



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:27 AM UTC

PDB ID : 8FHK / pdb_00008fhk
EMDB ID : EMD-29087
Title : Heterodimeric ABC transporter BmrCD in the occluded conformation bound to ATP: BmrCD_OC-ATP
Authors : Tang, Q.; Mchaourab, H.
Deposited on : 2022-12-14
Resolution : 2.90 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.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

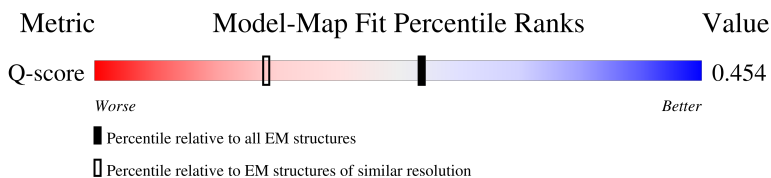
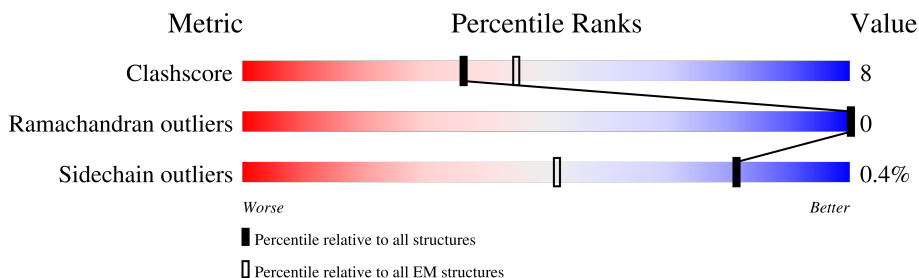
1 Overall quality at a glance

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	D	681	 79% 15% • 5%
2	C	607	 74% 18% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20406 atoms, of which 10286 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 Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	D	645	10395	3327	5234	880	937	17	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	154	ALA	CYS	engineered mutation	UNP O07549
D	256	ALA	CYS	engineered mutation	UNP O07549
D	351	ALA	CYS	engineered mutation	UNP O07549
D	592	GLN	GLU	engineered mutation	UNP O07549
D	674	LEU	-	expression tag	UNP O07549
D	675	GLU	-	expression tag	UNP O07549
D	676	HIS	-	expression tag	UNP O07549
D	677	HIS	-	expression tag	UNP O07549
D	678	HIS	-	expression tag	UNP O07549
D	679	HIS	-	expression tag	UNP O07549
D	680	HIS	-	expression tag	UNP O07549
D	681	HIS	-	expression tag	UNP O07549

- Molecule 2 is a protein called Probable multidrug resistance ABC transporter ATP-binding/permease protein YheI.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	574	9107	2917	4593	754	820	23	0	0

There are 24 discrepancies between the modelled and reference sequences:

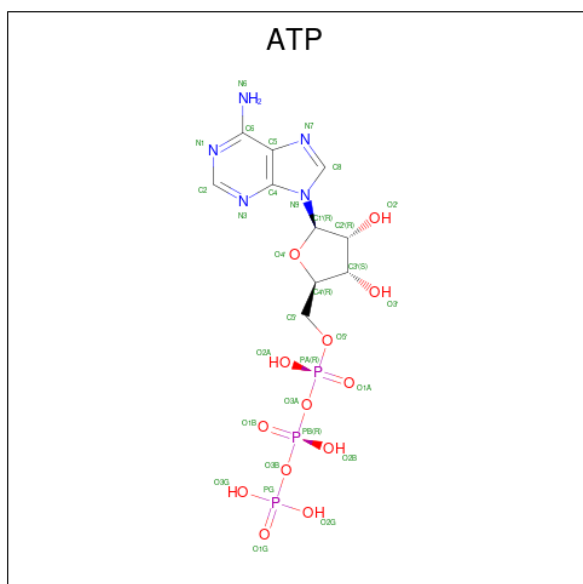
Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	initiating methionine	UNP O07550
C	-20	GLY	-	expression tag	UNP O07550
C	-19	SER	-	expression tag	UNP O07550

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	SER	-	expression tag	UNP O07550
C	-17	HIS	-	expression tag	UNP O07550
C	-16	HIS	-	expression tag	UNP O07550
C	-15	HIS	-	expression tag	UNP O07550
C	-14	HIS	-	expression tag	UNP O07550
C	-13	HIS	-	expression tag	UNP O07550
C	-12	HIS	-	expression tag	UNP O07550
C	-11	SER	-	expression tag	UNP O07550
C	-10	SER	-	expression tag	UNP O07550
C	-9	GLY	-	expression tag	UNP O07550
C	-8	LEU	-	expression tag	UNP O07550
C	-7	VAL	-	expression tag	UNP O07550
C	-6	PRO	-	expression tag	UNP O07550
C	-5	ARG	-	expression tag	UNP O07550
C	-4	GLY	-	expression tag	UNP O07550
C	-3	SER	-	expression tag	UNP O07550
C	-2	HIS	-	expression tag	UNP O07550
C	-1	MET	-	expression tag	UNP O07550
C	0	LEU	-	expression tag	UNP O07550
C	1	GLU	-	expression tag	UNP O07550
C	500	GLN	ASP	engineered mutation	UNP O07550

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf	
4	D	1	Total	C	H	O			0	
			46	17	26	3				
4	D	1	Total	C	H	N	O	P	0	
			24	5	13	1	4	1		
4	D	1	Total	C	H	N	O	P	0	
			69	22	38	1	7	1		
4	D	1	Total	C	H	O	P			0
			50	17	26	6	1			
4	D	1	Total	C	H	N	O	P	0	
			89	29	50	1	8	1		
4	D	1	Total	C	H	O	P			0
			76	25	42	8	1			
4	D	1	Total	C	H	O	P			0
			35	11	15	8	1			
4	D	1	Total	C	H	N	O	P	0	
			46	14	22	1	8	1		
4	D	1	Total	C	H	O	P			0
			45	15	21	8	1			

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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	H	O		0
			42	16	24	2		
4	D	1	Total	C	H	N	O	P
			38	11	18	1	7	1
4	C	1	Total	C	H	N	O	P
			58	18	30	1	8	1
4	C	1	Total	C	H			
			44	15	29			
4	C	1	Total	C	H	N	O	P
			69	22	39	1	6	1
4	C	1	Total	C	H	N	O	P
			60	19	33	1	6	1
4	C	1	Total	C	H	O	P	
			25	8	9	7	1	

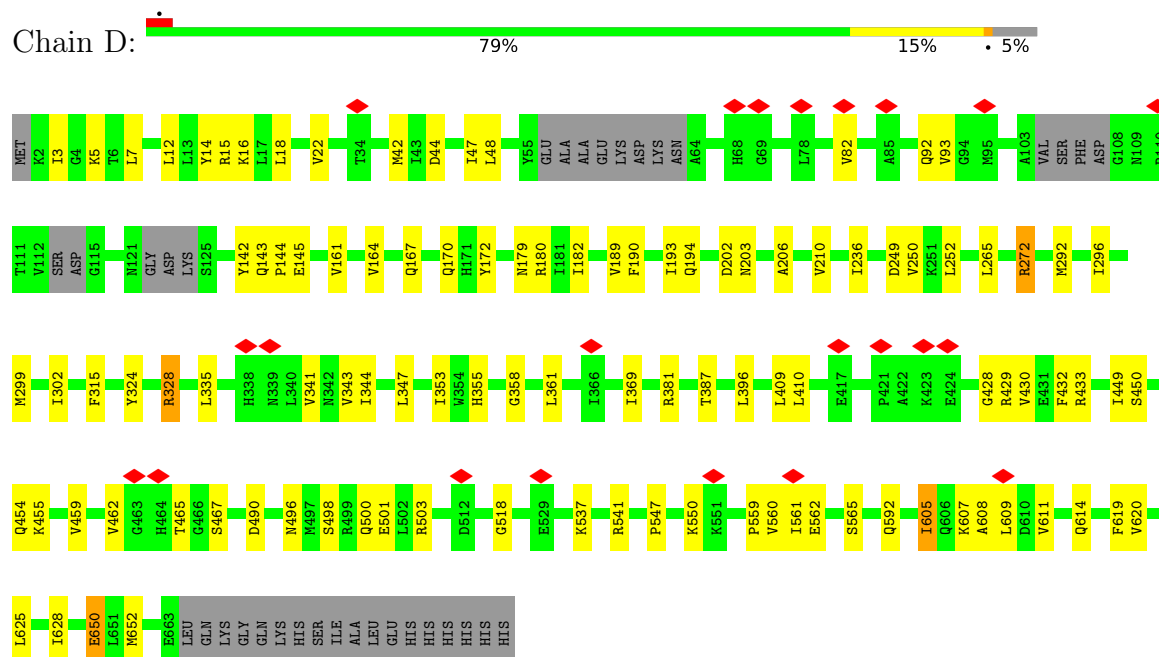
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	

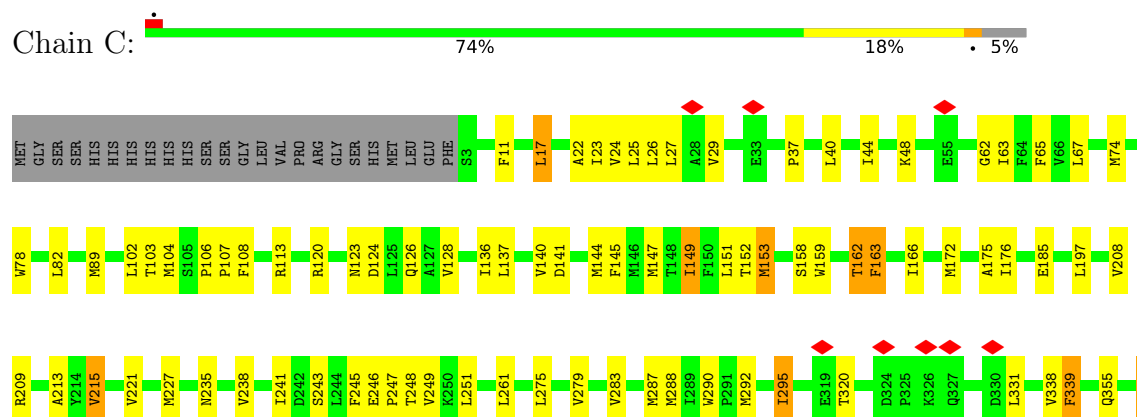
3 Residue-property plots

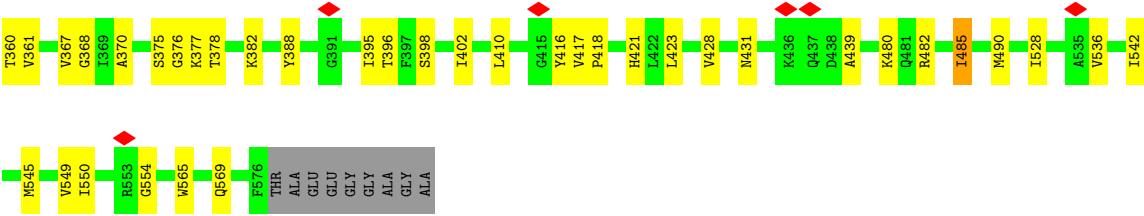
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH



- Molecule 2: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.905	Depositor
Minimum map value	-0.316	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.32	Depositor
Map size ($\text{\AA}$)	310.56, 310.56, 310.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.647, 0.647, 0.647	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, POV, MG

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	D	0.36	0/5257	0.64	11/7093 (0.2%)
2	C	0.51	4/4607 (0.1%)	0.80	13/6235 (0.2%)
All	All	0.43	4/9864 (0.0%)	0.72	24/13328 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	149	ILE	C-O	-7.01	1.15	1.24
2	C	295	ILE	C-O	-6.84	1.16	1.24
2	C	153	MET	C-O	-6.48	1.16	1.24
2	C	152	THR	C-O	-6.42	1.16	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	359	PHE	CA-C-O	-8.42	112.34	121.44
2	C	163	PHE	N-CA-C	-7.97	103.12	113.17
2	C	339	PHE	CA-C-N	7.72	133.39	120.88
2	C	339	PHE	C-N-CA	7.72	133.39	120.88
1	D	605	ILE	N-CA-C	-7.29	102.07	112.35
2	C	149	ILE	N-CA-C	-7.12	103.24	111.00
2	C	106	PRO	N-CA-C	6.86	119.07	110.70
1	D	315	PHE	CA-C-O	-6.78	113.62	121.07
2	C	17	LEU	N-CA-C	-6.68	105.70	114.31
2	C	162	THR	CB-CA-C	-6.63	98.40	109.55
1	D	496	ASN	N-CA-C	-6.13	105.66	113.02
1	D	344	ILE	N-CA-C	-5.99	104.47	111.00
1	D	369	ILE	N-CA-C	-5.91	107.05	112.96
2	C	153	MET	N-CA-C	-5.73	105.17	111.82
1	D	202	ASP	O-C-N	5.68	128.15	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	338	VAL	CB-CA-C	5.68	118.38	110.99
2	C	215	VAL	N-CA-C	5.66	121.11	109.34
2	C	251	LEU	CA-C-O	-5.63	114.88	121.07
2	C	485	ILE	CA-C-O	-5.54	115.51	121.27
1	D	650	GLU	N-CA-C	-5.25	105.58	112.72
1	D	328	ARG	N-CA-C	-5.24	106.86	113.20
1	D	592	GLN	CB-CA-C	5.14	119.31	111.80
1	D	343	VAL	CB-CA-C	-5.08	104.04	112.26
1	D	272	ARG	N-CA-C	-5.03	106.98	113.01

