L	703	3PE	C31-C32-C33-C34
10	A	201	CDL	C75-C76-C77-C78
9	J	202	7PH	O11-C1-C2-C3
9	J	202	7PH	O11-C1-C2-O21
9	M	602	7PH	O21-C2-C3-O31
8	J	201	3PE	C2D-C2E-C2F-C2G
8	N	502	3PE	C37-C38-C39-C3A
11	N	505	UQ8	C40-C39-C41-C42
8	J	201	3PE	C3B-C3C-C3D-C3E
8	L	701	3PE	O32-C31-O31-C3
10	A	201	CDL	C24-C25-C26-C27
11	N	505	UQ8	C30-C29-C31-C32
8	N	501	3PE	C3-C2-O21-C21
9	J	202	7PH	C1-C2-O21-C21
9	J	202	7PH	C38-C39-C3A-C3B
10	A	201	CDL	OB5-CB3-CB4-OB6
8	L	703	3PE	O22-C21-O21-C2
10	A	201	CDL	C43-C44-C45-C46
8	L	703	3PE	C22-C21-O21-C2
10	A	201	CDL	C15-C16-C17-C18
9	J	203	7PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
10	A	201	CDL	OA6-CA4-CA6-OA8
10	A	201	CDL	C55-C56-C57-C58
8	A	202	3PE	C1-O11-P-O13
8	N	503	3PE	C11-O13-P-O11
9	M	603	7PH	C29-C2A-C2B-C2C
9	M	602	7PH	C2A-C2B-C2C-C2D
10	A	201	CDL	CB4-CB3-OB5-PB2
8	J	201	3PE	C23-C24-C25-C26
8	L	701	3PE	C2A-C2B-C2C-C2D
8	H	401	3PE	O11-C1-C2-C3
8	J	201	3PE	O11-C1-C2-O21
9	H	403	7PH	O11-C1-C2-O21
8	N	501	3PE	C25-C26-C27-C28
8	N	502	3PE	C2A-C2B-C2C-C2D
9	M	603	7PH	C39-C3A-C3B-C3C
10	A	201	CDL	C62-C63-C64-C65
9	M	602	7PH	C24-C25-C26-C27
8	J	201	3PE	C32-C33-C34-C35
9	M	602	7PH	C39-C3A-C3B-C3C
8	N	501	3PE	C35-C36-C37-C38
8	N	504	3PE	C2-C1-O11-P
11	N	505	UQ8	C28-C29-C31-C32
11	N	505	UQ8	C20-C19-C21-C22
8	J	201	3PE	C37-C38-C39-C3A
8	L	701	3PE	C36-C37-C38-C39
8	N	502	3PE	C2B-C2C-C2D-C2E
8	J	201	3PE	C2B-C2C-C2D-C2E
11	N	505	UQ8	C38-C39-C41-C42
8	N	503	3PE	C2D-C2E-C2F-C2G
8	H	401	3PE	O11-C1-C2-O21
9	M	602	7PH	O11-C1-C2-O21
9	J	203	7PH	C36-C37-C38-C39
11	N	506	UQ8	C9-C11-C12-C13
11	N	505	UQ8	C18-C19-C21-C22
8	N	501	3PE	C2B-C2C-C2D-C2E
11	N	506	UQ8	C25-C24-C26-C27
9	M	603	7PH	C2A-C2B-C2C-C2D
8	L	703	3PE	O31-C31-C32-C33
8	L	702	3PE	C3A-C3B-C3C-C3D
9	M	602	7PH	C25-C26-C27-C28
11	N	505	UQ8	C5-C4-O4-C4M
8	N	502	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
8	H	401	3PE	C32-C33-C34-C35
8	H	401	3PE	C26-C27-C28-C29
8	L	702	3PE	O21-C21-C22-C23
8	H	401	3PE	C23-C24-C25-C26
8	N	502	3PE	C3C-C3D-C3E-C3F
9	J	202	7PH	C39-C3A-C3B-C3C
8	H	402	3PE	C39-C3A-C3B-C3C
8	L	703	3PE	O32-C31-C32-C33
8	N	503	3PE	C2C-C2D-C2E-C2F
8	A	202	3PE	C37-C38-C39-C3A
8	L	703	3PE	C23-C24-C25-C26
8	H	402	3PE	C11-O13-P-O12
8	L	701	3PE	C11-O13-P-O12
8	L	702	3PE	C11-O13-P-O12
8	N	503	3PE	C11-O13-P-O14
11	N	505	UQ8	C9-C11-C12-C13
8	J	201	3PE	C3F-C3G-C3H-C3I
8	N	502	3PE	C28-C29-C2A-C2B
11	N	505	UQ8	C15-C14-C16-C17
8	L	702	3PE	O22-C21-C22-C23
8	J	201	3PE	C26-C27-C28-C29
9	H	403	7PH	O21-C21-C22-C23
8	M	601	3PE	O21-C21-C22-C23
8	N	503	3PE	C33-C34-C35-C36
8	L	702	3PE	C36-C37-C38-C39
11	N	505	UQ8	C29-C31-C32-C33

There are no ring outliers.

17 monomers are involved in 49 short contacts:

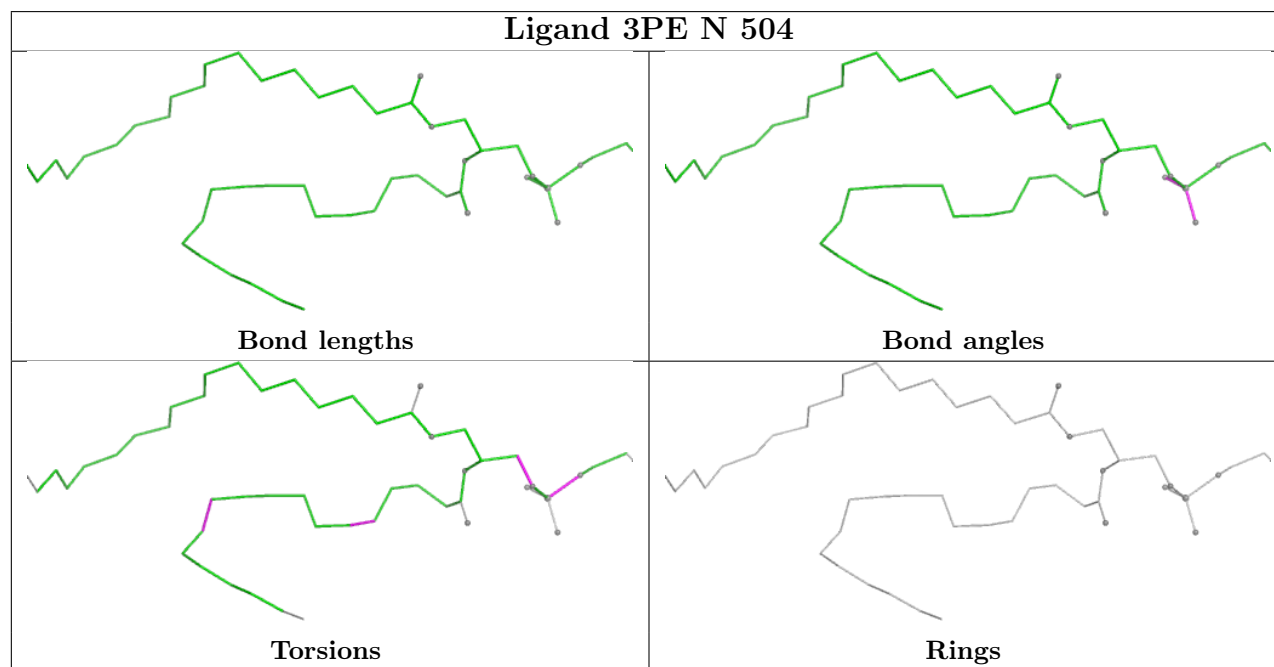
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	504	3PE	1	0
10	A	201	CDL	10	0
8	L	701	3PE	4	0
9	J	203	7PH	1	0
9	M	603	7PH	4	0
8	M	601	3PE	2	0
8	J	201	3PE	7	0
9	J	202	7PH	2	0
8	A	202	3PE	2	0
9	H	403	7PH	1	0
8	H	401	3PE	6	0