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	D	5161	5234	5230	68	0
2	C	4514	4593	4592	94	0
3	C	31	12	12	2	0
3	D	31	12	12	1	0
4	C	116	140	140	12	0
4	D	265	295	295	6	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10120	10286	10281	157	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 (157) 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:D:252:LEU:HD21	1:D:355:HIS:CG	2.28	0.68
2:C:545:MET:SD	2:C:550:ILE:HG22	2.37	0.65
2:C:22:ALA:HB1	2:C:78:TRP:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:TYR:HB3	1:D:145:GLU:HB2	1.81	0.61
1:D:430:VAL:HG21	1:D:619:PHE:CZ	2.35	0.60
2:C:245:PHE:O	2:C:248:THR:HG22	2.01	0.60
1:D:324:TYR:CZ	1:D:328:ARG:HD2	2.35	0.59
2:C:63:ILE:O	2:C:67:LEU:HG	2.05	0.57
4:C:604:POV:H13A	4:C:604:POV:H1	1.87	0.57
2:C:421:HIS:HB3	2:C:480:LYS:HZ3	1.70	0.56
4:C:604:POV:H13A	4:C:604:POV:O12	2.05	0.56
1:D:500:GLN:HA	2:C:215:VAL:HG11	1.87	0.56
1:D:500:GLN:HA	2:C:215:VAL:CG1	2.37	0.55
2:C:361:VAL:HG22	2:C:367:VAL:HG21	1.89	0.54
2:C:22:ALA:HB1	2:C:78:TRP:HD1	1.71	0.54
2:C:378:THR:HG22	2:C:382:LYS:HE2	1.89	0.53
2:C:423:LEU:HD11	2:C:480:LYS:HG3	1.91	0.53
1:D:433:ARG:O	1:D:449:ILE:O	2.28	0.52
1:D:44:ASP:HA	1:D:48:LEU:HD12	1.92	0.52
2:C:104:MET:HE2	2:C:320:THR:HA	1.91	0.51
1:D:193:ILE:HG22	1:D:409:LEU:HD11	1.92	0.51
1:D:252:LEU:HD21	1:D:355:HIS:CD2	2.45	0.51
1:D:299:MET:HA	1:D:302:ILE:HG12	1.93	0.50
2:C:149:ILE:HG21	2:C:288:MET:HB2	1.94	0.50
2:C:158:SER:O	2:C:162:THR:HG23	2.12	0.50
2:C:376:GLY:HA2	3:C:601:ATP:C5'	2.42	0.50
1:D:430:VAL:HG21	1:D:619:PHE:CE1	2.47	0.49
4:C:604:POV:H23	4:C:604:POV:H13	1.94	0.49
2:C:396:THR:HG22	2:C:398:SER:O	2.11	0.49
2:C:368:GLY:HA3	2:C:536:VAL:HG23	1.94	0.48
1:D:462:VAL:HG11	1:D:467:SER:HB2	1.96	0.48
2:C:23:ILE:O	2:C:26:LEU:HG	2.13	0.48
2:C:172:MET:HE1	2:C:249:VAL:HG13	1.95	0.48
1:D:47:ILE:HG21	2:C:275:LEU:HD21	1.95	0.48
2:C:370:ALA:HA	2:C:377:LYS:HE2	1.96	0.48
2:C:339:PHE:HB2	2:C:359:PHE:HB3	1.96	0.48
1:D:14:TYR:O	1:D:18:LEU:HD23	2.14	0.47
1:D:324:TYR:CE2	1:D:328:ARG:HD2	2.48	0.47
2:C:238:VAL:O	2:C:241:ILE:HG22	2.14	0.47
1:D:625:LEU:HD13	1:D:628:ILE:HD11	1.97	0.47
2:C:159:TRP:HD1	4:C:602:POV:H14A	1.79	0.47
2:C:163:PHE:O	2:C:163:PHE:CD2	2.68	0.47
1:D:92:GLN:OE1	2:C:48:LYS:HE3	2.15	0.47
2:C:123:ASN:OD1	2:C:126:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:THR:O	1:D:465:THR:HG22	2.15	0.47
2:C:144:MET:SD	2:C:145:PHE:N	2.88	0.47
2:C:26:LEU:HA	2:C:29:VAL:HG22	1.97	0.47
2:C:44:ILE:HD11	2:C:279:VAL:HB	1.96	0.47
2:C:23:ILE:O	2:C:27:LEU:HG	2.16	0.46
2:C:439:ALA:HB1	2:C:490:MET:CE	2.44	0.46
2:C:29:VAL:HG13	2:C:74:MET:HE3	1.96	0.46
2:C:368:GLY:HA2	2:C:528:ILE:CG2	2.45	0.46
1:D:22:VAL:HG23	1:D:236:ILE:HD11	1.97	0.46
1:D:161:VAL:HA	1:D:164:VAL:HB	1.97	0.46
1:D:562:GLU:HG3	2:C:113:ARG:HH12	1.81	0.46
2:C:82:LEU:HD23	2:C:137:LEU:HB2	1.96	0.46
1:D:42:MET:HE1	2:C:261:LEU:HD23	1.97	0.46
2:C:377:LYS:HG2	3:C:601:ATP:O2B	2.15	0.46
2:C:136:ILE:O	2:C:140:VAL:HG22	2.15	0.46
1:D:429:ARG:HB3	1:D:490:ASP:OD1	2.16	0.46
2:C:25:LEU:HD11	2:C:74:MET:HG3	1.97	0.46
1:D:189:VAL:HA	1:D:410:LEU:HD21	1.98	0.45
2:C:65:PHE:CD2	4:C:603:POV:H31G	2.51	0.45
1:D:93:VAL:O	1:D:93:VAL:HG23	2.15	0.45
2:C:107:PRO:HG3	2:C:388:TYR:CD1	2.51	0.45
2:C:428:VAL:O	2:C:431:ASN:OD1	2.34	0.45
2:C:208:VAL:HG13	2:C:209:ARG:N	2.32	0.45
1:D:396:LEU:C	1:D:396:LEU:HD23	2.41	0.45
1:D:537:LYS:O	1:D:541:ARG:N	2.50	0.45
2:C:144:MET:SD	2:C:144:MET:C	3.00	0.45
1:D:430:VAL:HG21	1:D:619:PHE:HZ	1.77	0.45
1:D:650:GLU:C	1:D:652:MET:HE2	2.41	0.45
2:C:159:TRP:CD1	4:C:602:POV:H14A	2.51	0.45
2:C:172:MET:O	2:C:176:ILE:HD12	2.17	0.45
2:C:23:ILE:HG13	2:C:24:VAL:N	2.32	0.45
2:C:175:ALA:HB1	2:C:245:PHE:HE1	1.82	0.45
2:C:292:MET:O	2:C:295:ILE:HG22	2.16	0.45
1:D:14:TYR:CZ	1:D:180:ARG:HB3	2.51	0.45
1:D:143:GLN:HB2	1:D:144:PRO:HD3	1.99	0.45
1:D:465:THR:HG23	3:D:701:ATP:O1G	2.17	0.44
1:D:194:GLN:OE1	2:C:221:VAL:HG23	2.18	0.44
1:D:547:PRO:HA	1:D:550:LYS:HG2	2.00	0.44
2:C:162:THR:O	2:C:166:ILE:HG12	2.18	0.44
1:D:607:LYS:O	1:D:611:VAL:HG22	2.17	0.44
1:D:428:GLY:O	1:D:454:GLN:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:LEU:CD1	2:C:480:LYS:HG3	2.47	0.44
1:D:341:VAL:HG11	1:D:387:THR:CG2	2.48	0.44
1:D:498:SER:O	1:D:501:GLU:HG2	2.17	0.44
4:D:711:POV:H21D	4:D:711:POV:H27	1.99	0.44
2:C:528:ILE:HG23	2:C:528:ILE:O	2.17	0.44
2:C:542:ILE:N	2:C:554:GLY:O	2.49	0.44
2:C:331:LEU:H	2:C:331:LEU:HD23	1.83	0.43
1:D:608:ALA:O	1:D:611:VAL:HG23	2.18	0.43
2:C:120:ARG:O	2:C:124:ASP:HB2	2.18	0.43
1:D:179:ASN:O	1:D:182:ILE:HG12	2.18	0.43
1:D:560:VAL:HG11	1:D:565:SER:HB2	1.99	0.43
1:D:561:ILE:HB	2:C:113:ARG:NH1	2.33	0.43
2:C:246:GLU:N	2:C:247:PRO:HD2	2.34	0.43
2:C:482:ARG:HA	2:C:485:ILE:HG22	2.00	0.43
2:C:17:LEU:C	2:C:17:LEU:HD23	2.43	0.43
4:C:604:POV:H23	4:C:604:POV:H14	2.00	0.43
4:C:604:POV:H15	4:C:604:POV:H26	2.01	0.43
1:D:335:LEU:HD12	1:D:335:LEU:O	2.18	0.43
1:D:605:ILE:HG23	1:D:609:LEU:HD12	2.01	0.43
2:C:78:TRP:CH2	2:C:137:LEU:HG	2.54	0.43
2:C:359:PHE:O	2:C:360:THR:HG23	2.19	0.43
2:C:368:GLY:HA2	2:C:528:ILE:HG23	2.00	0.43
1:D:432:PHE:O	1:D:450:SER:HA	2.19	0.43
2:C:153:MET:HB3	2:C:162:THR:HG22	2.01	0.43
1:D:82:VAL:HG23	1:D:82:VAL:O	2.19	0.42
1:D:172:TYR:CZ	4:D:709:POV:O14	2.72	0.42
1:D:5:LYS:HA	4:D:705:POV:H1A	2.00	0.42
1:D:292:MET:O	1:D:296:ILE:HG12	2.19	0.42
1:D:518:GLY:O	1:D:559:PRO:HD2	2.19	0.42
2:C:37:PRO:HG3	2:C:287:MET:HE1	2.02	0.42
2:C:37:PRO:CG	2:C:287:MET:HE1	2.49	0.42
2:C:197:LEU:HD13	2:C:227:MET:HE1	2.00	0.42
2:C:163:PHE:HB2	4:C:602:POV:H25	2.00	0.42
2:C:375:SER:O	2:C:545:MET:CE	2.67	0.42
1:D:12:LEU:O	1:D:15:ARG:HG3	2.18	0.42
2:C:355:GLN:HB3	2:C:549:VAL:HG22	2.01	0.42
1:D:561:ILE:CG2	2:C:113:ARG:CZ	2.98	0.42
2:C:402:ILE:HD11	2:C:410:LEU:HD11	2.02	0.42
1:D:190:PHE:HA	1:D:193:ILE:HG12	2.02	0.42
2:C:102:LEU:O	2:C:103:THR:HG22	2.20	0.42
2:C:565:TRP:O	2:C:569:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:628:ILE:O	1:D:628:ILE:HD12	2.20	0.42
1:D:381:ARG:NE	2:C:290:TRP:CH2	2.88	0.42
1:D:459:VAL:HG12	1:D:620:VAL:HB	2.02	0.42
2:C:62:GLY:HA2	4:C:603:POV:H313	2.01	0.42
1:D:265:LEU:HD11	4:D:707:POV:H33A	2.02	0.41
2:C:147:MET:O	2:C:151:LEU:HD13	2.20	0.41
2:C:11:PHE:CG	2:C:89:MET:SD	3.13	0.41
2:C:166:ILE:O	2:C:166:ILE:HG22	2.20	0.41
2:C:153:MET:HB3	2:C:162:THR:CG2	2.51	0.41
2:C:235:ASN:O	2:C:238:VAL:HG12	2.20	0.41
2:C:359:PHE:CE1	2:C:361:VAL:CG2	3.04	0.41
1:D:503:ARG:HD2	2:C:213:ALA:HA	2.01	0.41
2:C:124:ASP:O	2:C:128:VAL:HG23	2.21	0.41
2:C:283:VAL:HG12	2:C:287:MET:HE2	2.03	0.41
1:D:358:GLY:O	1:D:361:LEU:HD22	2.20	0.41
4:C:604:POV:H13	4:C:604:POV:C22	2.51	0.41
1:D:167:GLN:HA	1:D:170:GLN:HG3	2.03	0.41
1:D:455:LYS:HD3	1:D:614:GLN:O	2.20	0.41
2:C:159:TRP:HB2	4:C:602:POV:H14A	2.01	0.41
2:C:375:SER:O	2:C:545:MET:HE2	2.21	0.40
2:C:417:VAL:N	2:C:418:PRO:HD3	2.35	0.40
1:D:3:ILE:O	1:D:7:LEU:HD23	2.21	0.40
1:D:272:ARG:HD2	4:D:706:POV:H34A	2.03	0.40
2:C:243:SER:O	2:C:247:PRO:HD3	2.21	0.40
1:D:16:LYS:HB2	4:D:704:POV:H25	2.03	0.40
1:D:206:ALA:O	1:D:210:VAL:HG23	2.21	0.40
1:D:249:ASP:OD1	1:D:250:VAL:N	2.55	0.40
1:D:353:ILE:HD11	2:C:40:LEU:HD12	2.04	0.40
2:C:140:VAL:HG23	2:C:141:ASP:N	2.36	0.40
2:C:185:GLU:OE1	2:C:185:GLU:N	2.53	0.40
2:C:395:ILE:HB	2:C:402:ILE:HB	2.03	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	D	635/681 (93%)	596 (94%)	39 (6%)	0	100	100
2	C	572/607 (94%)	527 (92%)	45 (8%)	0	100	100
All	All	1207/1288 (94%)	1123 (93%)	84 (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	D	550/581 (95%)	548 (100%)	2 (0%)	84	94
2	C	484/508 (95%)	482 (100%)	2 (0%)	84	94
All	All	1034/1089 (95%)	1030 (100%)	4 (0%)	81	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	203	ASN
1	D	347	LEU
2	C	108	PHE
2	C	416	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	66	GLN
1	D	293	ASN
1	D	322	HIS
1	D	346	ASN
1	D	538	ASN
2	C	112	ASN

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Mol	Chain	Res	Type
2	C	573	GLN
2	C	574	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	D	710	-	23,23,51	0.53	0	26,28,59	0.66	1 (3%)
4	POV	D	702	-	19,19,51	0.37	0	19,19,59	0.28	0
4	POV	C	605	-	26,26,51	0.38	0	31,32,59	0.48	0
4	POV	D	708	-	19,19,51	0.90	1 (5%)	20,23,59	0.88	1 (5%)
4	POV	D	709	-	23,23,51	0.38	0	29,31,59	0.65	1 (3%)
3	ATP	C	601	5	32,33,33	0.77	1 (3%)	48,52,52	1.32	5 (10%)
4	POV	D	706	-	38,38,51	0.34	0	44,46,59	0.39	0
4	POV	C	602	-	27,27,51	0.42	0	33,35,59	0.42	0
4	POV	D	703	-	10,10,51	1.19	1 (10%)	15,15,59	0.88	1 (6%)
4	POV	C	606	-	15,15,51	1.19	2 (13%)	17,19,59	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	D	712	-	19,19,51	0.58	0	24,26,59	0.49	0
4	POV	C	603	-	14,14,51	0.21	0	13,13,59	0.08	0
4	POV	D	704	-	30,30,51	0.52	0	35,37,59	0.42	0
4	POV	D	705	-	23,23,51	0.57	0	26,26,59	0.57	1 (3%)
4	POV	C	604	-	29,29,51	0.41	0	34,35,59	0.50	0
4	POV	D	711	-	17,17,51	0.38	0	17,17,59	0.23	0
3	ATP	D	701	5	32,33,33	0.83	1 (3%)	48,52,52	0.80	0
4	POV	D	707	-	33,33,51	0.48	0	36,38,59	0.61	1 (2%)