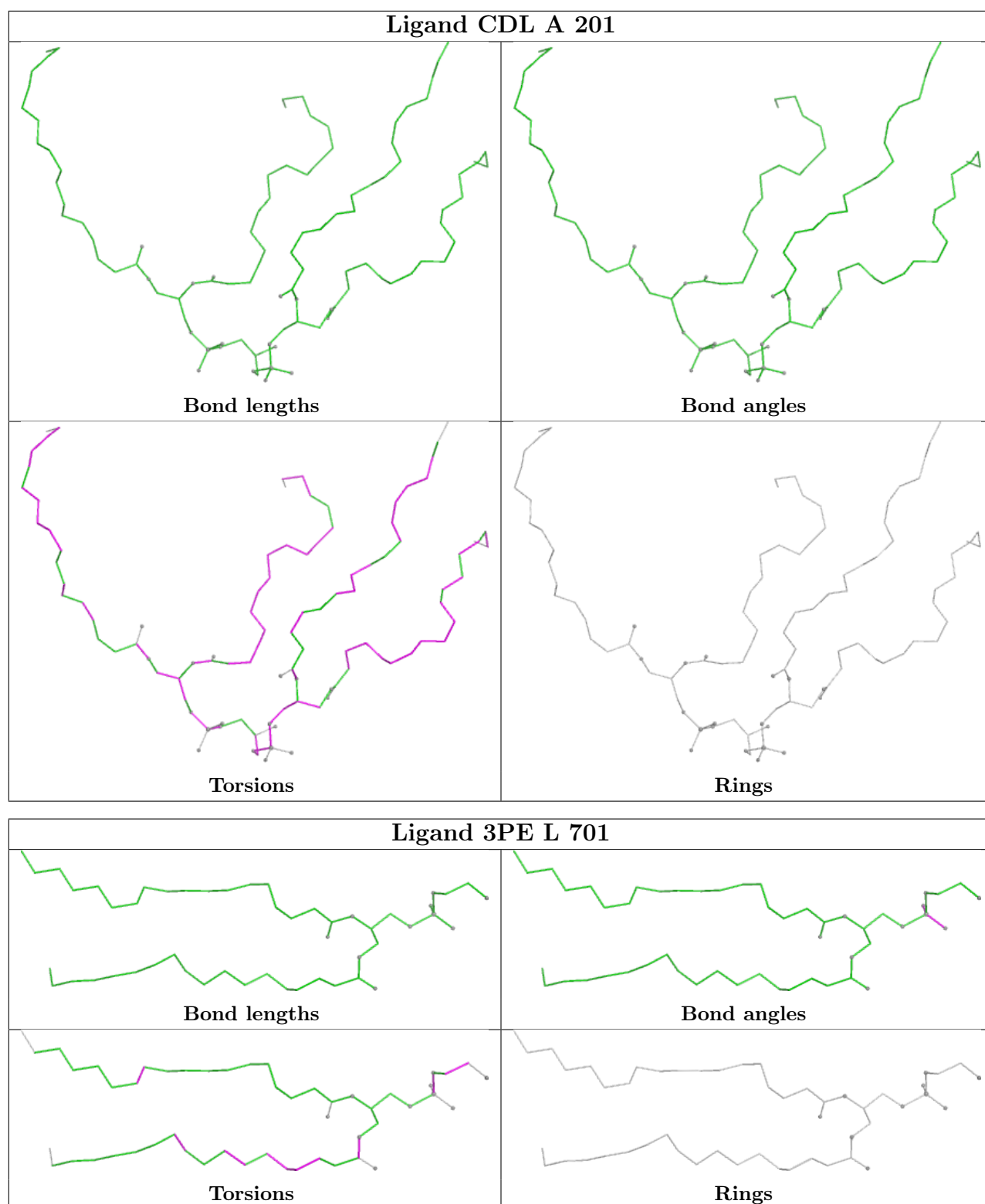
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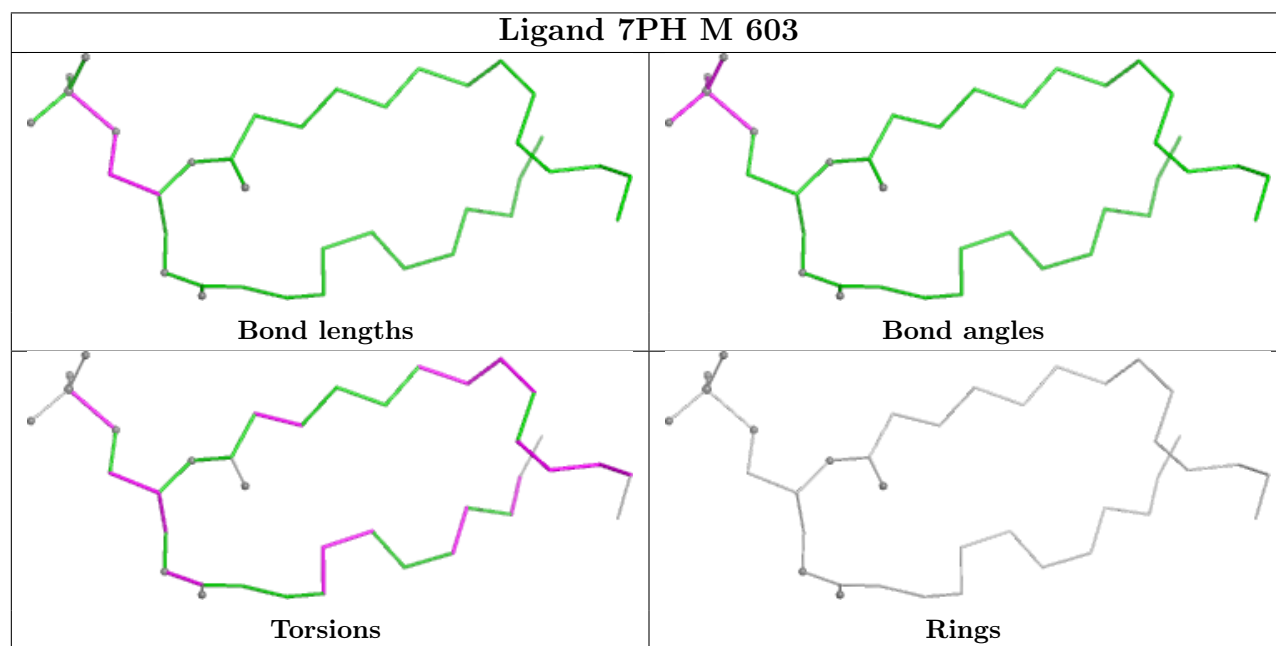
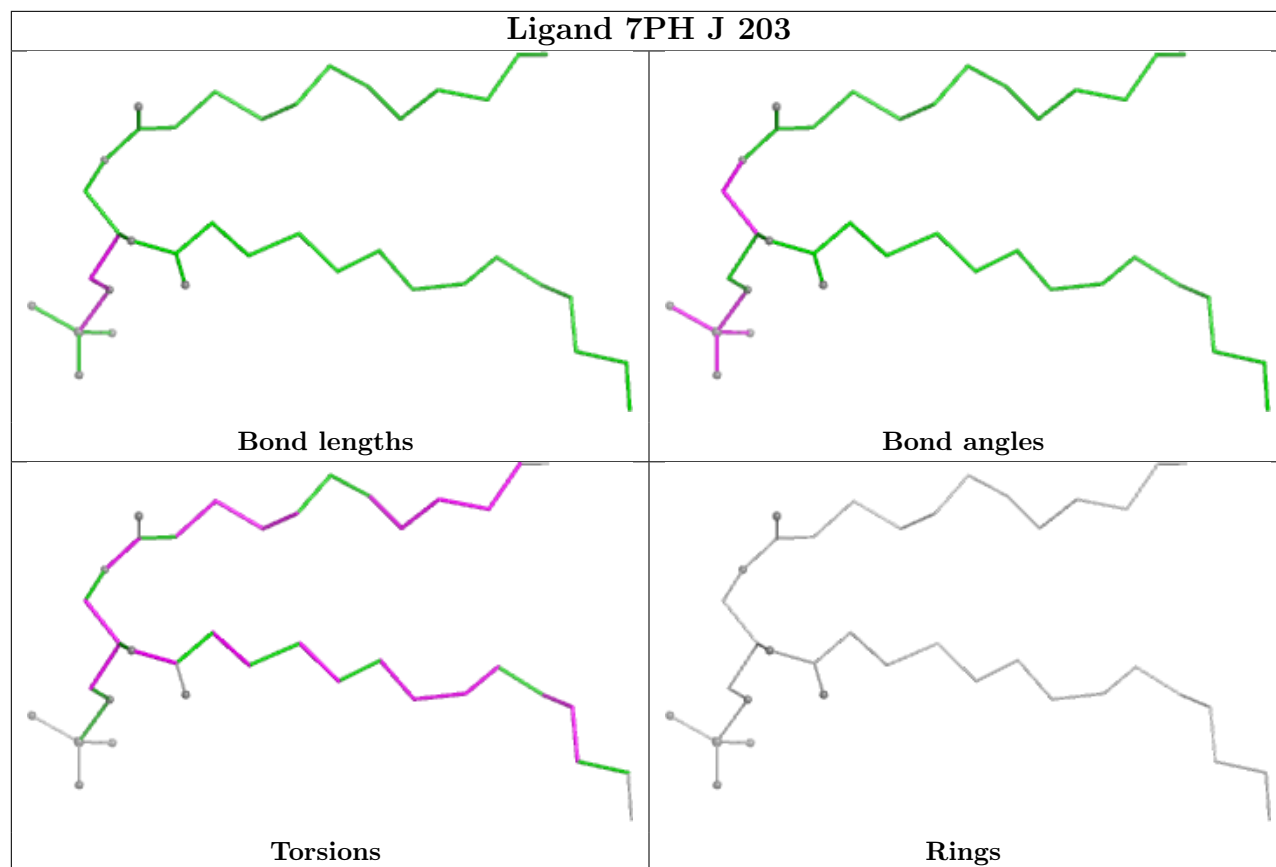
Continued from previous page...

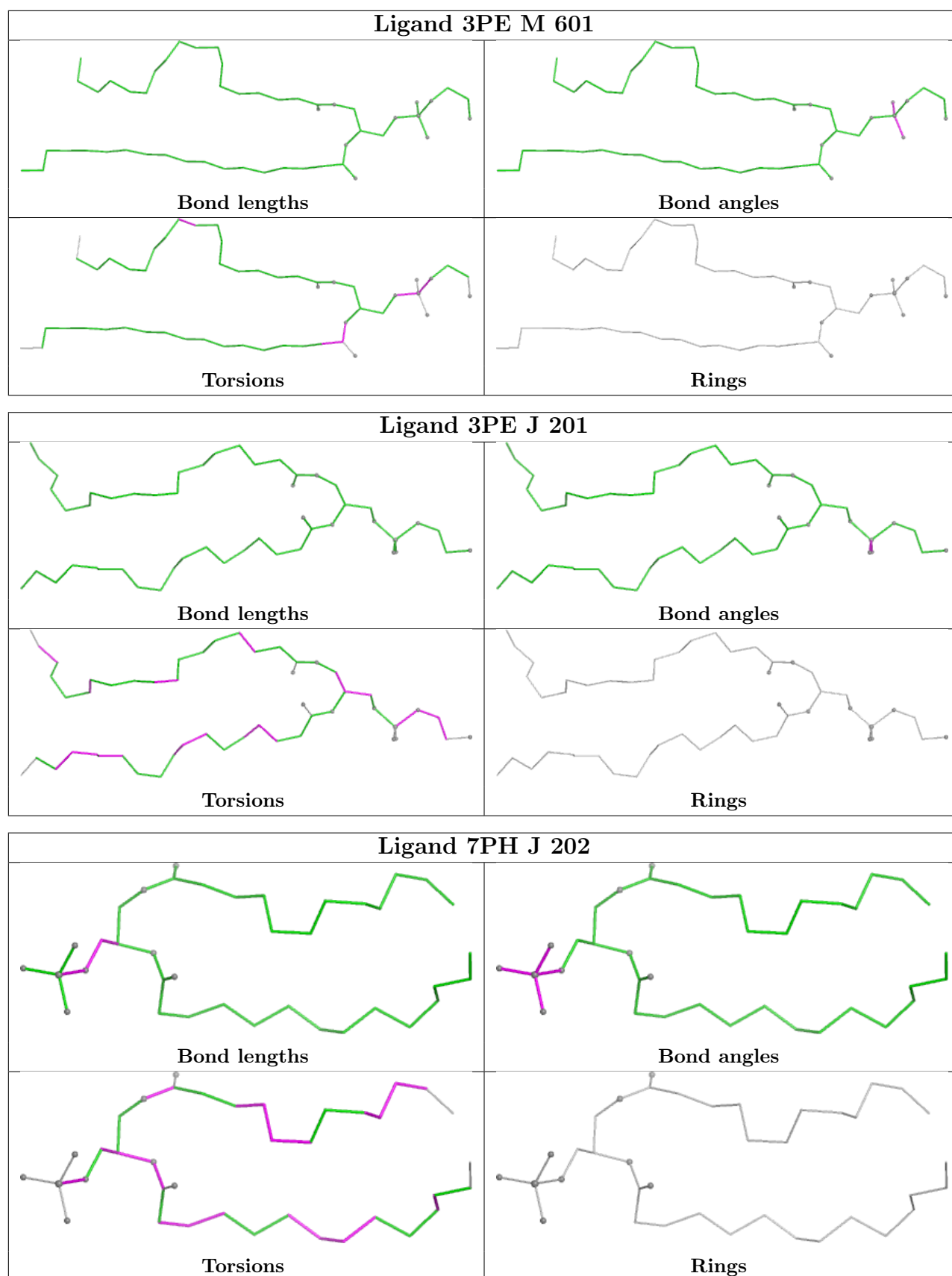
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	502	3PE	1	0
11	N	506	UQ8	3	0
11	N	505	UQ8	3	0
8	N	501	3PE	1	0
9	M	602	7PH	2	0
8	L	703	3PE	3	0

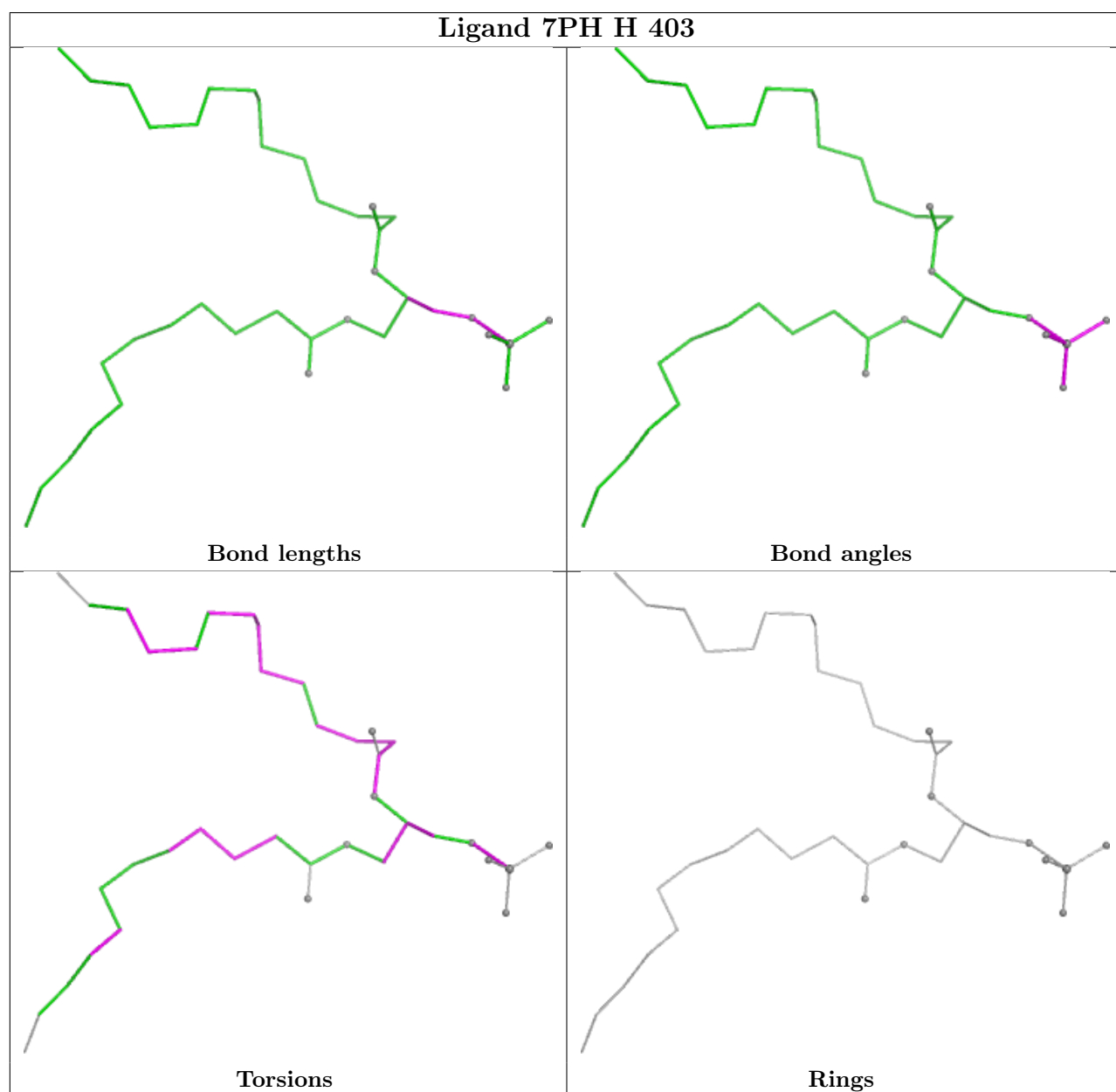
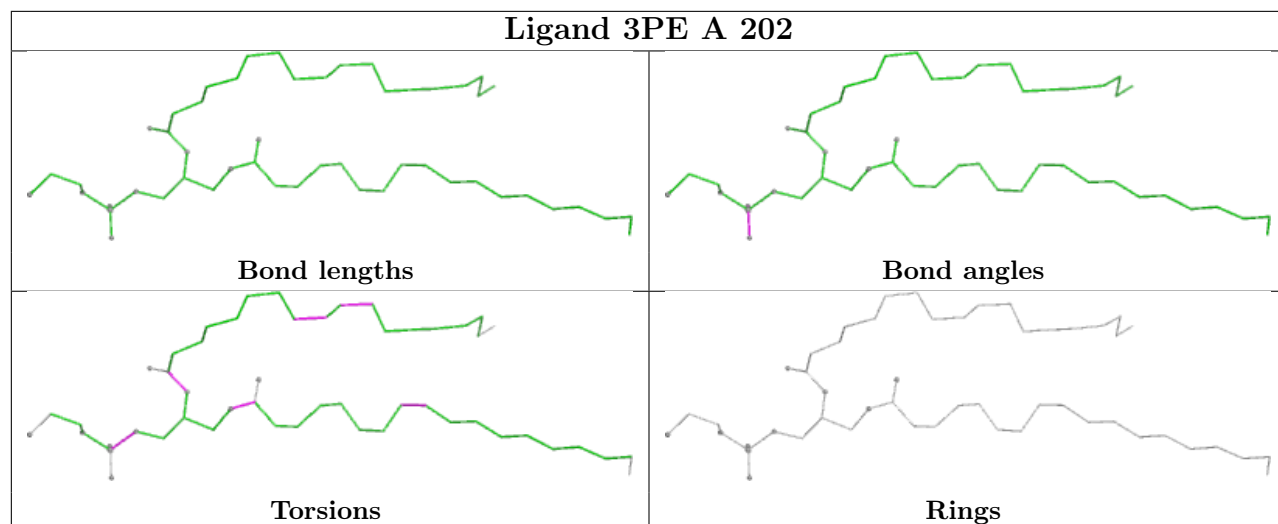
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

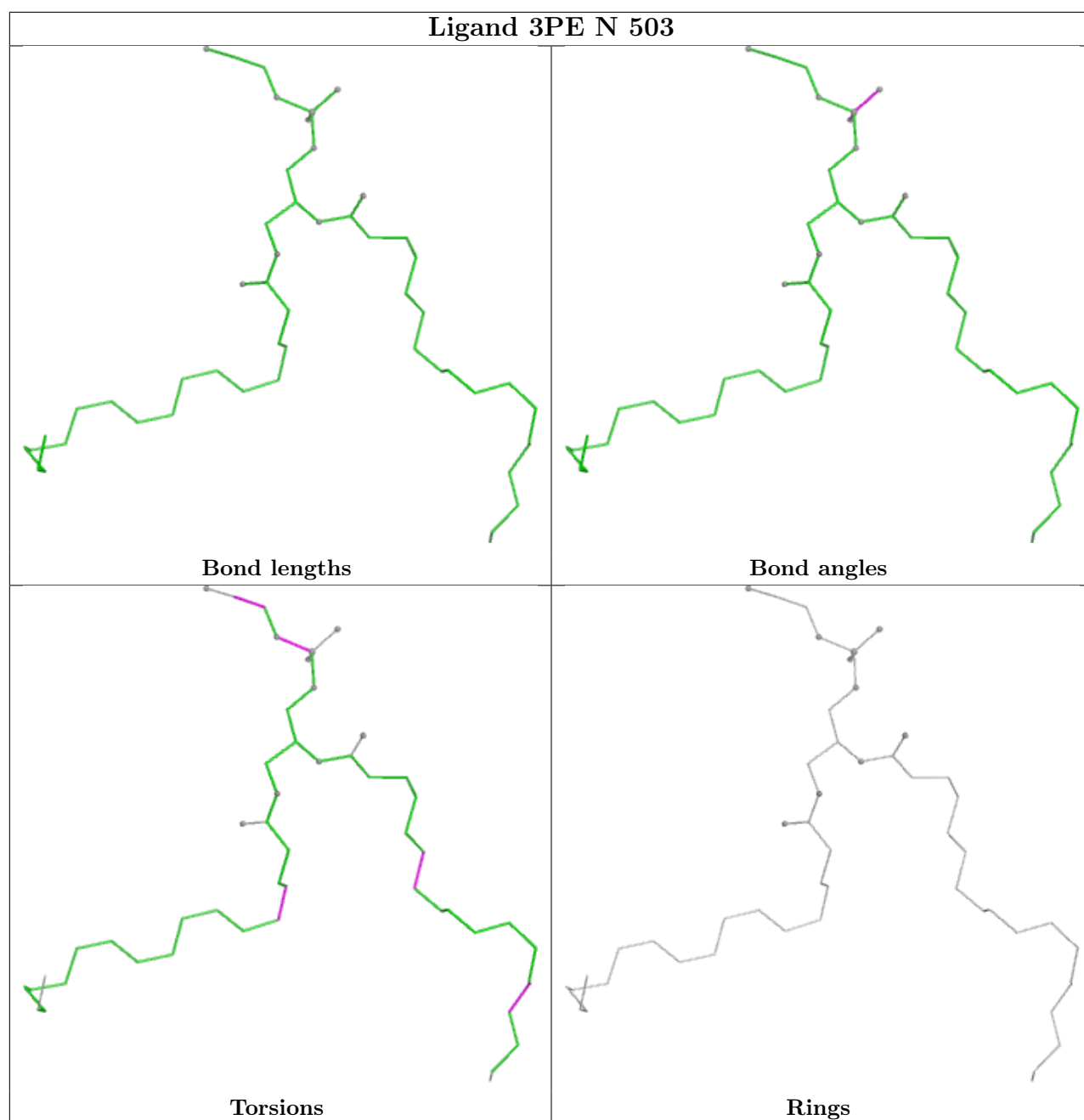


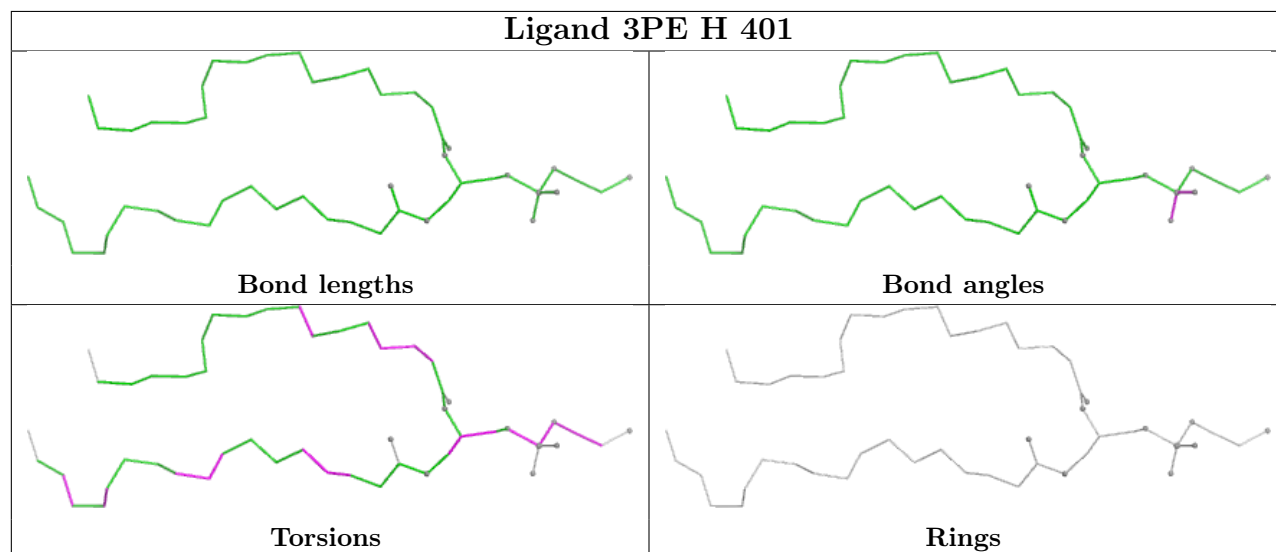
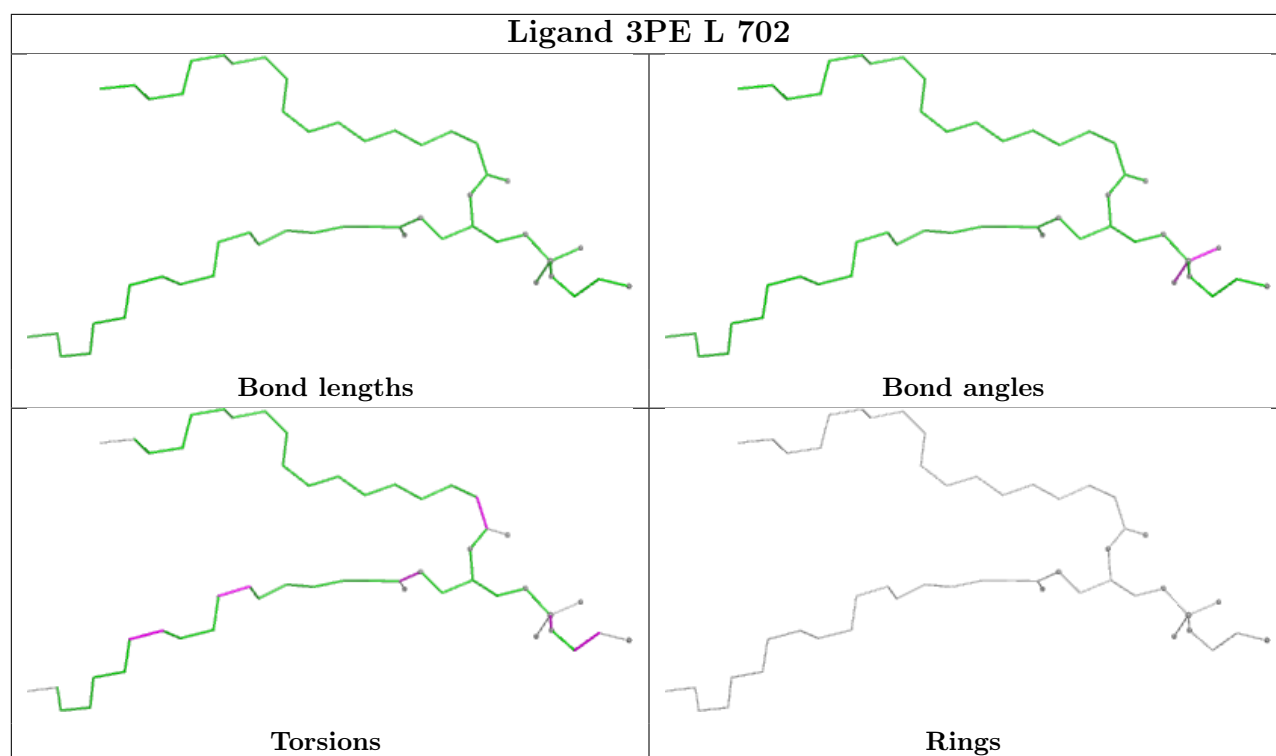