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
4	POV	D	710	-	-	7/25/25/55	-
4	POV	D	702	-	-	7/18/18/55	-
4	POV	C	605	-	-	10/27/27/55	-
4	POV	D	708	-	-	1/20/20/55	-
4	POV	D	709	-	-	8/26/26/55	-
3	ATP	C	601	5	-	6/22/38/38	0/3/3/3
4	POV	D	706	-	-	15/42/42/55	-
4	POV	C	602	-	-	9/31/31/55	-
4	POV	D	703	-	-	4/8/8/55	-
4	POV	C	606	-	-	6/16/16/55	-
4	POV	D	712	-	-	12/21/21/55	-
4	POV	C	603	-	-	5/12/12/55	-
4	POV	D	704	-	-	13/33/33/55	-
4	POV	D	705	-	-	6/22/22/55	-
4	POV	C	604	-	-	7/30/30/55	-
4	POV	D	711	-	-	9/16/16/55	-
3	ATP	D	701	5	-	11/22/38/38	0/3/3/3
4	POV	D	707	-	-	12/35/35/55	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	POV	P-O14	3.40	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	708	POV	P-O14	3.34	1.60	1.50
4	D	703	POV	P-O14	3.33	1.60	1.50
3	D	701	ATP	PG-O2G	-2.81	1.44	1.54
4	C	606	POV	O21-C21	-2.35	1.34	1.42
3	C	601	ATP	PB-O2B	-2.19	1.45	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ATP	O2B-PB-O3B	-4.75	94.43	107.27
3	C	601	ATP	O2G-PG-O3B	4.17	118.62	104.64
4	D	708	POV	O13-P-O12	3.24	119.97	107.80
3	C	601	ATP	O2B-PB-O3A	3.00	115.38	107.27
4	C	606	POV	O13-P-O12	2.93	118.78	107.80
4	D	703	POV	O13-P-O11	2.86	118.53	107.80
4	D	705	POV	O13-P-O14	2.39	120.15	110.83
3	C	601	ATP	O2A-PA-O3A	-2.37	100.86	107.27
4	D	709	POV	O13-P-O14	2.28	123.05	112.44
4	D	710	POV	O13-P-O14	2.26	119.65	110.83
4	D	707	POV	O13-P-O14	2.25	119.61	110.83
3	C	601	ATP	O2A-PA-O1A	2.08	122.11	112.44

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	701	ATP	C5'-O5'-PA-O1A
3	C	601	ATP	C5'-O5'-PA-O2A
4	D	704	POV	C2-C1-O11-P
4	D	704	POV	C210-C211-C212-C213
4	D	705	POV	O11-C1-C2-O21
4	D	706	POV	C1-O11-P-O12
4	D	706	POV	C11-O12-P-O11
4	D	706	POV	C11-O12-P-O13
4	D	706	POV	O12-C11-C12-N
4	D	706	POV	C22-C21-O21-C2
4	D	707	POV	O21-C2-C3-O31
4	D	708	POV	O22-C21-O21-C2
4	D	709	POV	C1-O11-P-O12
4	D	709	POV	C1-O11-P-O13
4	D	709	POV	O12-C11-C12-N
4	D	709	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
4	D	711	POV	C22-C21-O21-C2
4	D	712	POV	C1-O11-P-O12
4	D	712	POV	C1-O11-P-O14
4	D	712	POV	C11-O12-P-O13
4	C	604	POV	C11-O12-P-O14
4	C	604	POV	O12-C11-C12-N
4	C	605	POV	C1-O11-P-O14
4	D	709	POV	O22-C21-O21-C2
4	D	711	POV	O22-C21-O21-C2
4	D	702	POV	O22-C21-O21-C2
4	D	706	POV	O22-C21-O21-C2
4	D	702	POV	C22-C21-O21-C2
4	D	704	POV	C211-C210-C29-C28
4	D	706	POV	C32-C31-O31-C3
4	D	709	POV	O32-C31-O31-C3
4	D	706	POV	O32-C31-O31-C3
4	D	709	POV	C32-C31-O31-C3
4	C	604	POV	C211-C210-C29-C28
4	D	710	POV	C32-C31-O31-C3
4	C	606	POV	C32-C31-O31-C3
4	D	710	POV	O32-C31-O31-C3
4	C	605	POV	C211-C210-C29-C28
4	D	703	POV	C11-C12-N-C14
4	D	704	POV	C21-C22-C23-C24
4	C	606	POV	O32-C31-O31-C3
4	D	706	POV	C211-C210-C29-C28
4	D	705	POV	C1-C2-O21-C21
4	D	702	POV	O11-C1-C2-O21
4	C	604	POV	O11-C1-C2-O21
4	C	605	POV	C22-C21-O21-C2
4	D	707	POV	C2-C1-O11-P
4	C	605	POV	O22-C21-O21-C2
4	D	703	POV	C11-C12-N-C13
4	C	605	POV	C23-C24-C25-C26
4	D	704	POV	C25-C26-C27-C28
4	D	711	POV	C211-C212-C213-C214
4	C	602	POV	C32-C31-O31-C3
4	C	603	POV	C312-C313-C314-C315
3	D	701	ATP	O4'-C4'-C5'-O5'
4	D	707	POV	C23-C24-C25-C26
4	D	706	POV	C21-C22-C23-C24
4	D	703	POV	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
4	C	602	POV	O32-C31-O31-C3
4	D	707	POV	O22-C21-O21-C2
4	D	707	POV	C22-C21-O21-C2
4	D	707	POV	C211-C212-C213-C214
4	D	705	POV	C211-C210-C29-C28
4	D	706	POV	C33-C34-C35-C36
4	D	711	POV	C25-C26-C27-C28
4	C	606	POV	O11-C1-C2-C3
4	D	711	POV	C24-C25-C26-C27
4	D	707	POV	C1-C2-C3-O31
4	D	704	POV	C24-C25-C26-C27
4	C	605	POV	C24-C25-C26-C27
3	D	701	ATP	PB-O3B-PG-O1G
4	D	706	POV	C22-C23-C24-C25
4	D	707	POV	O32-C31-O31-C3
4	D	702	POV	C211-C210-C29-C28
4	D	707	POV	C32-C31-O31-C3
4	C	604	POV	C211-C212-C213-C214
4	D	704	POV	O21-C2-C3-O31
4	D	712	POV	O21-C2-C3-O31
4	C	604	POV	C27-C28-C29-C210
4	C	602	POV	C2-C3-O31-C31
4	D	706	POV	C25-C26-C27-C28
4	D	705	POV	C2-C1-O11-P
4	C	605	POV	C2-C1-O11-P
4	D	707	POV	O11-C1-C2-O21
4	D	712	POV	O11-C1-C2-O21
4	C	606	POV	O11-C1-C2-O21
3	C	601	ATP	C4'-C5'-O5'-PA
4	D	704	POV	C12-C11-O12-P
4	D	712	POV	C12-C11-O12-P
4	C	602	POV	C12-C11-O12-P
4	C	602	POV	O21-C2-C3-O31
4	D	712	POV	C2-C1-O11-P
3	D	701	ATP	C2'-C1'-N9-C8
3	D	701	ATP	PG-O3B-PB-O2B
4	D	703	POV	O12-C11-C12-N
4	D	704	POV	O12-C11-C12-N
4	C	602	POV	O12-C11-C12-N
4	C	605	POV	O11-C1-C2-O21
4	D	704	POV	C22-C23-C24-C25
4	D	705	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
4	D	702	POV	C24-C25-C26-C27
4	D	707	POV	O11-C1-C2-C3
4	D	711	POV	C212-C213-C214-C215
4	C	604	POV	C25-C26-C27-C28
4	D	711	POV	C27-C28-C29-C210
4	D	710	POV	O21-C2-C3-O31
4	D	704	POV	C1-C2-C3-O31
4	D	710	POV	C1-C2-C3-O31
4	D	712	POV	C1-C2-C3-O31
3	C	601	ATP	C5'-O5'-PA-O1A
3	C	601	ATP	C5'-O5'-PA-O3A
4	D	704	POV	C1-O11-P-O12
4	D	706	POV	C1-O11-P-O14
4	D	712	POV	C11-O12-P-O11
4	D	712	POV	C11-O12-P-O14
4	C	602	POV	C11-O12-P-O14
4	D	710	POV	C2-C1-O11-P
4	D	710	POV	C1-O11-P-O14
4	D	712	POV	O11-C1-C2-C3
4	C	605	POV	C27-C28-C29-C210
4	D	706	POV	C29-C210-C211-C212
4	D	711	POV	C29-C210-C211-C212
4	C	603	POV	C311-C310-C39-C38
4	C	605	POV	C25-C26-C27-C28
4	D	704	POV	C3-C2-O21-C21
4	D	710	POV	C3-C2-O21-C21
3	D	701	ATP	C2'-C1'-N9-C4
3	D	701	ATP	O4'-C1'-N9-C8
3	D	701	ATP	C3'-C4'-C5'-O5'
4	C	606	POV	C1-C2-O21-C21
4	C	606	POV	C3-C2-O21-C21
4	D	702	POV	C25-C26-C27-C28
4	C	602	POV	C1-C2-C3-O31
3	D	701	ATP	PB-O3B-PG-O3G
4	D	712	POV	C3-C2-O21-C21
4	D	709	POV	C12-C11-O12-P
4	D	705	POV	C24-C25-C26-C27
3	C	601	ATP	PB-O3A-PA-O1A
3	C	601	ATP	PB-O3A-PA-O2A
4	C	603	POV	C34-C35-C36-C37
4	D	702	POV	C26-C27-C28-C29
4	D	707	POV	C24-C25-C26-C27

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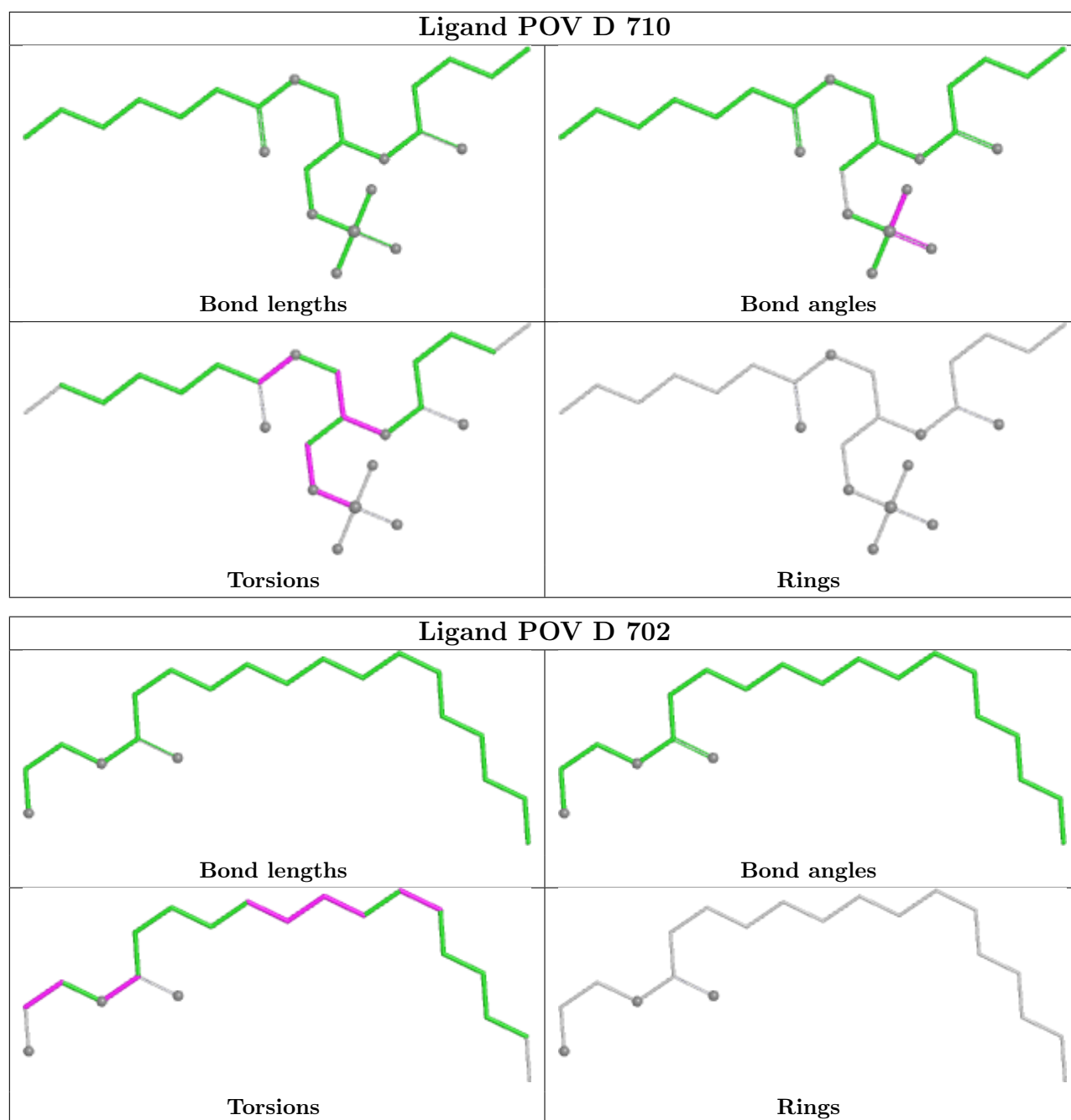
Mol	Chain	Res	Type	Atoms
4	C	602	POV	C1-C2-O21-C21
4	C	603	POV	C311-C312-C313-C314
3	D	701	ATP	PG-O3B-PB-O1B
3	D	701	ATP	PB-O3A-PA-O2A
4	D	711	POV	C26-C27-C28-C29
4	C	603	POV	C37-C38-C39-C310