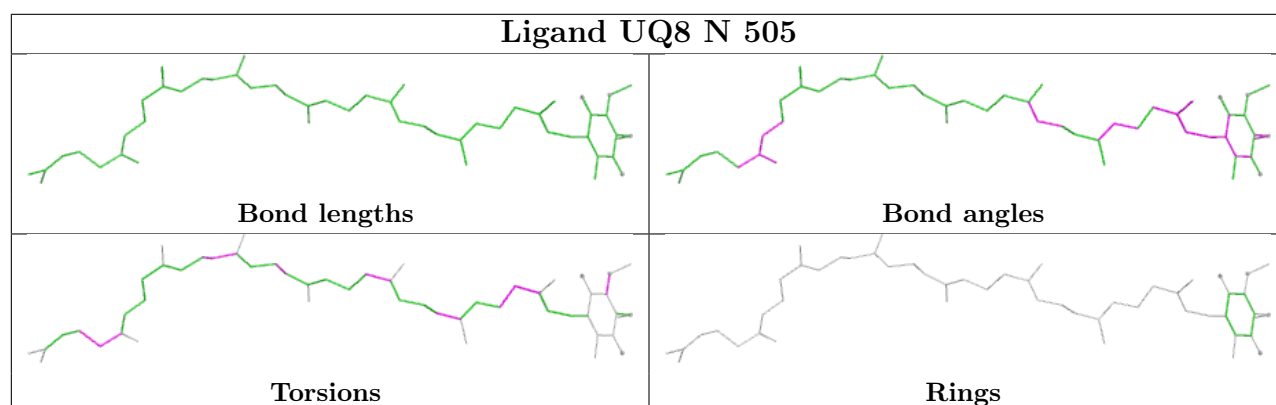
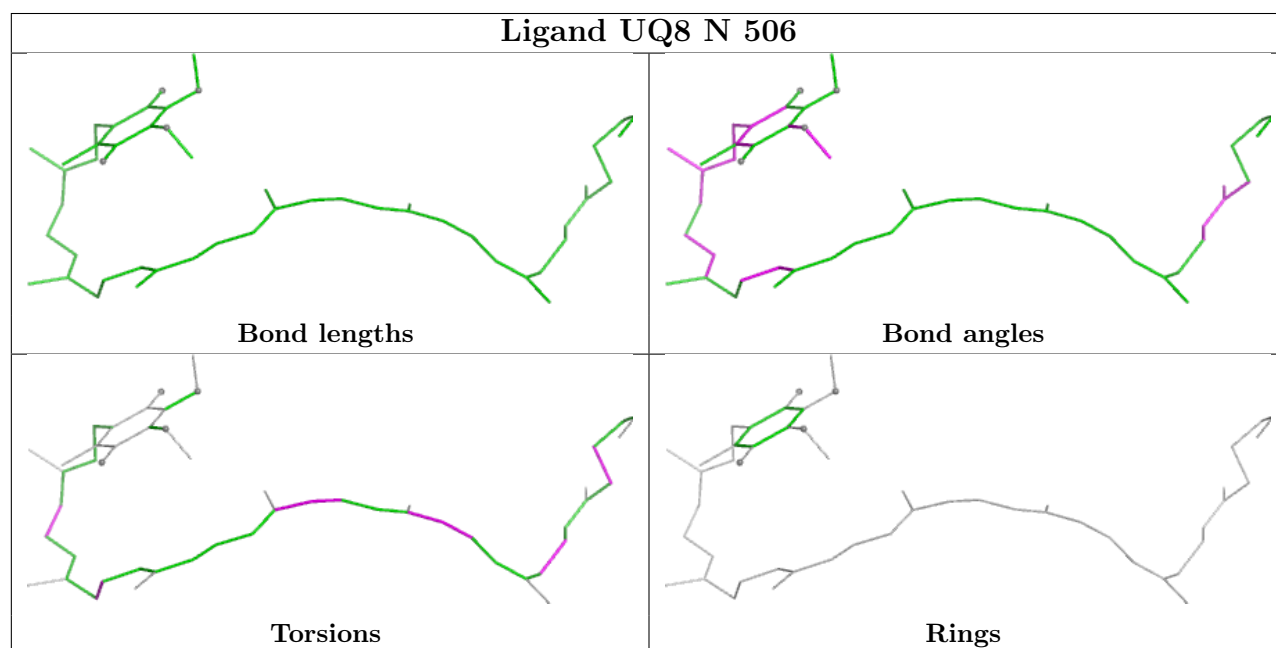
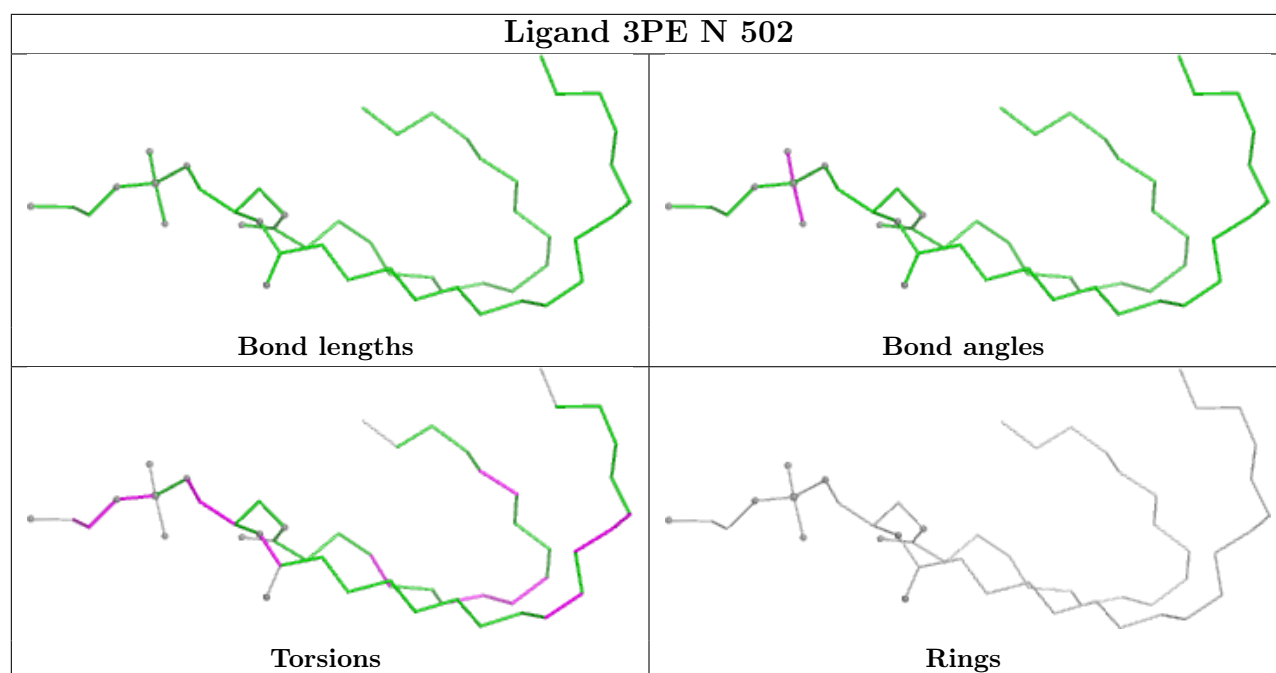