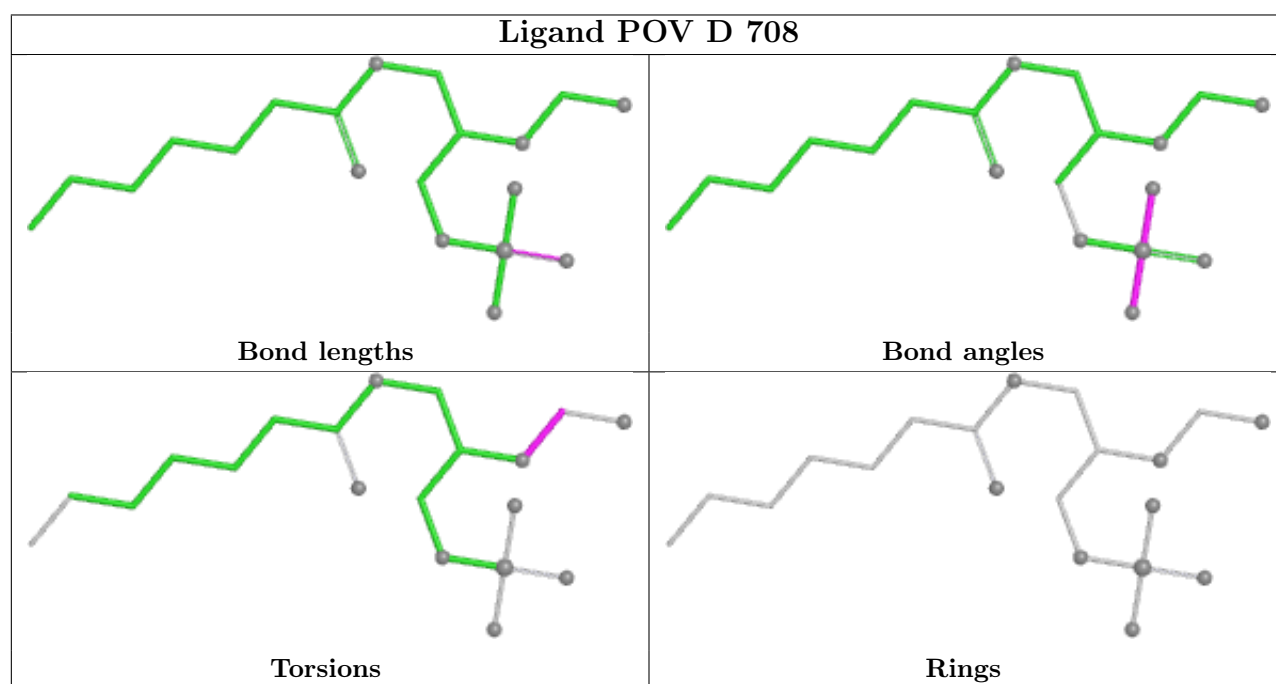
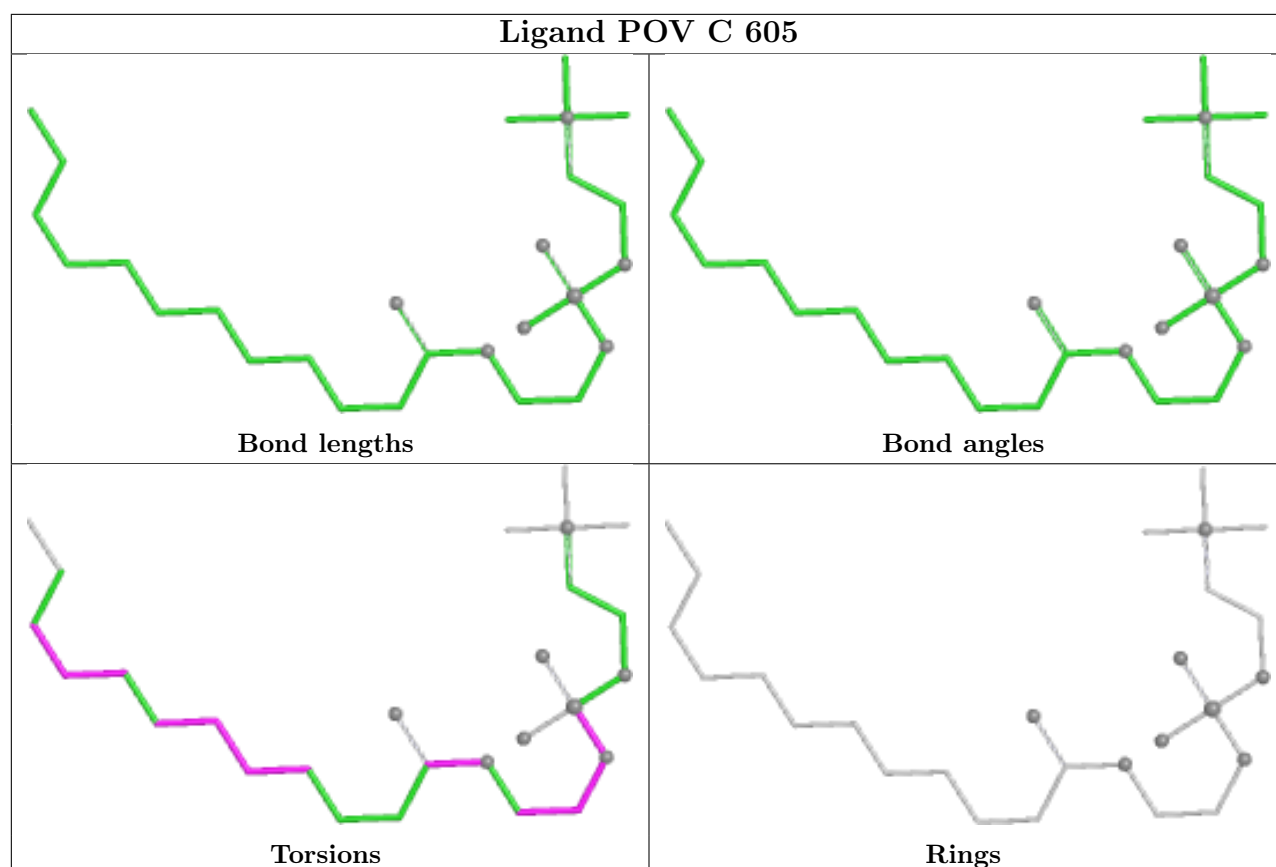
There are no ring outliers.

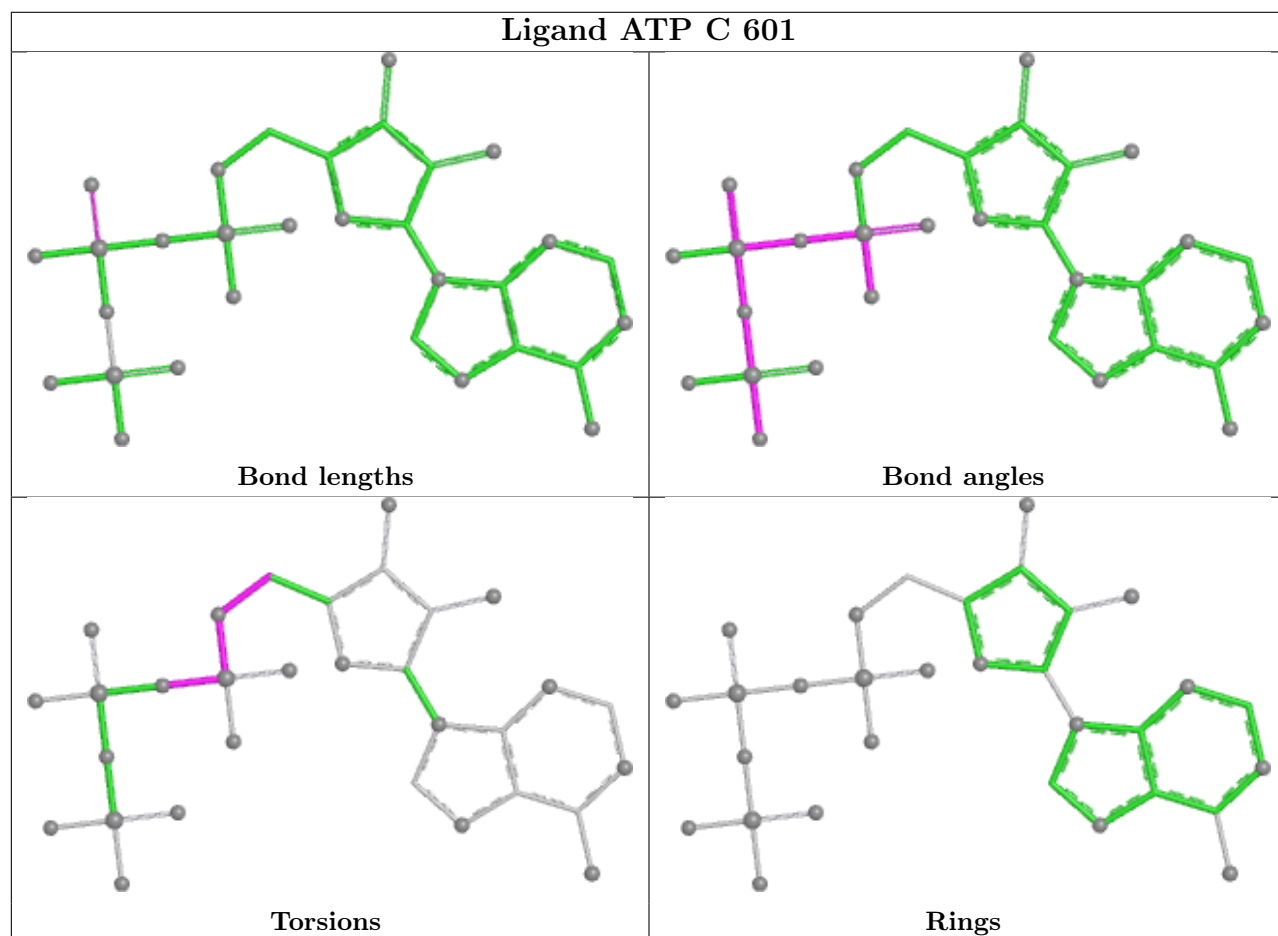
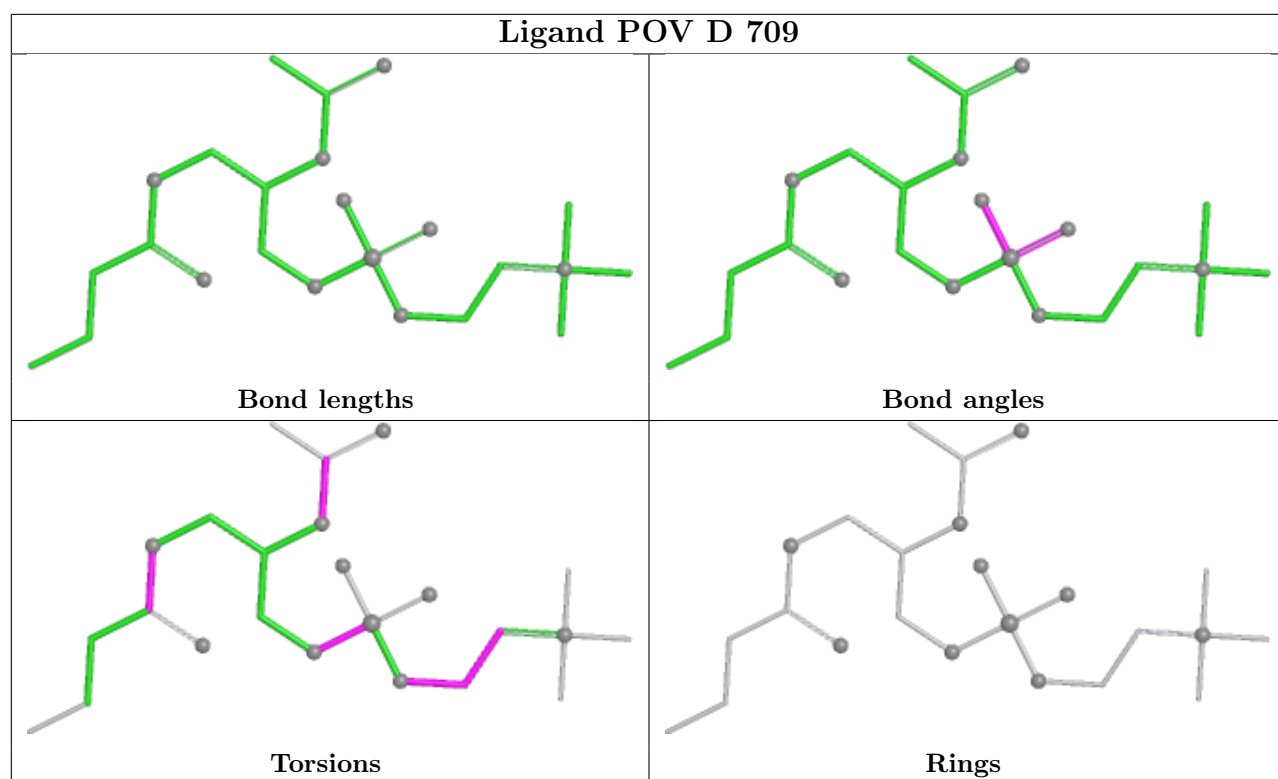
11 monomers are involved in 21 short contacts:

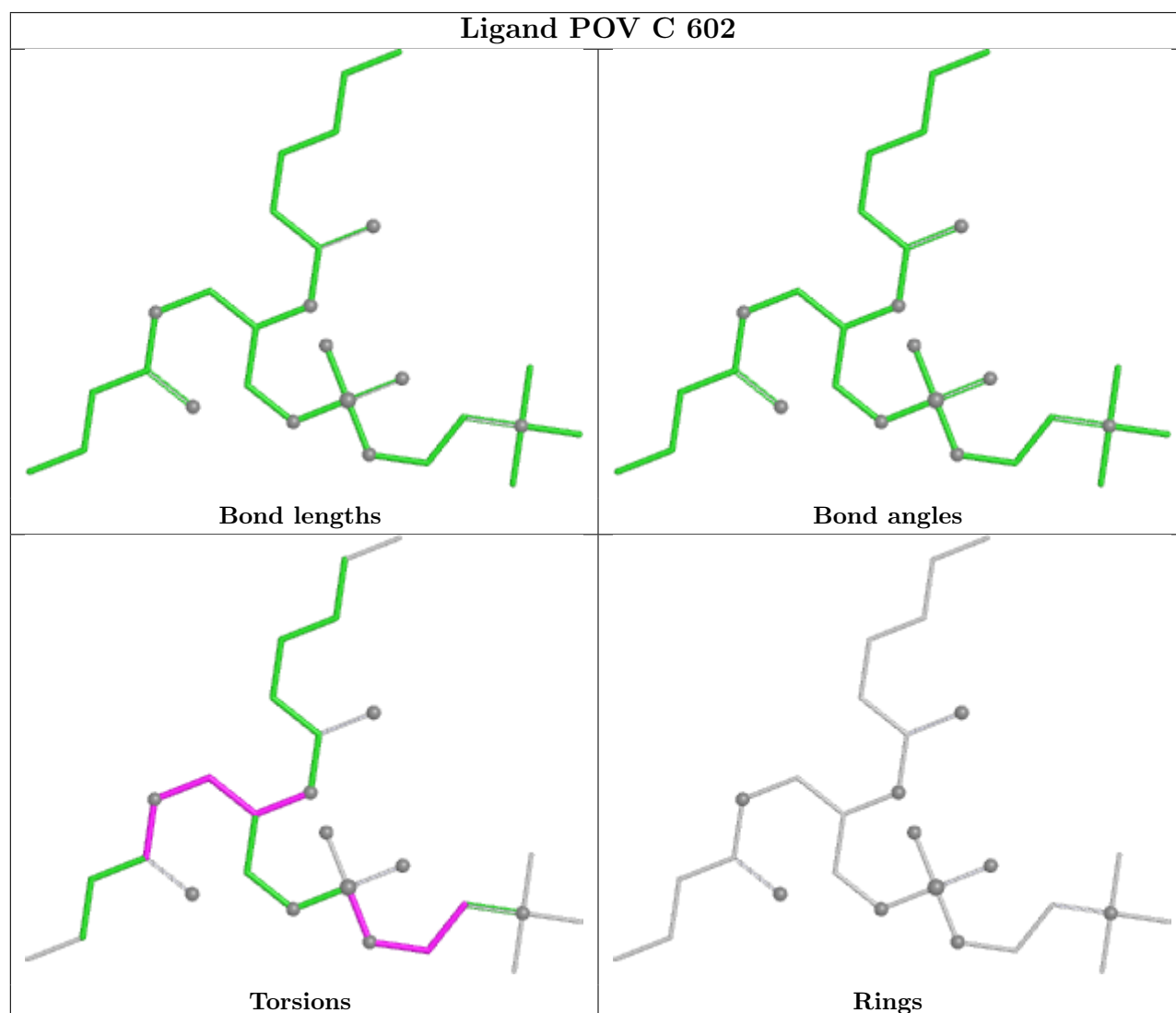
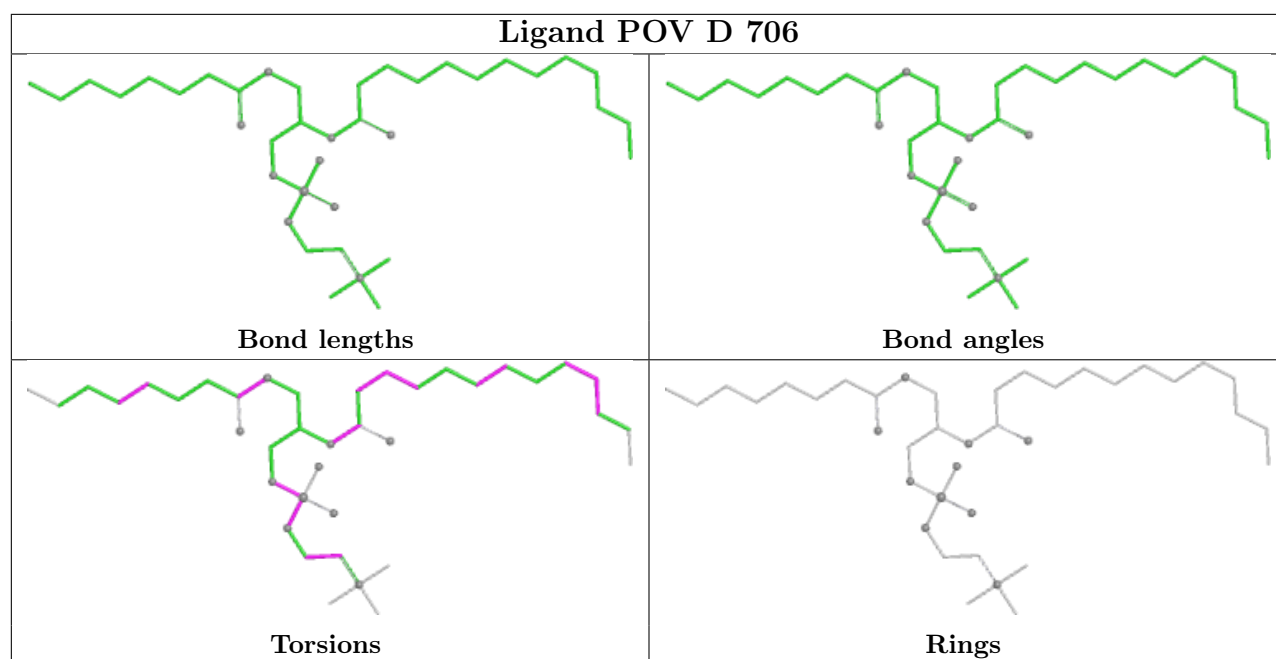
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	709	POV	1	0
3	C	601	ATP	2	0
4	D	706	POV	1	0
4	C	602	POV	4	0
4	C	603	POV	2	0
4	D	704	POV	1	0
4	D	705	POV	1	0
4	C	604	POV	6	0
4	D	711	POV	1	0
3	D	701	ATP	1	0
4	D	707	POV	1	0

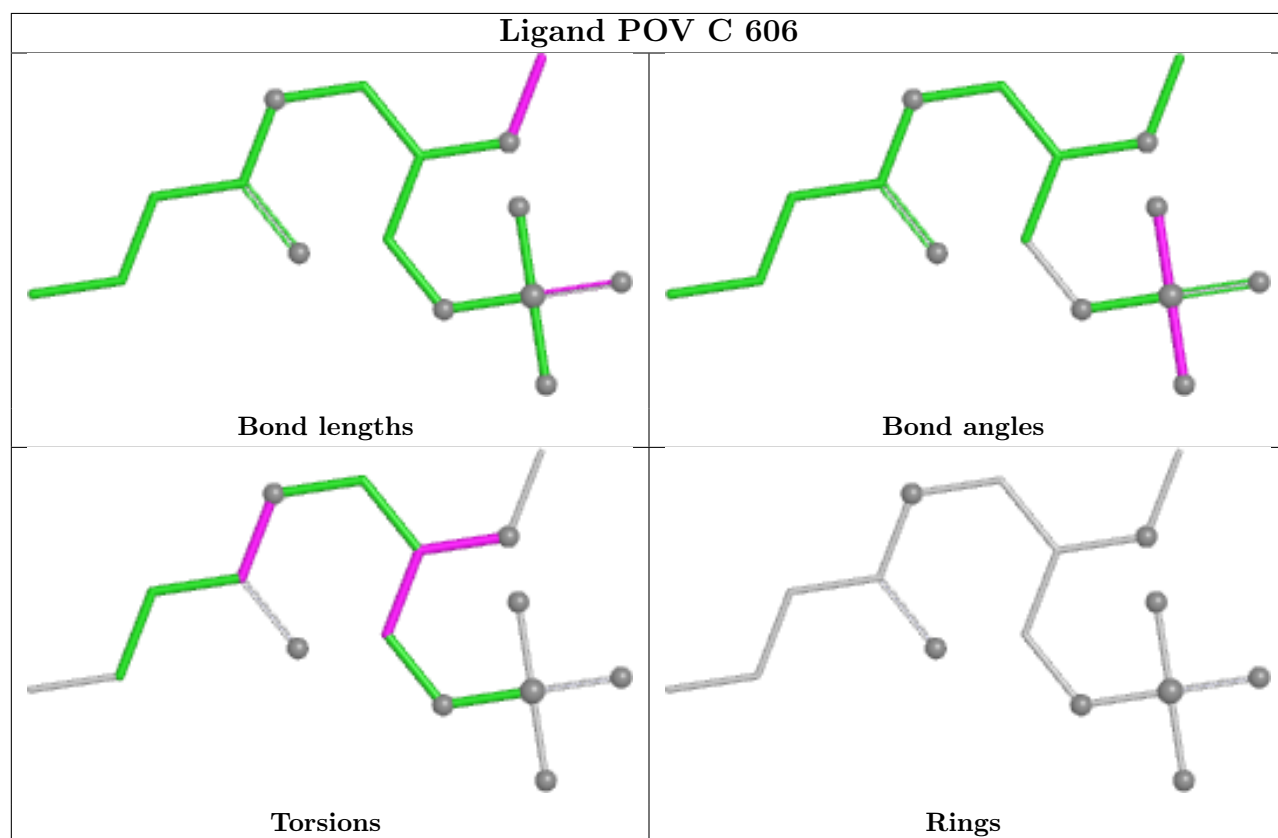
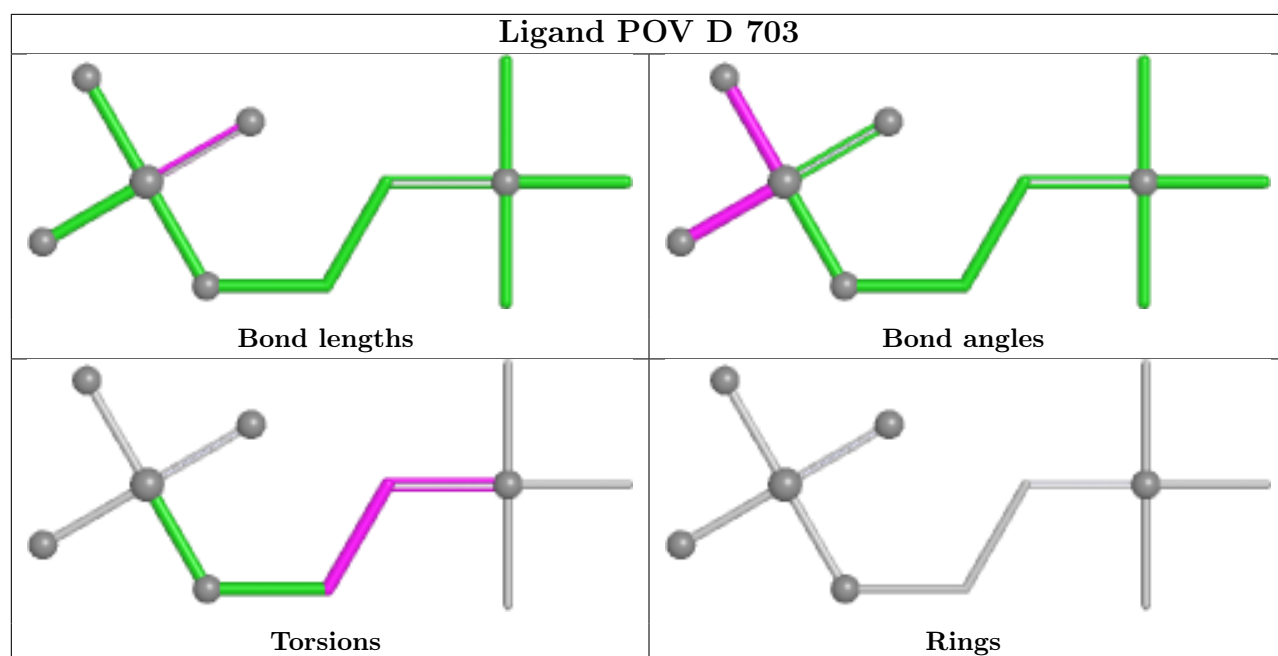
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