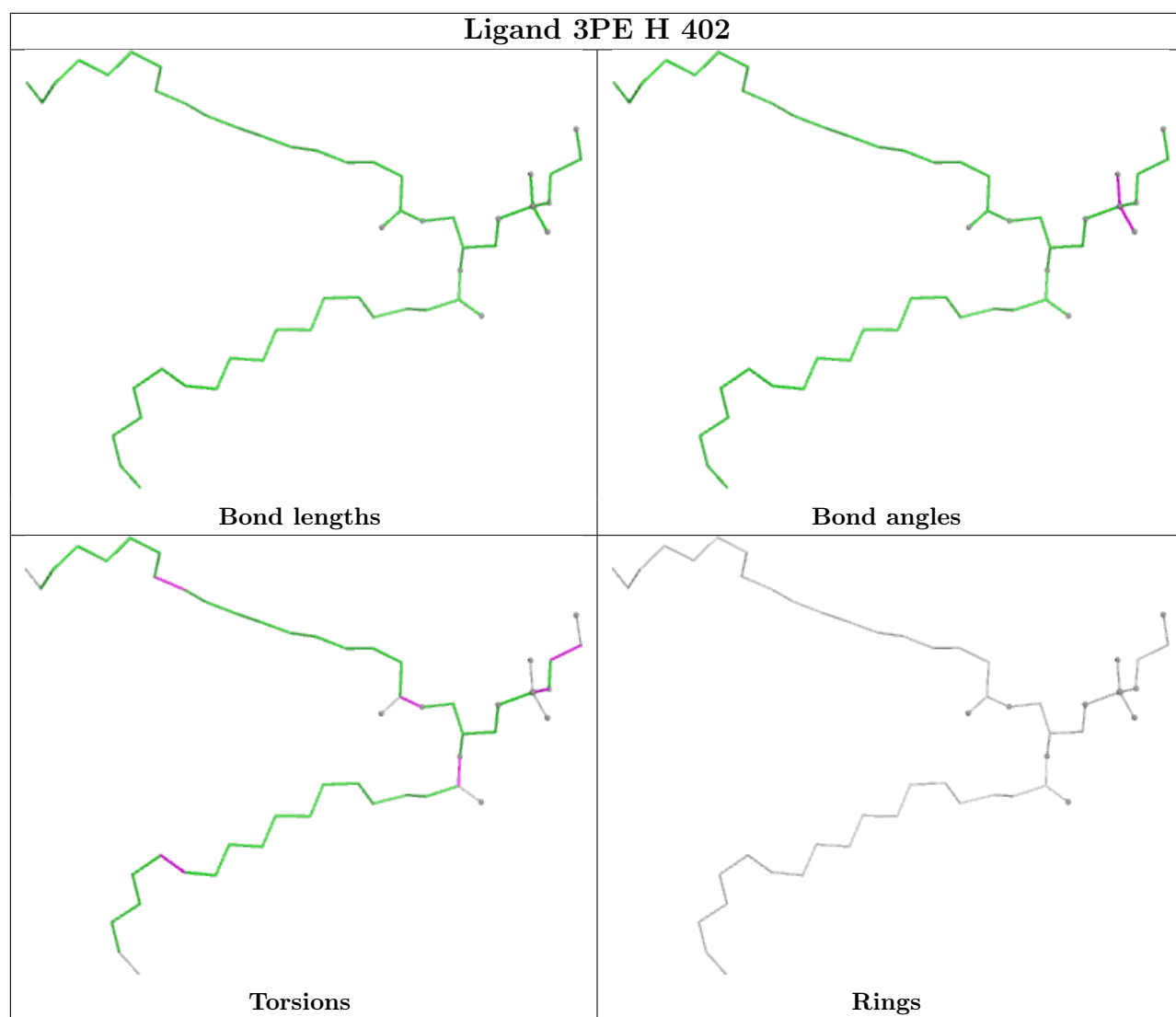


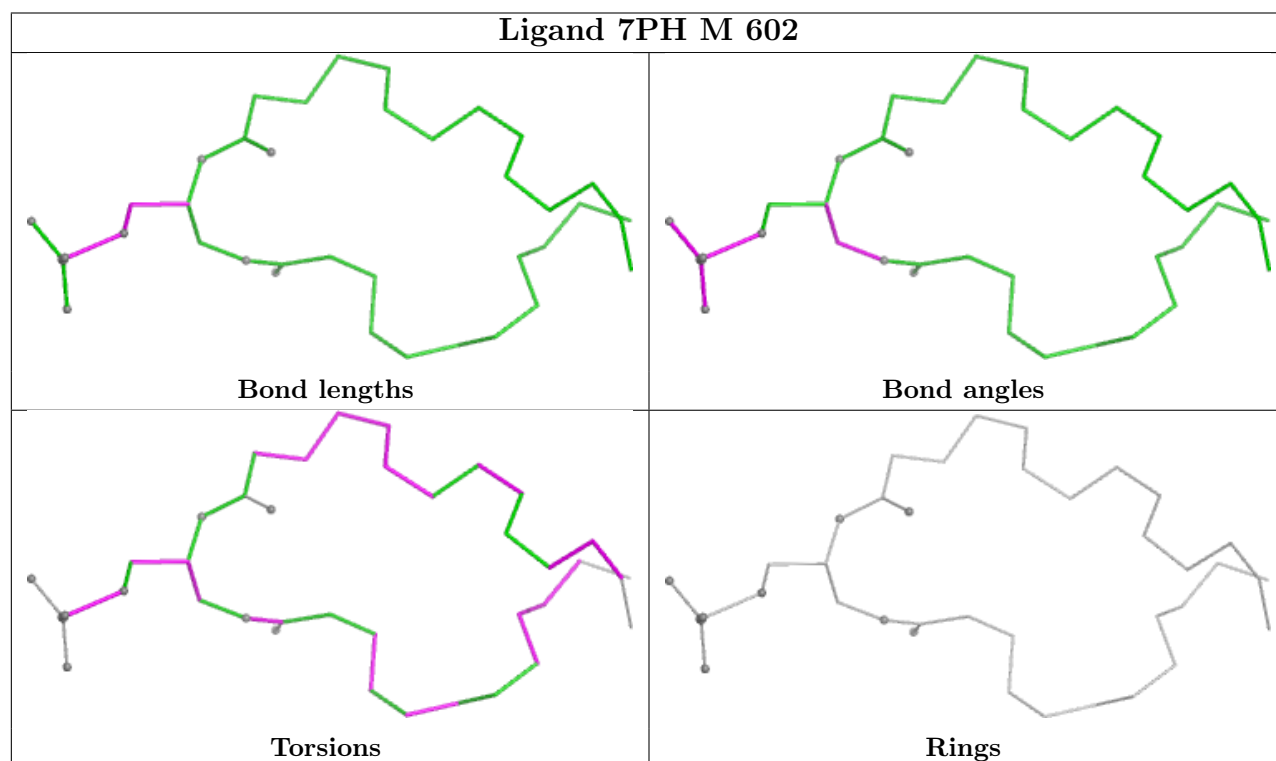
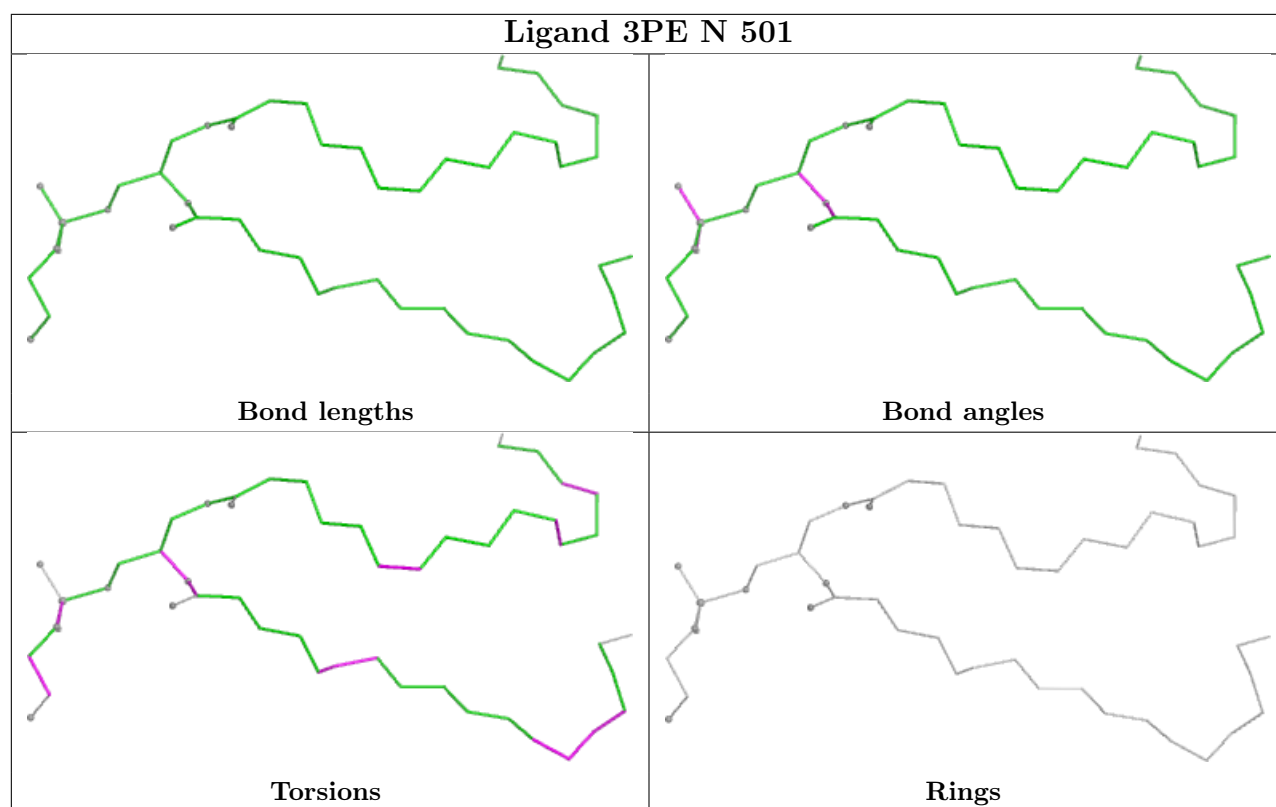


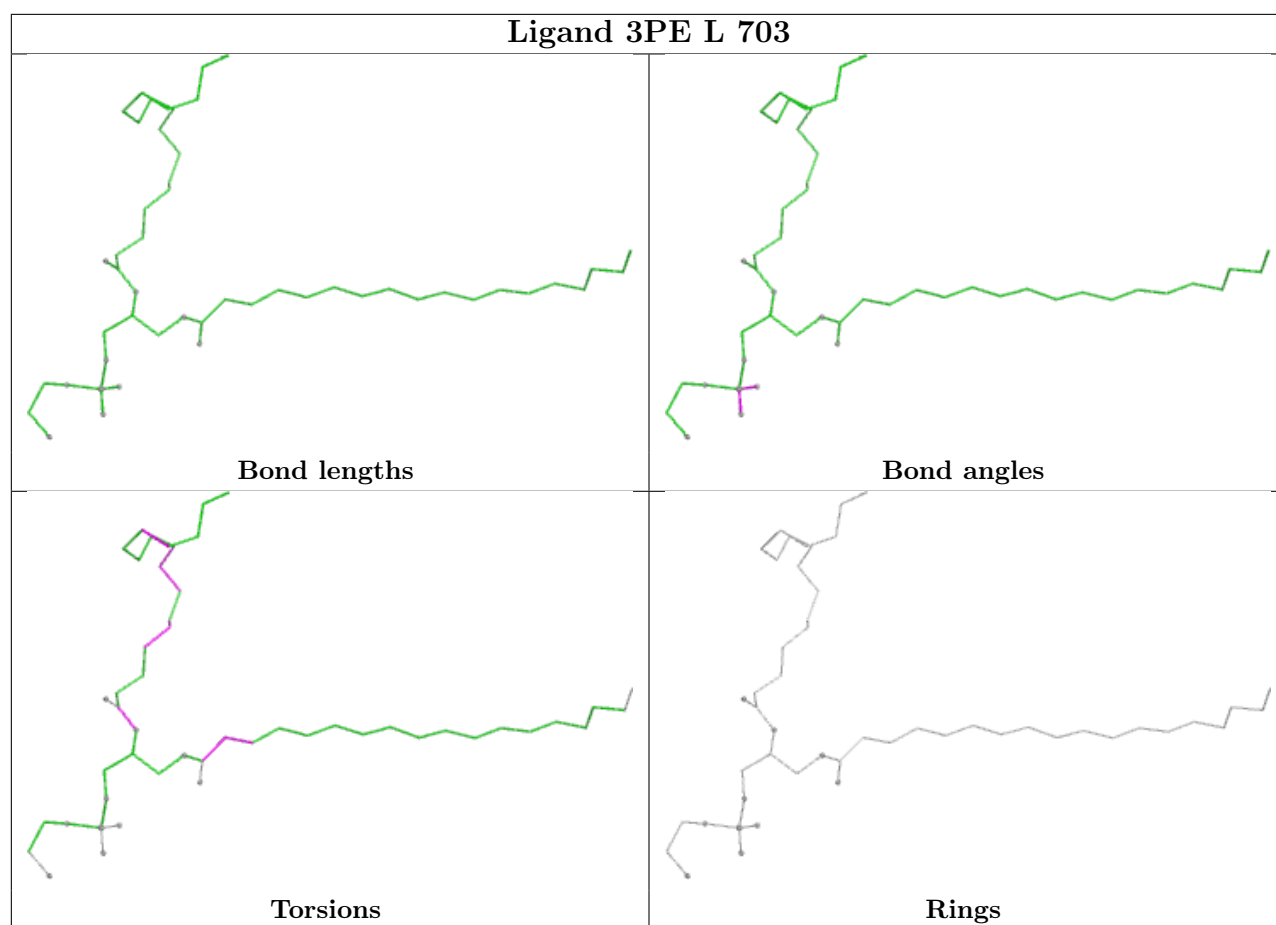












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

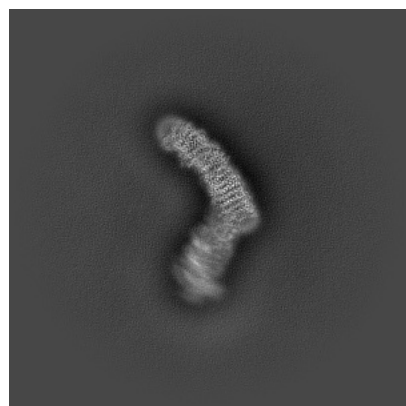
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55753. These allow visual inspection of the internal detail of the map and identification of artifacts.

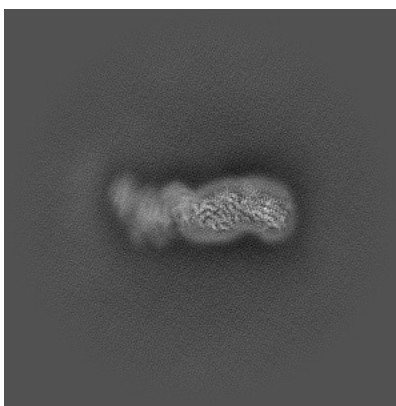
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

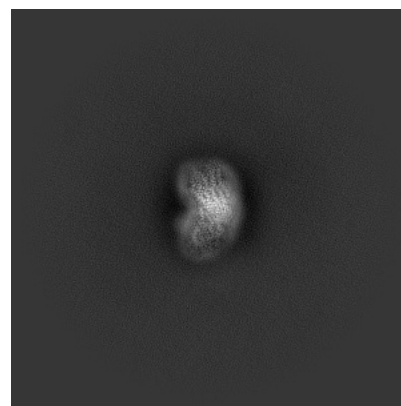
6.1.1 Primary map



X

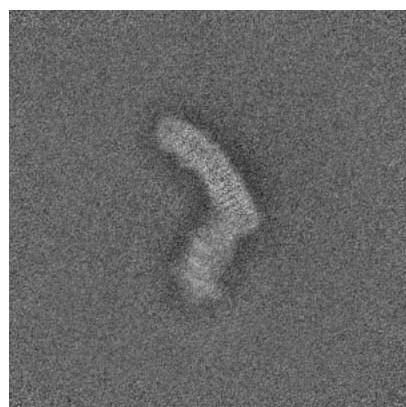


Y

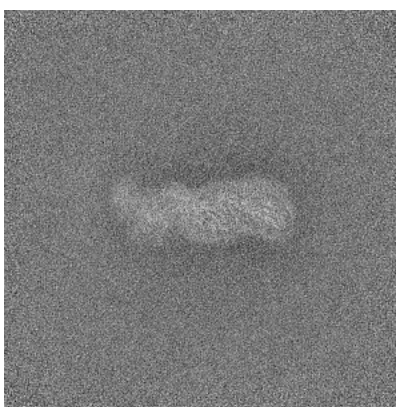


Z

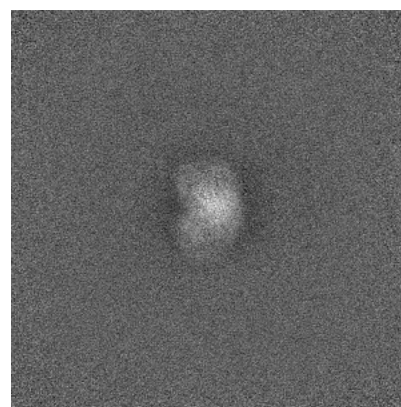
6.1.2 Raw map



X



Y



Z

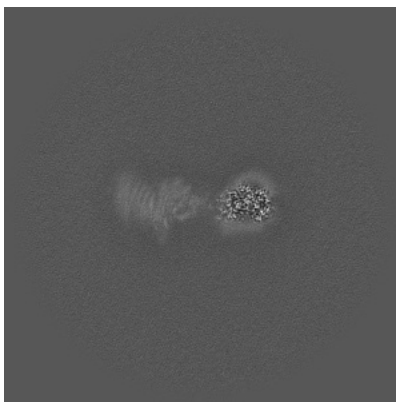
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