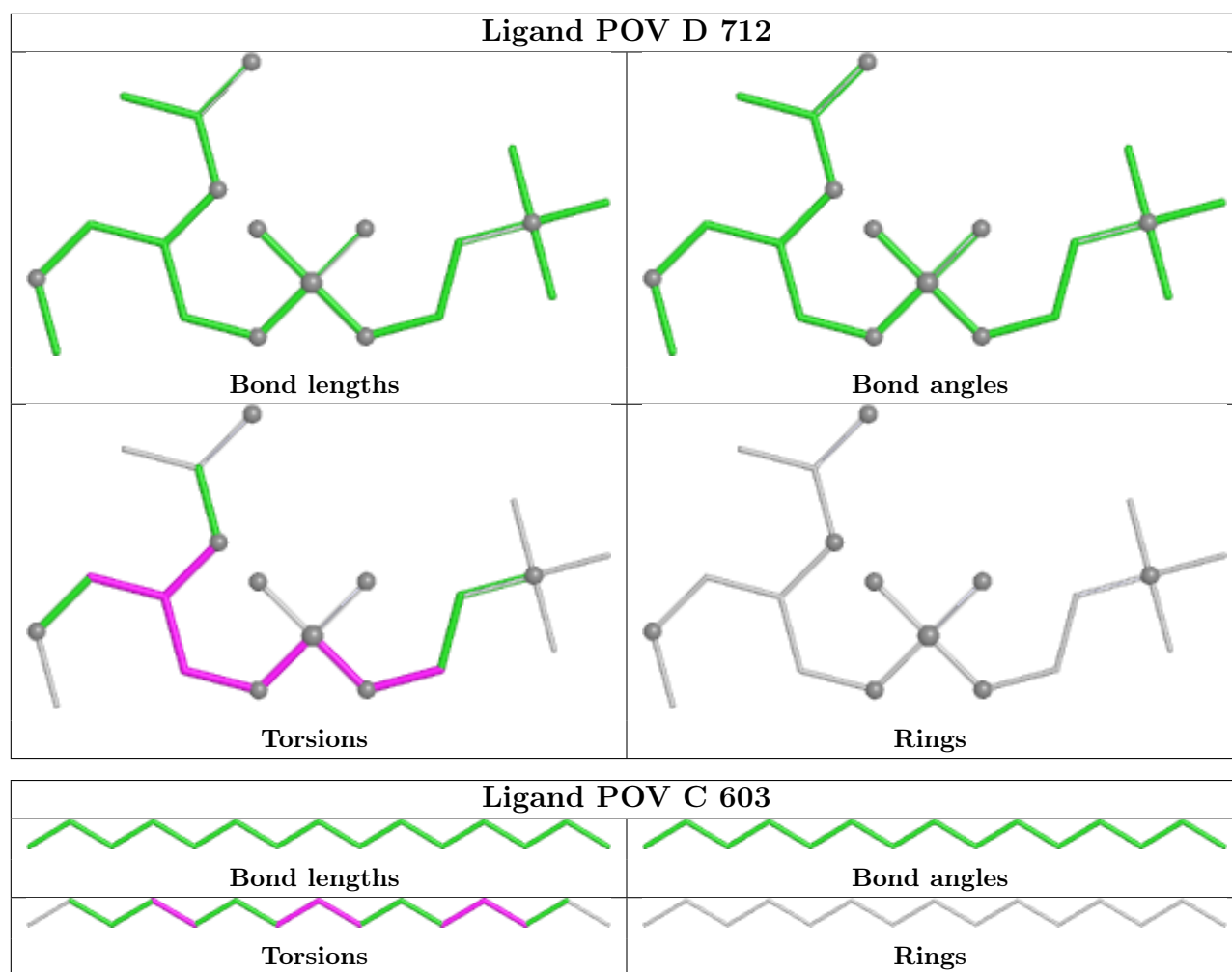


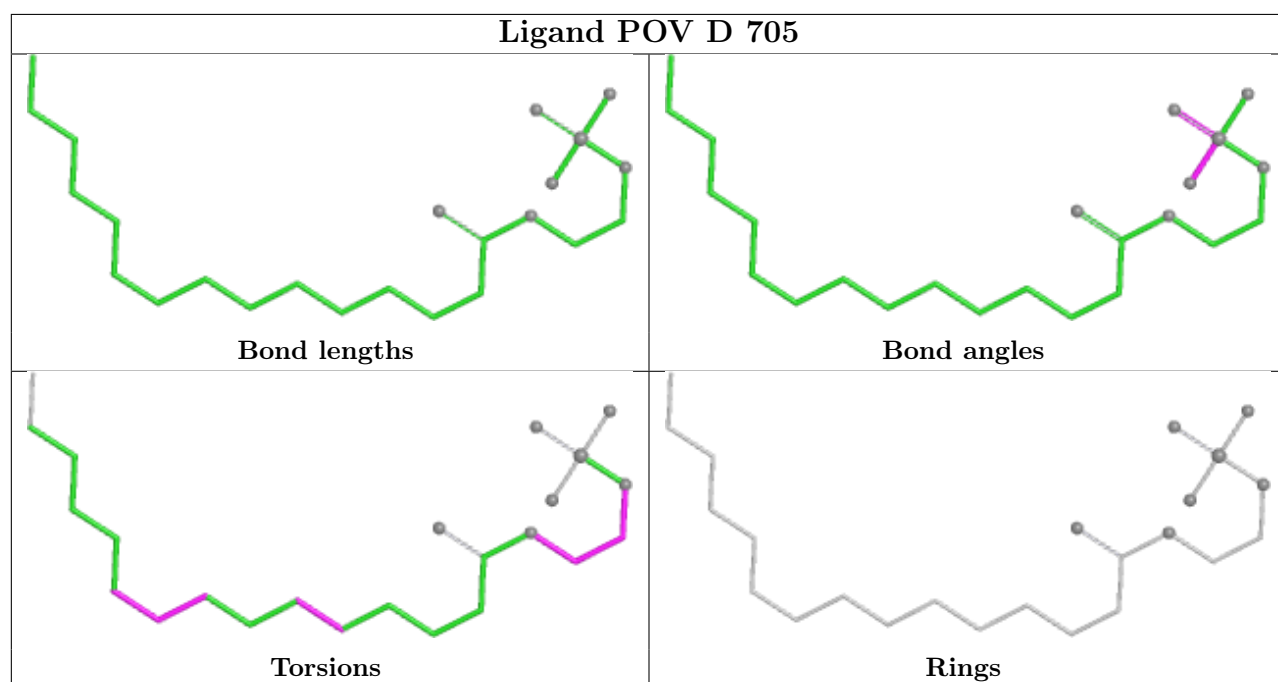
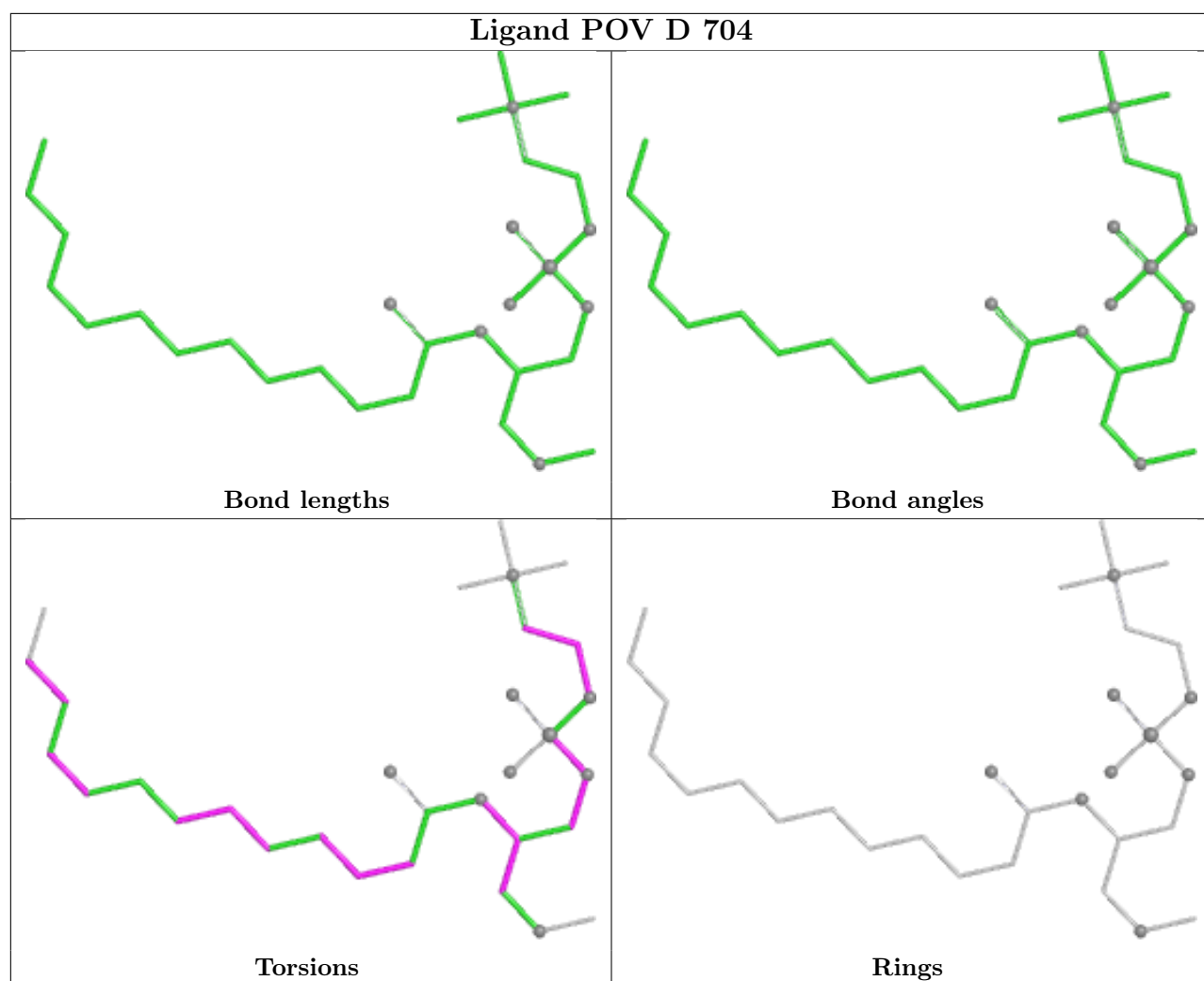


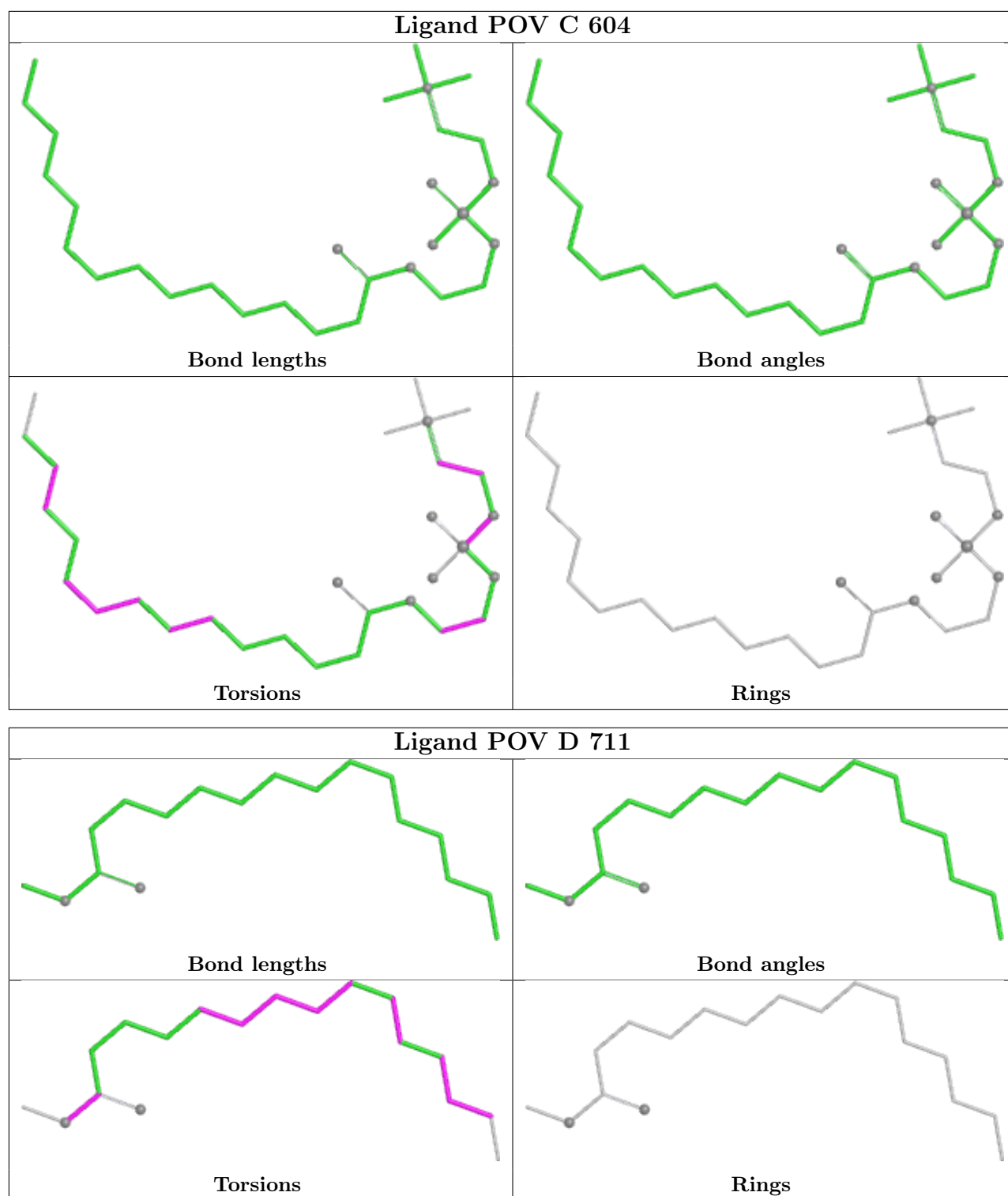


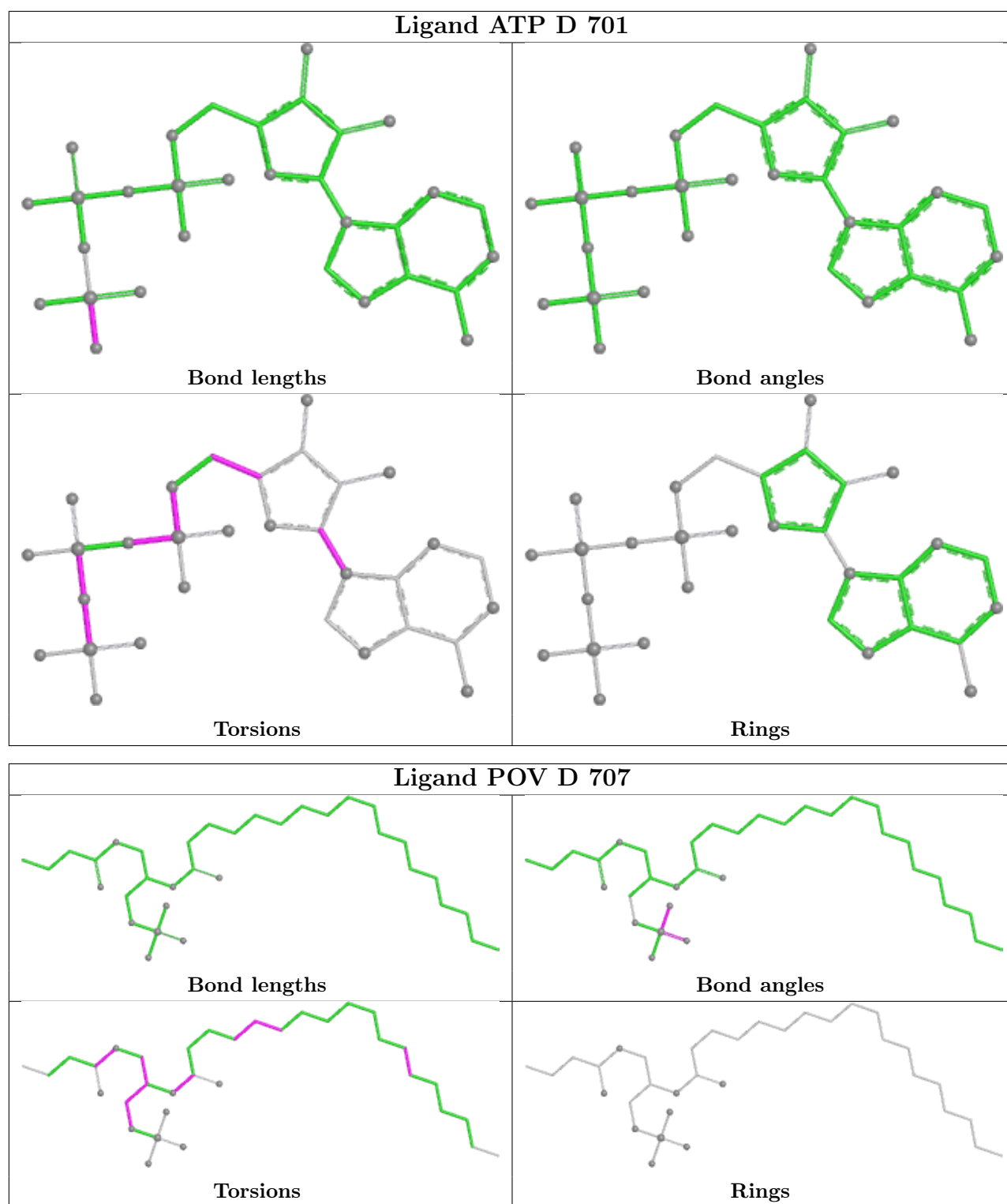












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

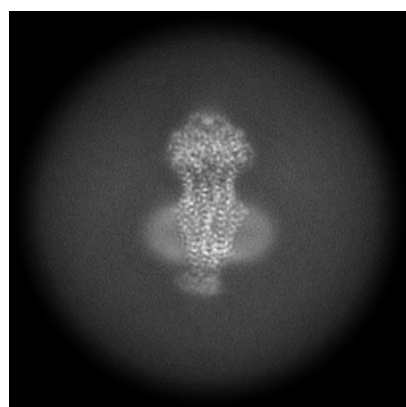
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29087. These allow visual inspection of the internal detail of the map and identification of artifacts.

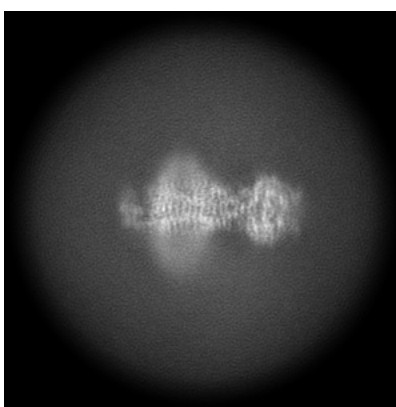
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

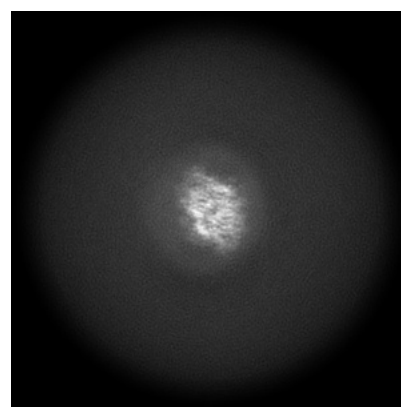
6.1.1 Primary map



X



Y

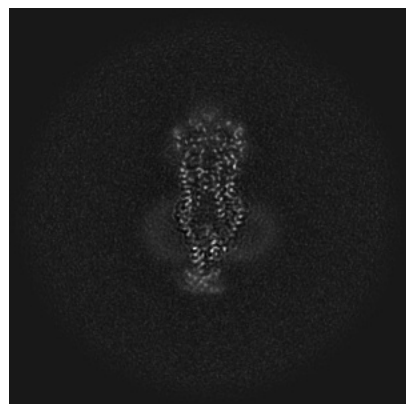


Z

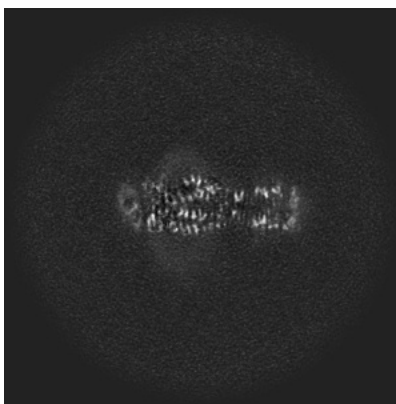
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

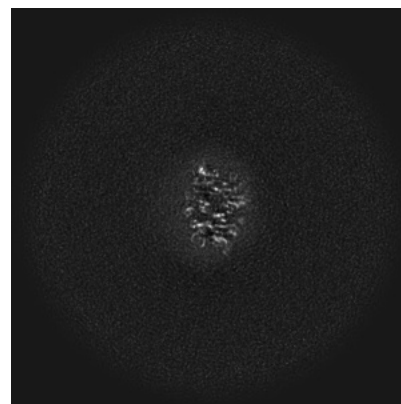
6.2.1 Primary map



X Index: 240



Y Index: 240

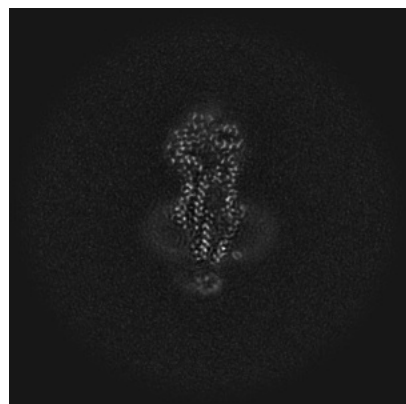


Z Index: 240

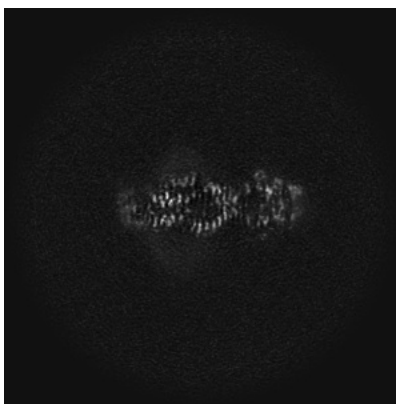
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

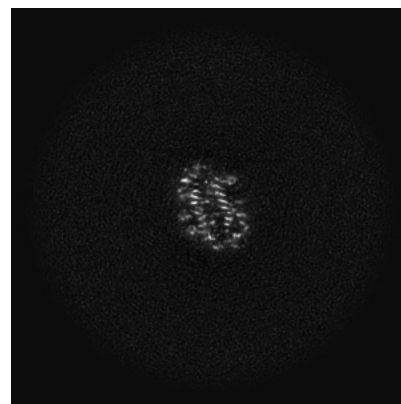
6.3.1 Primary map



X Index: 247



Y Index: 234

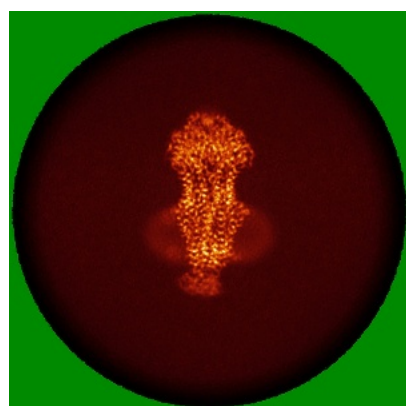


Z Index: 314

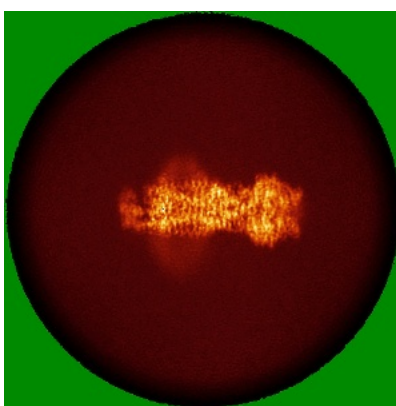
The images above show the largest variance slices of the map in three orthogonal directions.

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

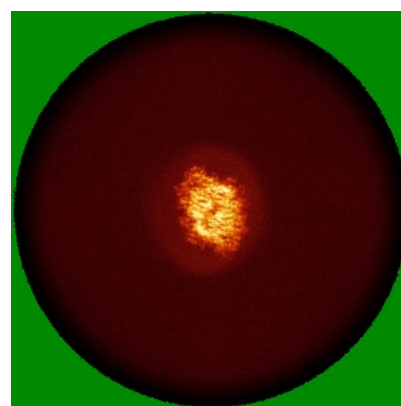
6.4.1 Primary map



X



Y

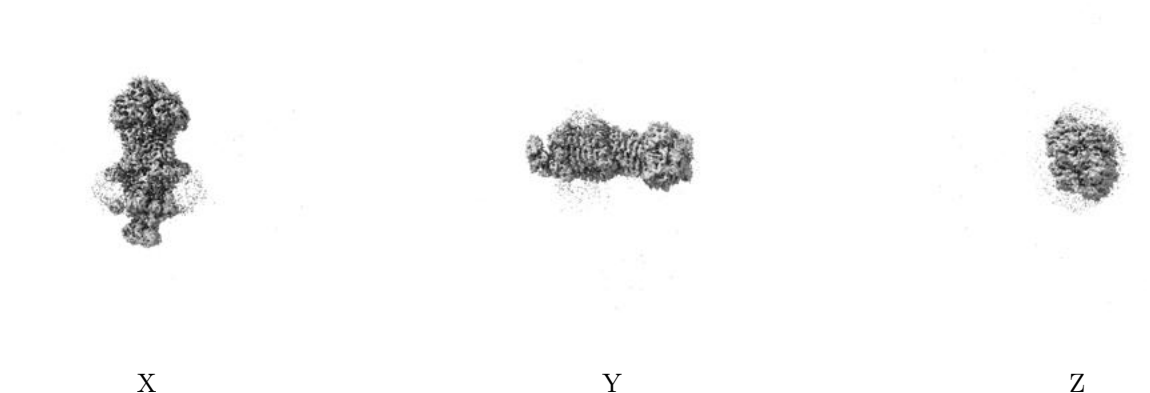


Z

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

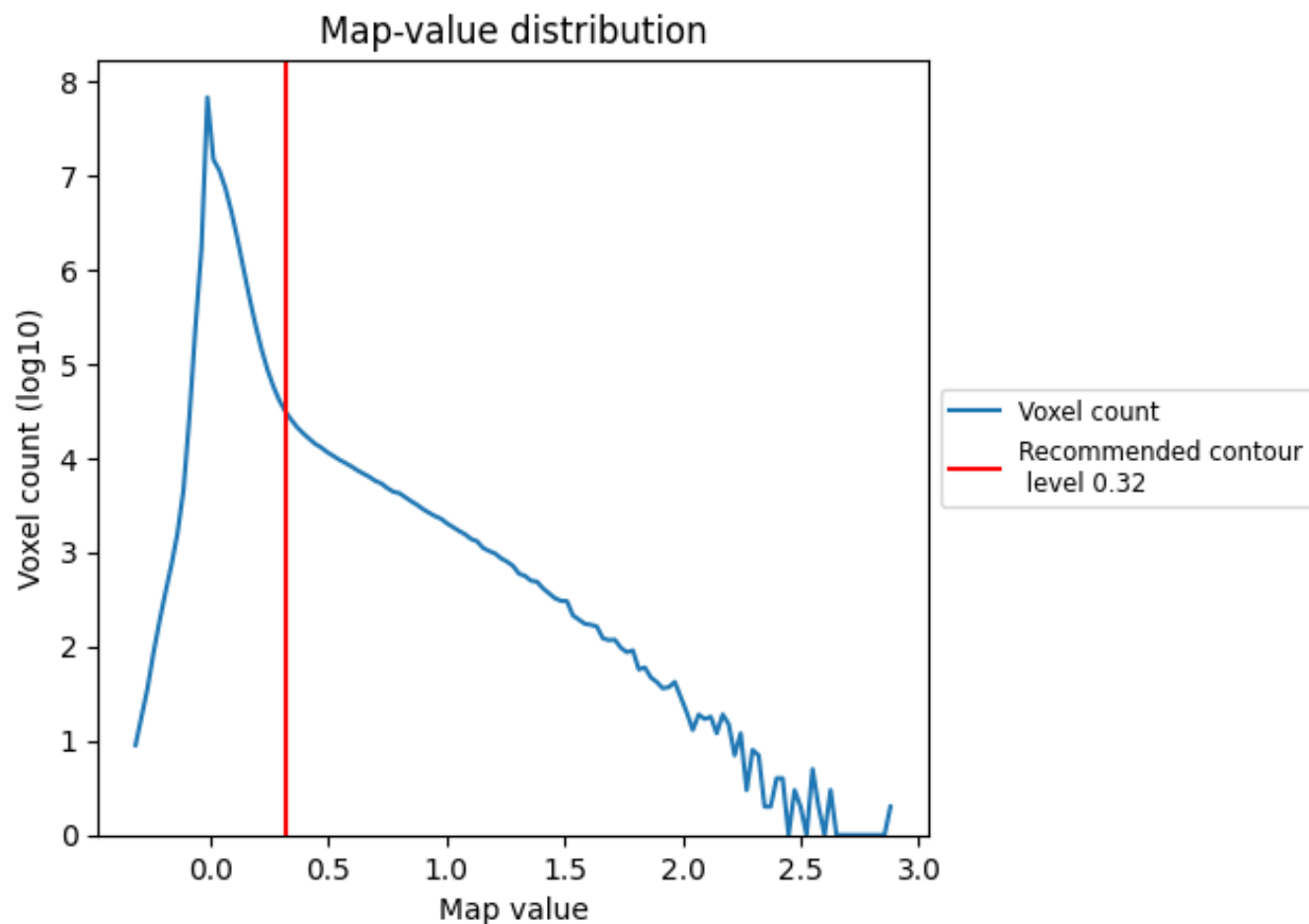
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

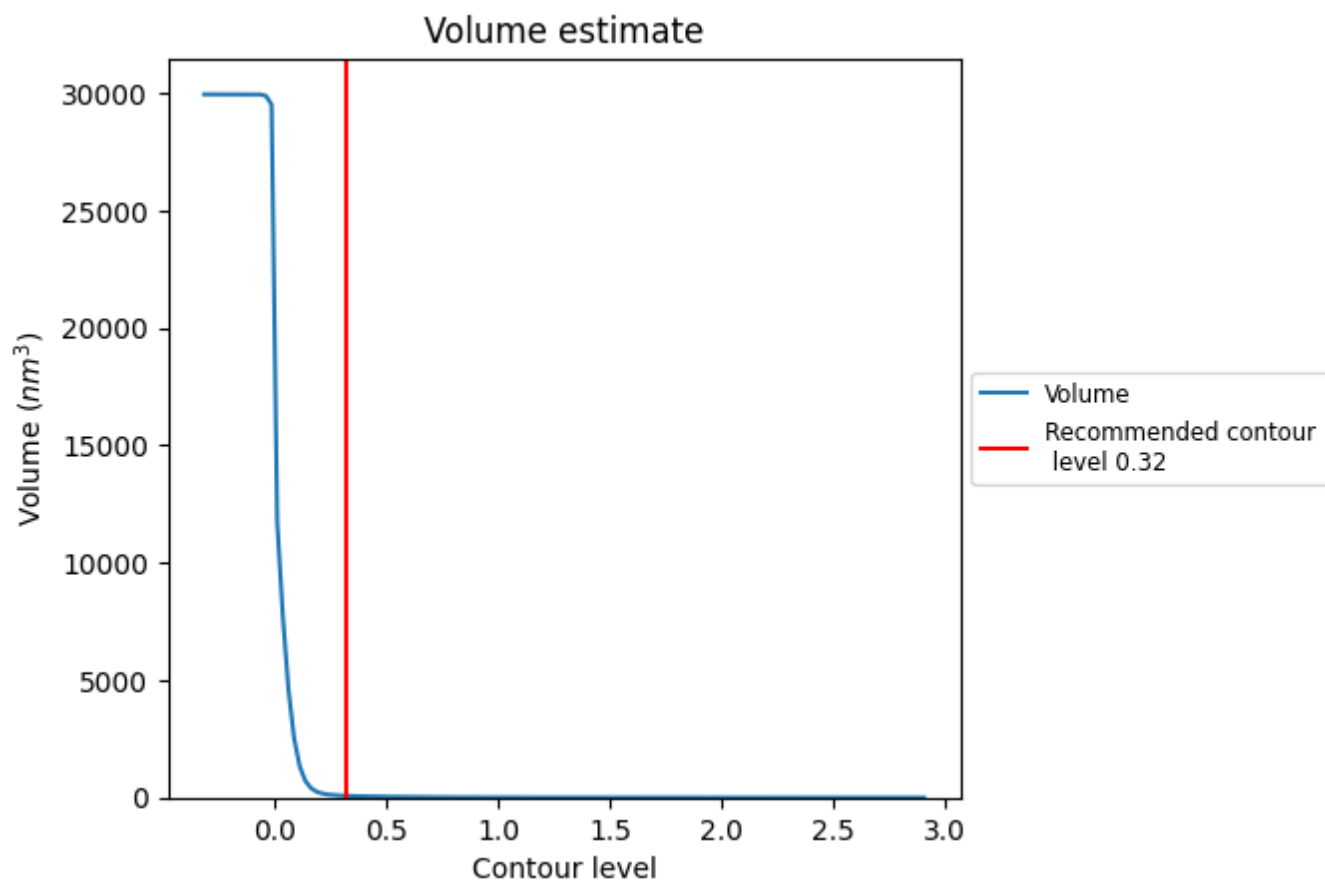
This section contains the results of statistical analysis of the map.