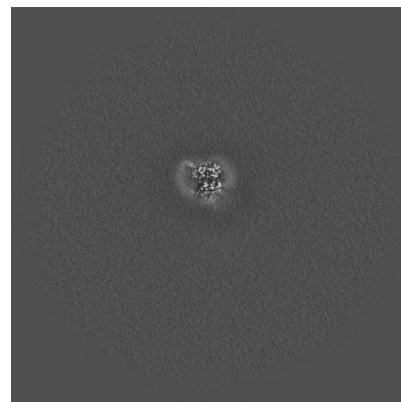
6.2.1 Primary map



X Index: 355

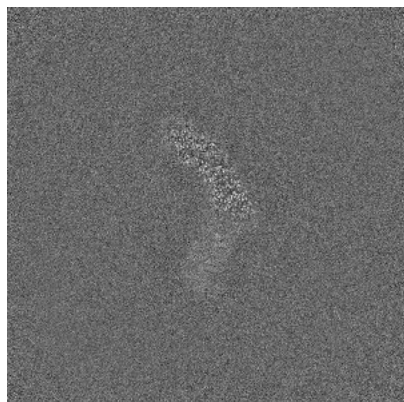


Y Index: 355

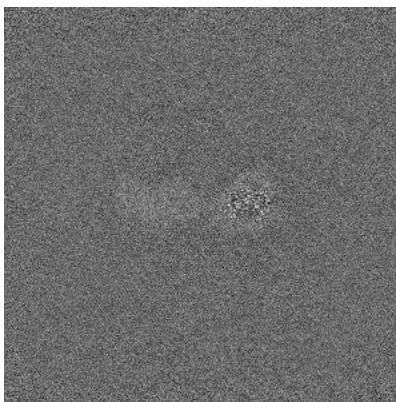


Z Index: 355

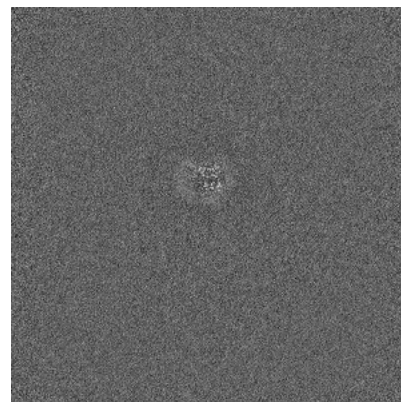
6.2.2 Raw map



X Index: 355



Y Index: 355

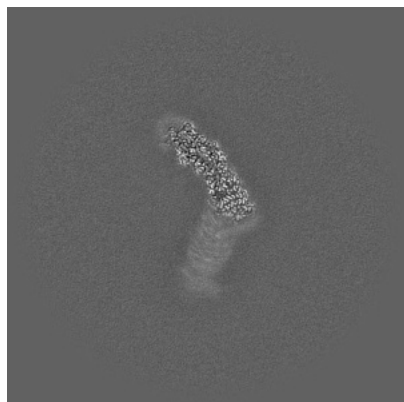


Z Index: 355

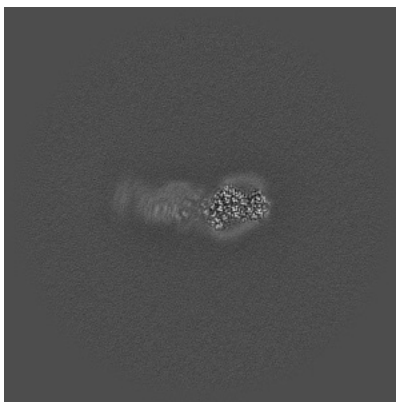
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

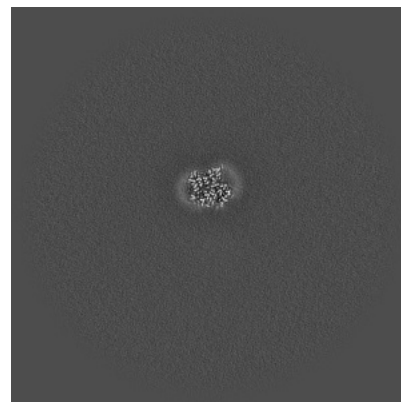
6.3.1 Primary map



X Index: 358

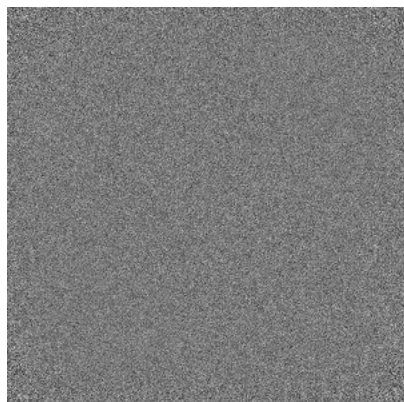


Y Index: 370

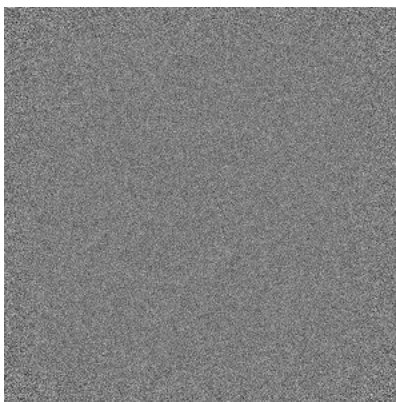


Z Index: 385

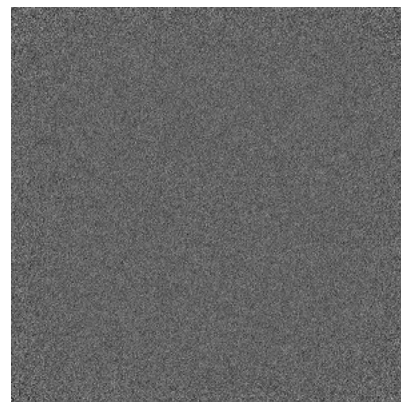
6.3.2 Raw map



X Index: 0



Y Index: 0

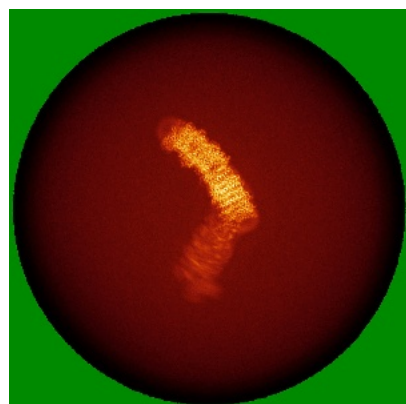


Z Index: 709

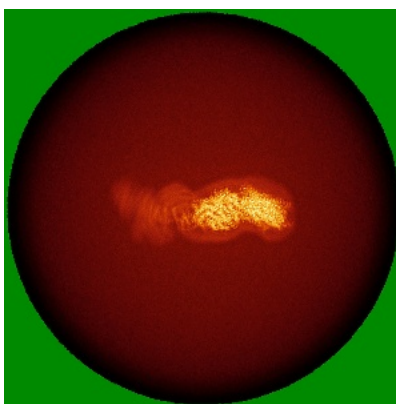
The images above show the largest variance slices of the map in three orthogonal directions.

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

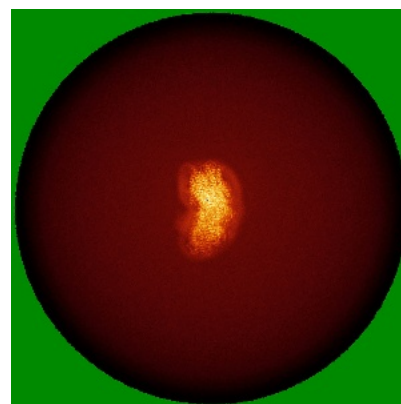
6.4.1 Primary map



X

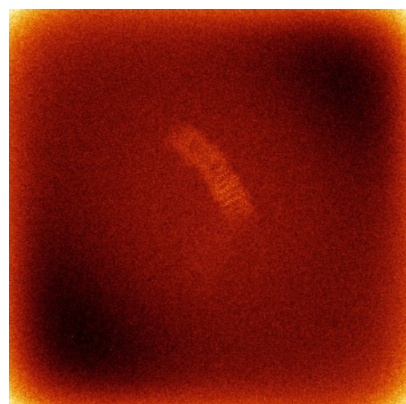


Y

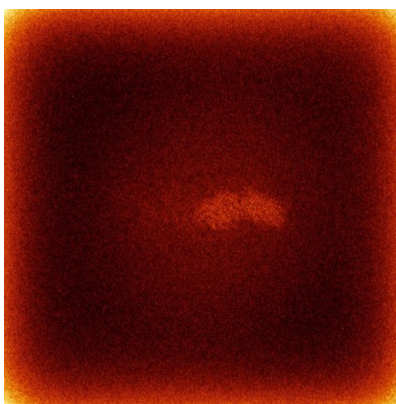


Z

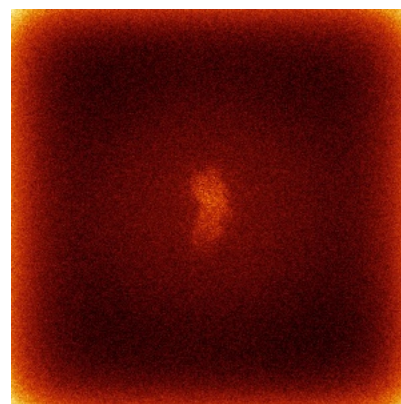
6.4.2 Raw map



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



X



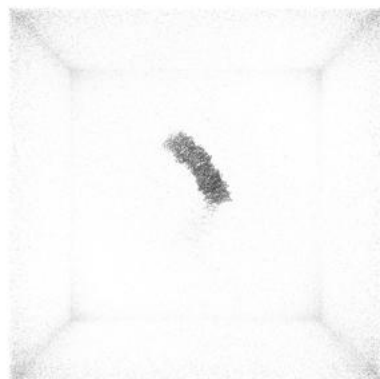
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

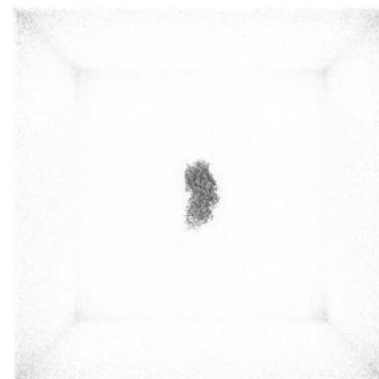
6.5.2 Raw map



X



Y



Z

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

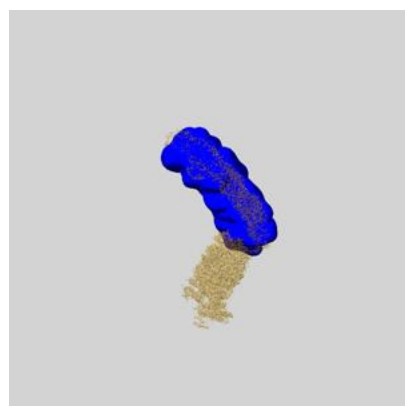
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

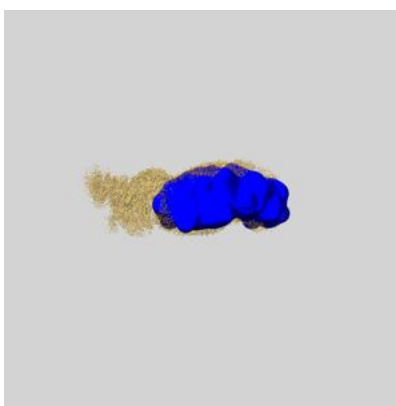
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

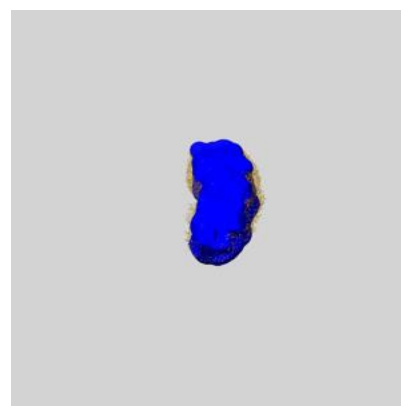
6.6.1 emd_55753_msk_1.map [i](#)