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.

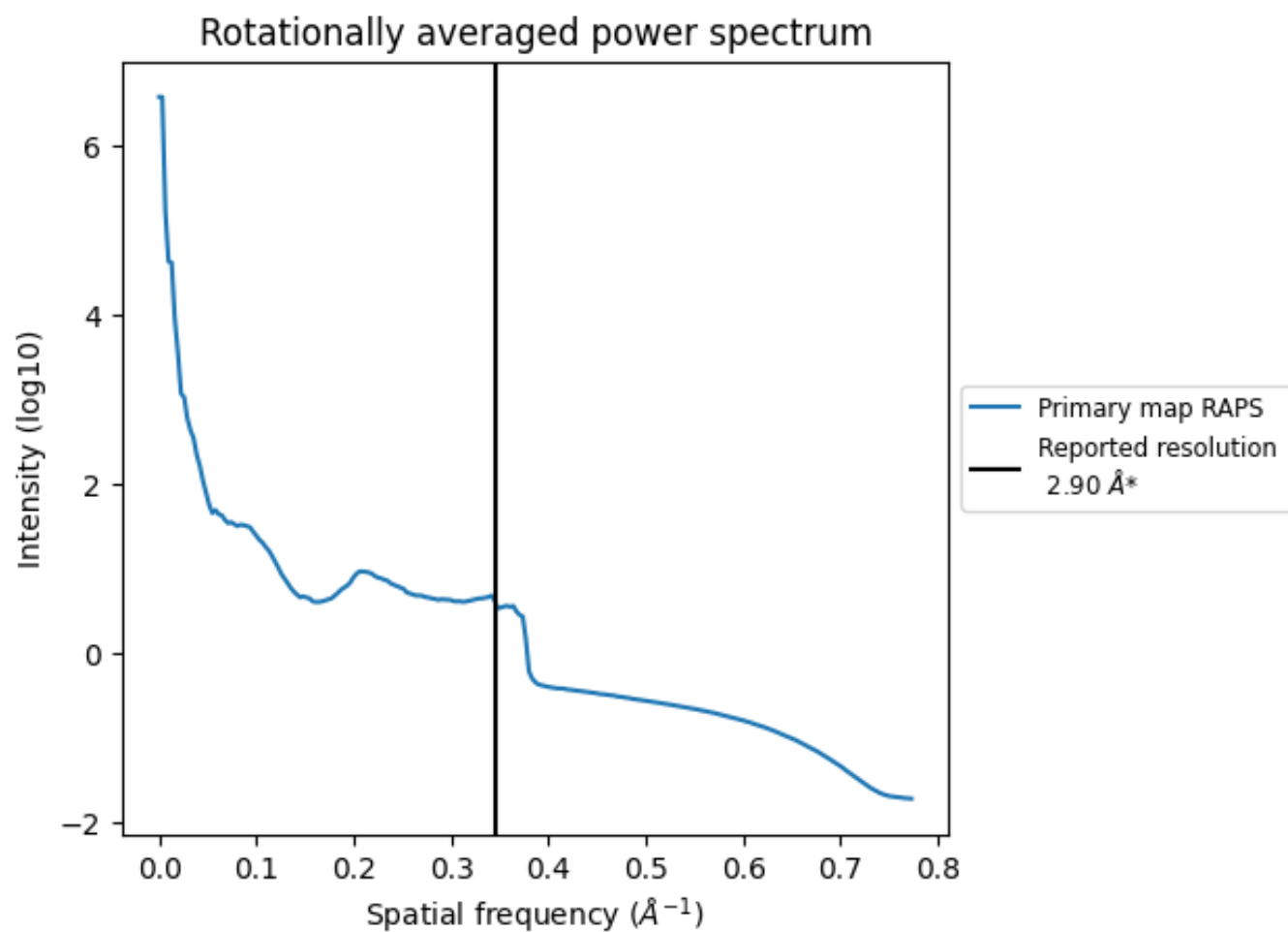
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 0.345 Å⁻¹

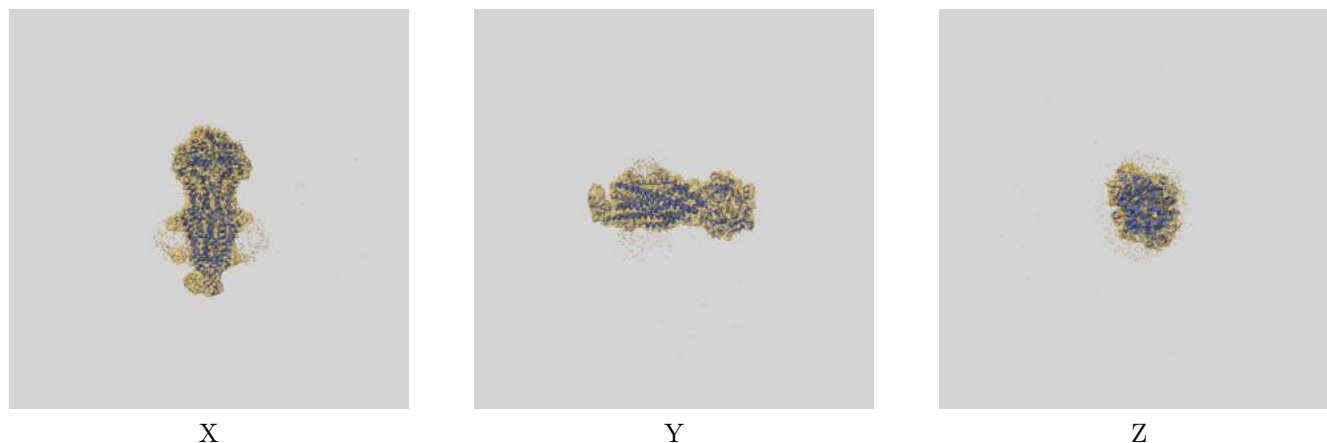
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

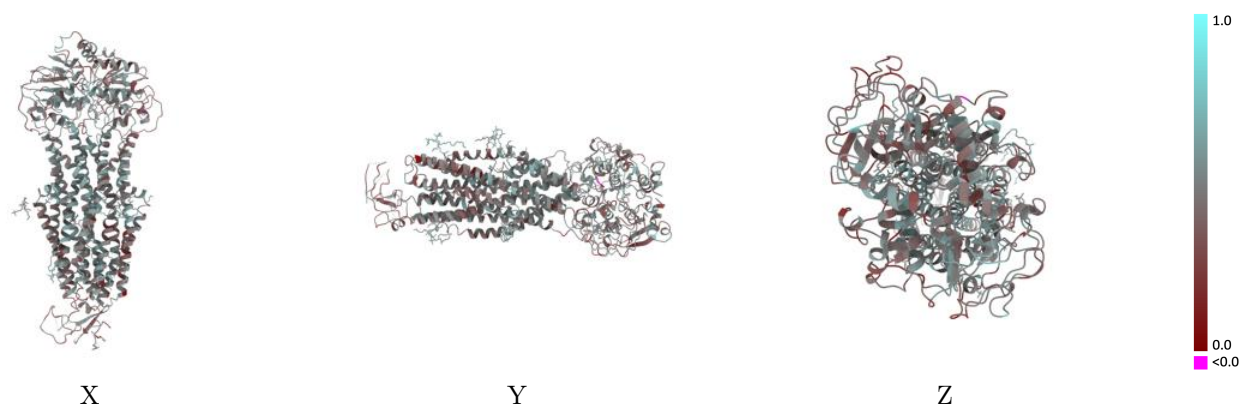
This section contains information regarding the fit between EMDB map EMD-29087 and PDB model 8FHK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



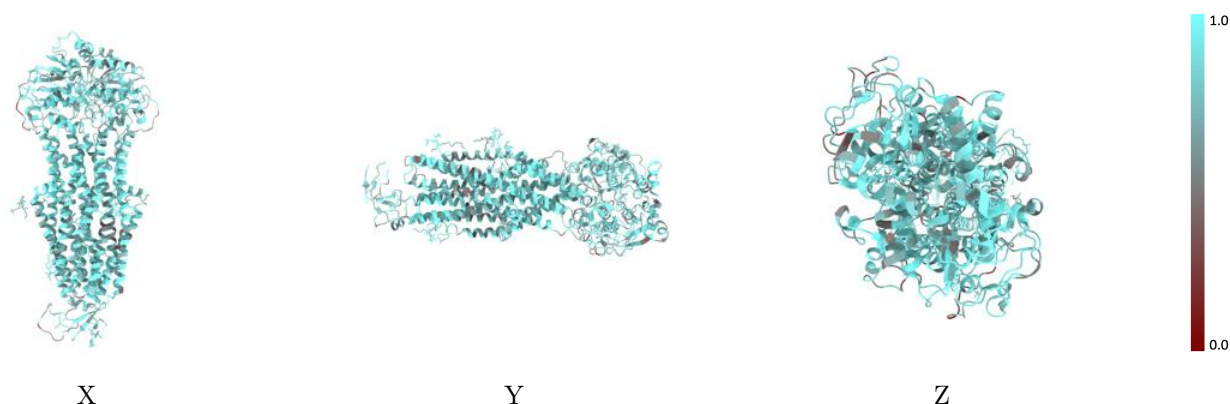
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



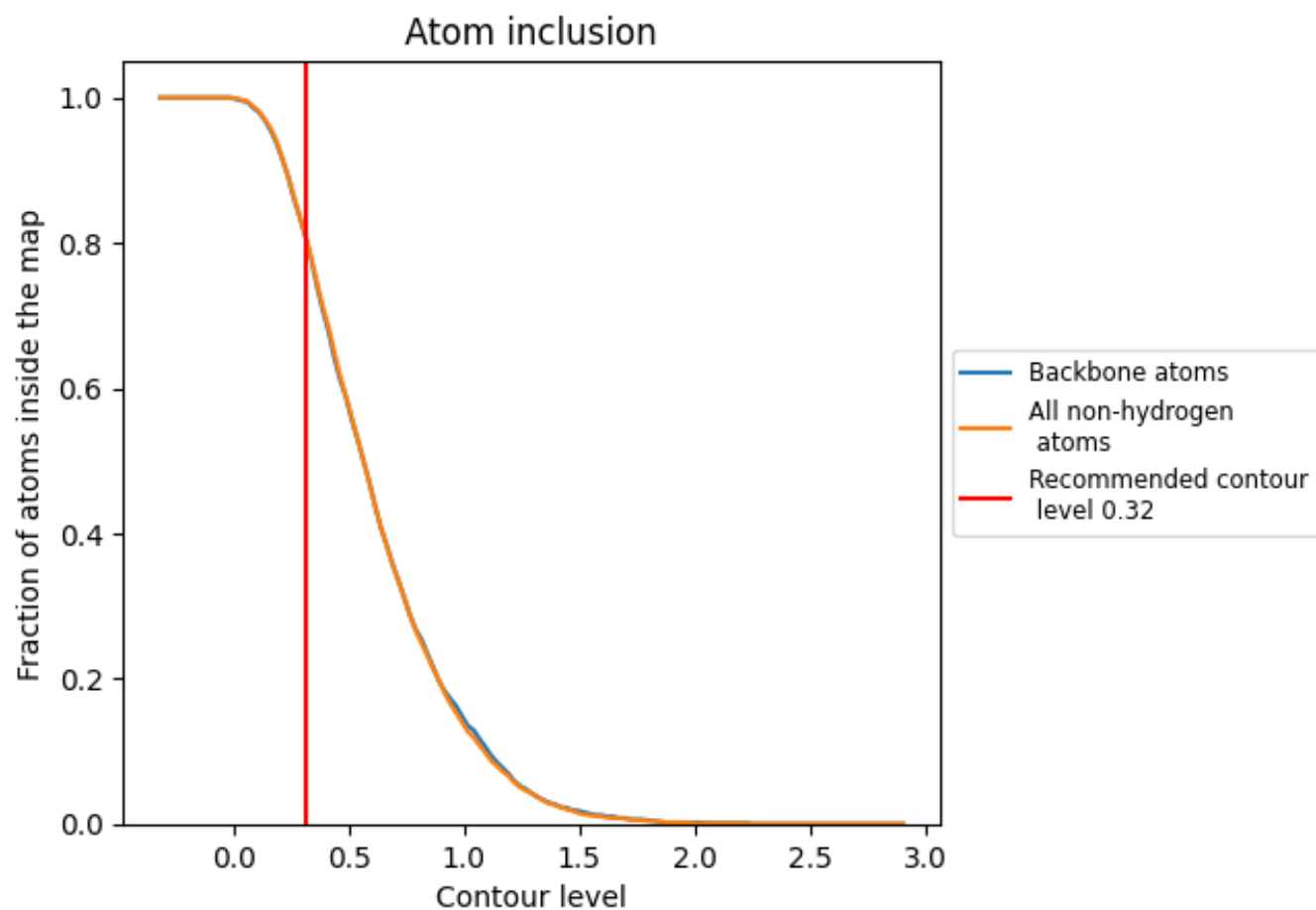
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4540
C	0.8110	0.4550
D	0.8040	0.4540