X



Y

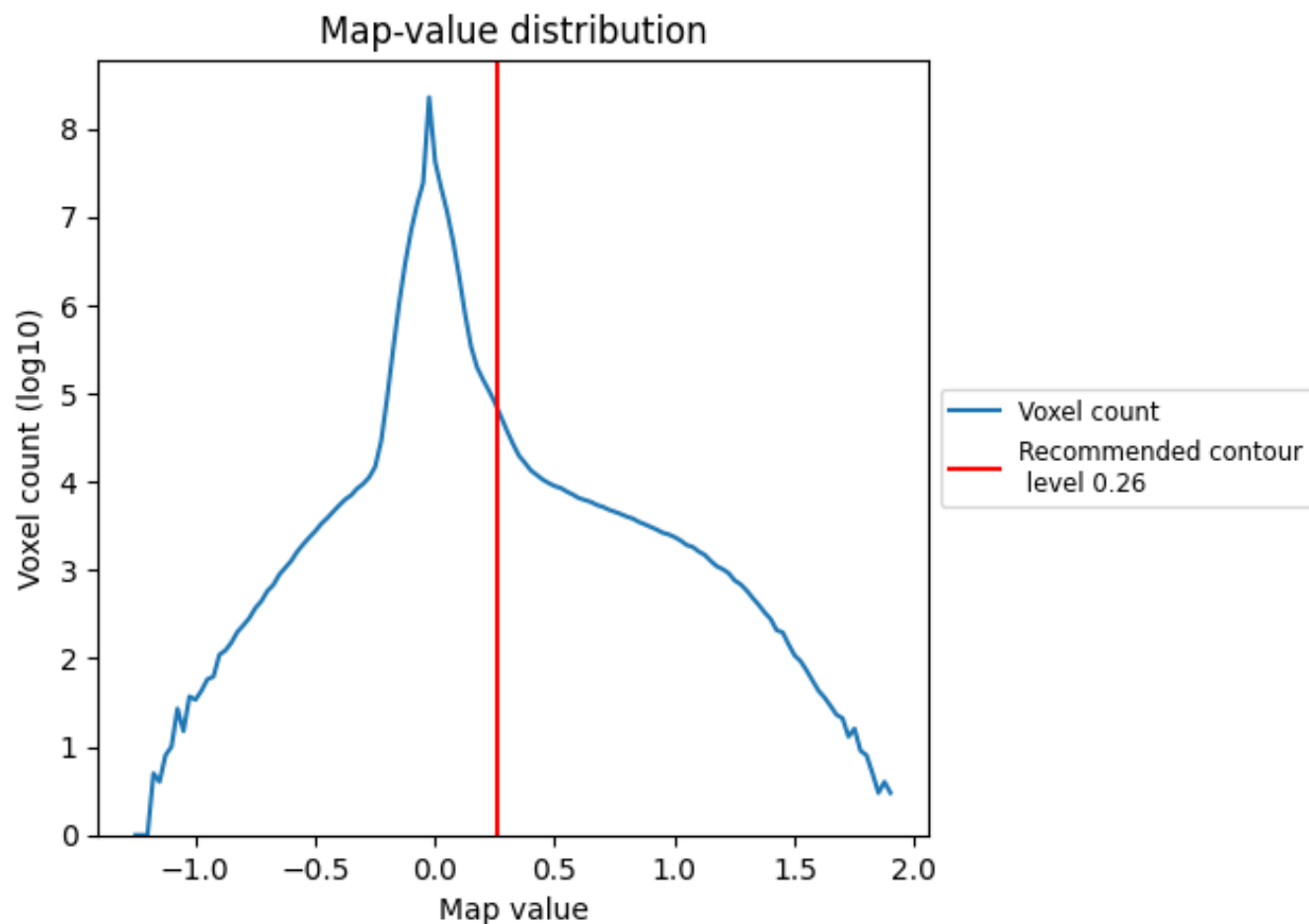


Z

7 Map analysis [i](#)

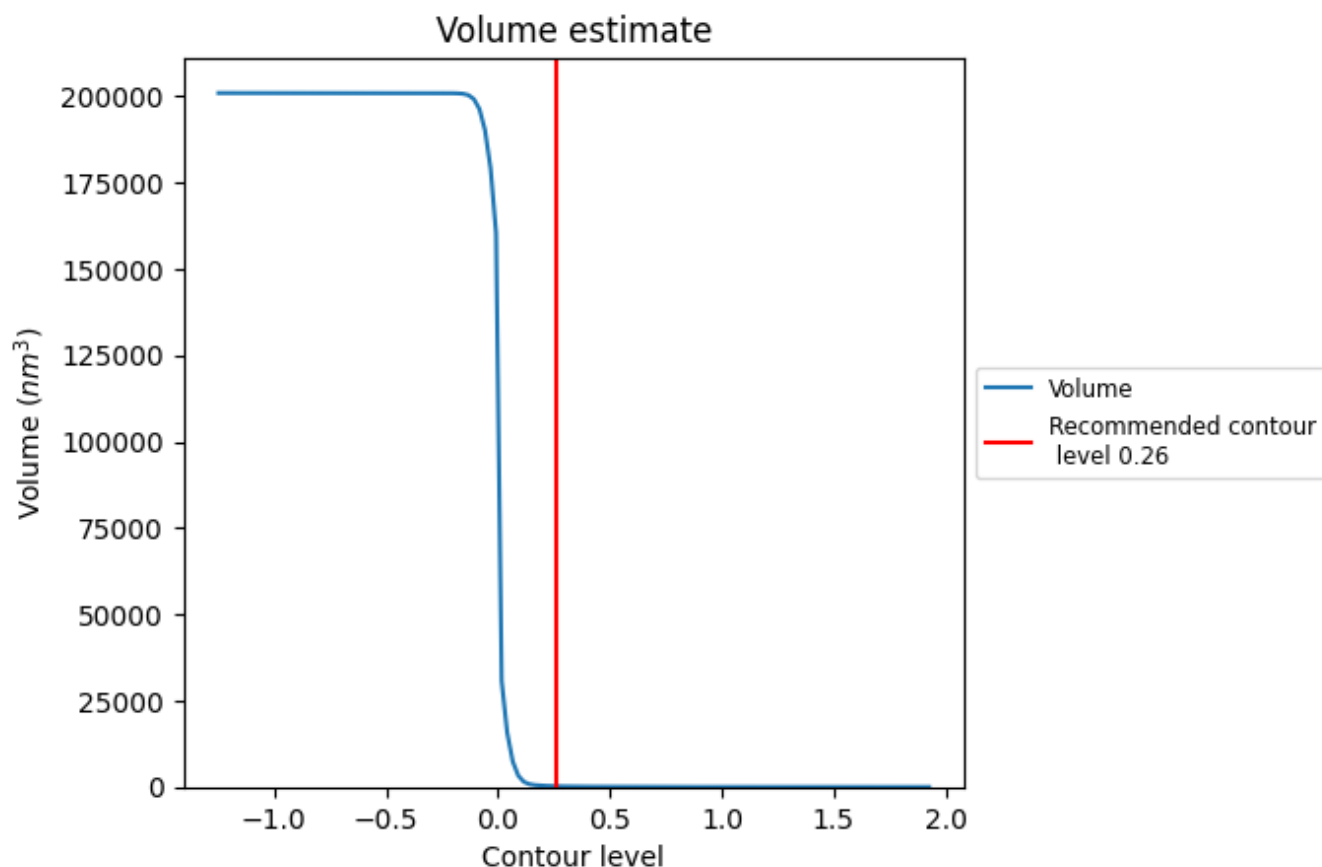
This section contains the results of statistical analysis of the map.

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.

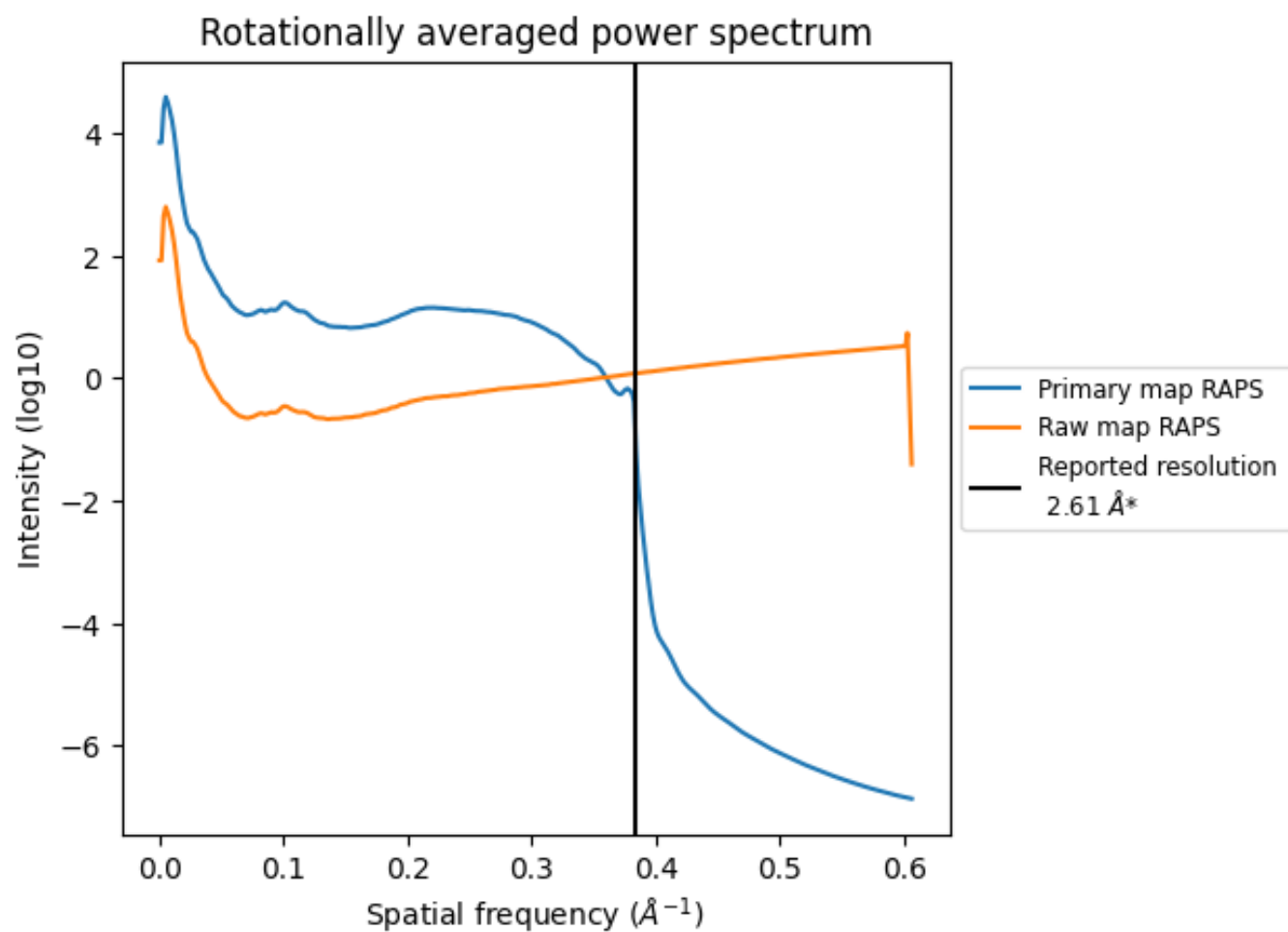
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

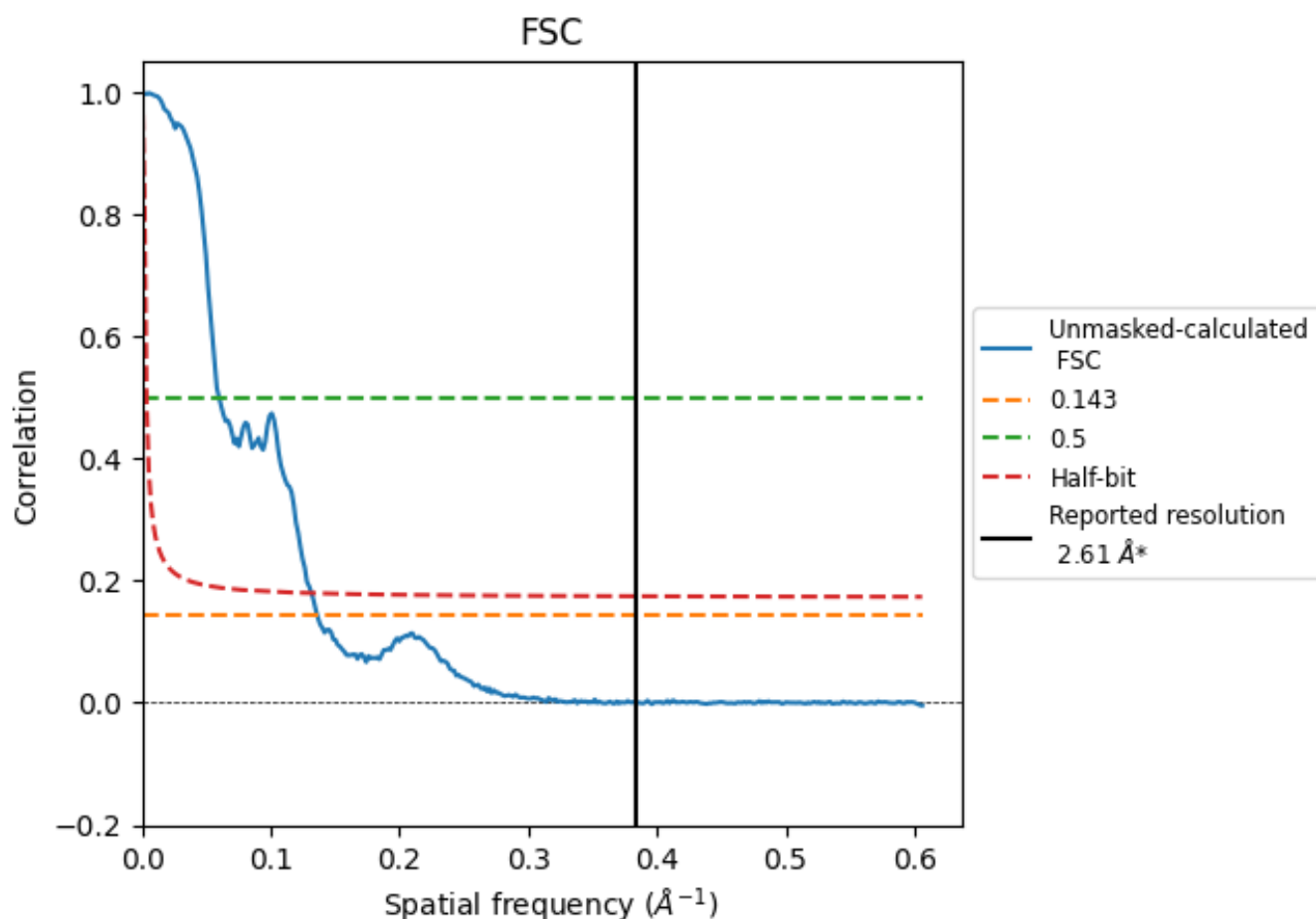


*Reported resolution corresponds to spatial frequency of 0.383 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.383 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

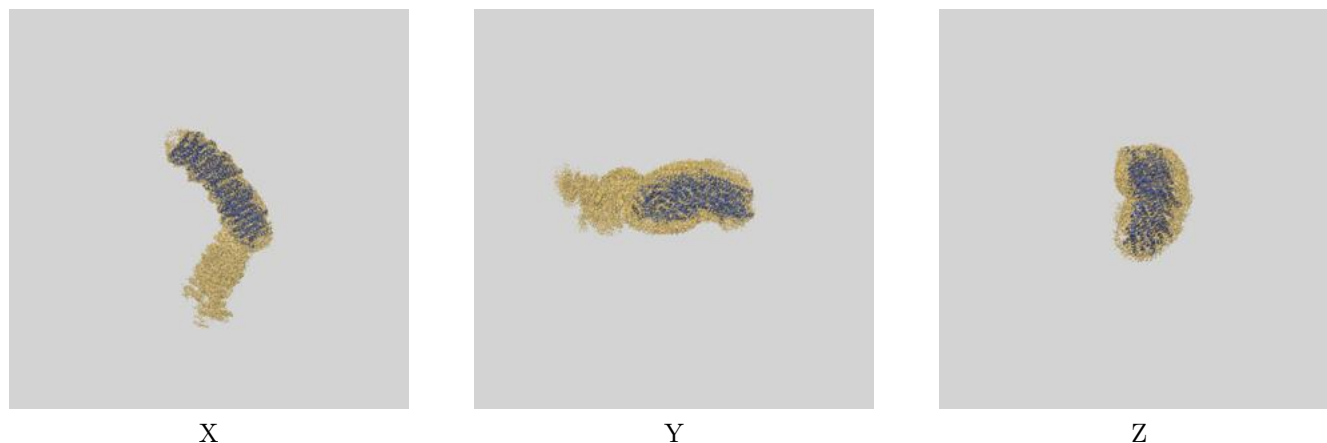
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.35	16.78	7.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.35 differs from the reported value 2.61 by more than 10 %

9 Map-model fit [i](#)

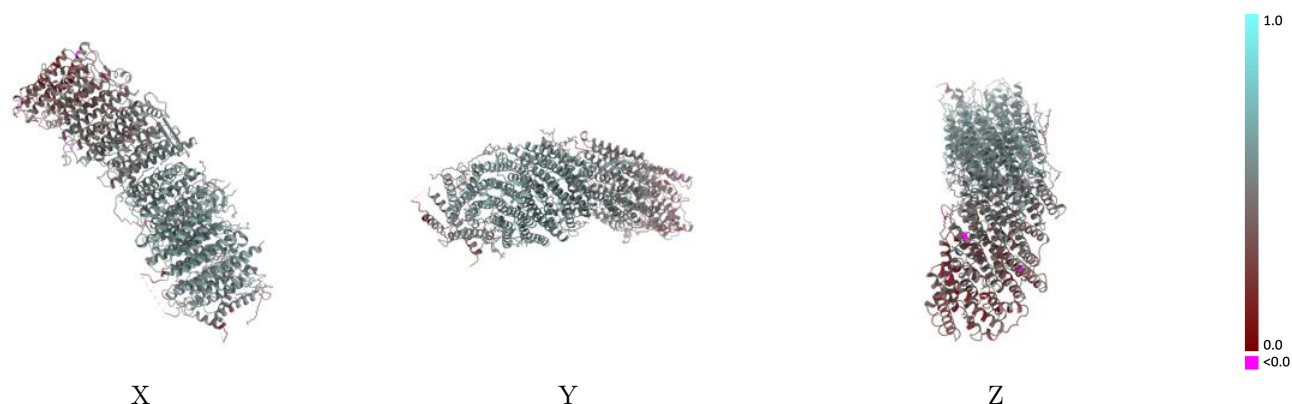
This section contains information regarding the fit between EMDB map EMD-55753 and PDB model 9TAO. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



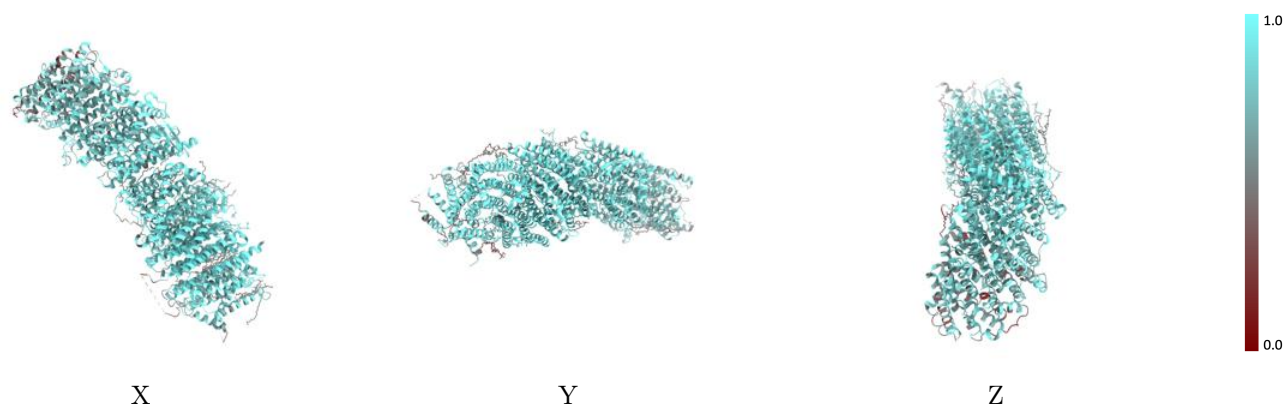
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



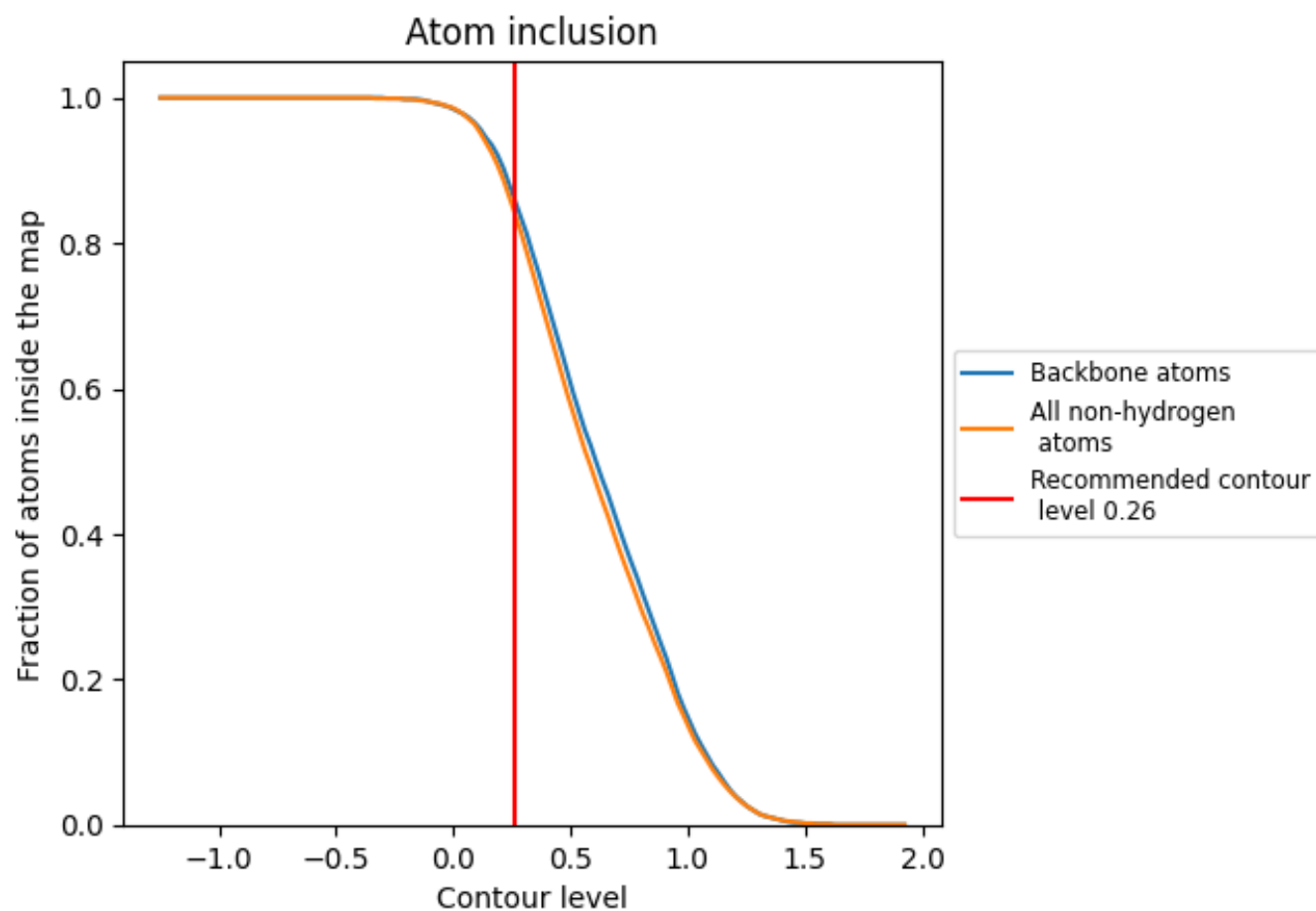
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.4920
A	0.8030	0.5180
H	0.8610	0.5240
J	0.9050	0.5600
K	0.9450	0.5860
L	0.7530	0.3820
M	0.8600	0.4840
N	0.9100	0.5640

1.0

0.0

<0.0