



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:36 PM UTC

PDB ID : 7U2X / pdb_00007u2x
EMDB ID : EMD-26321
Title : Cryo-EM structure of the pancreatic ATP-sensitive potassium channel in the presence of carbamazepine and ATP with Kir6.2-CTD in the down conformation
Authors : Shyng, S.L.; Sung, M.W.; Driggers, C.M.
Deposited on : 2022-02-25
Resolution : 4.10 Å (reported)
Based on initial models : 6PZ9, 6BAA

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:

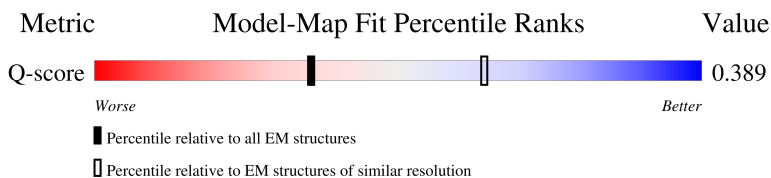
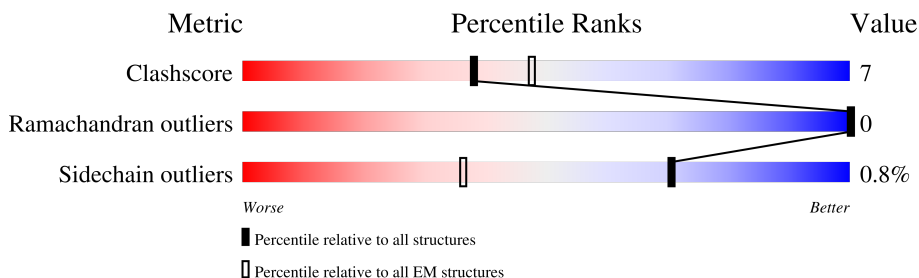
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	390	 5% 74% 15% 11%
1	B	390	 1% 68% 15% 16%
1	C	390	 1% 72% 12% 16%

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Mol	Chain	Length	Quality of chain
1	D	390	
2	E	1582	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19480 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.

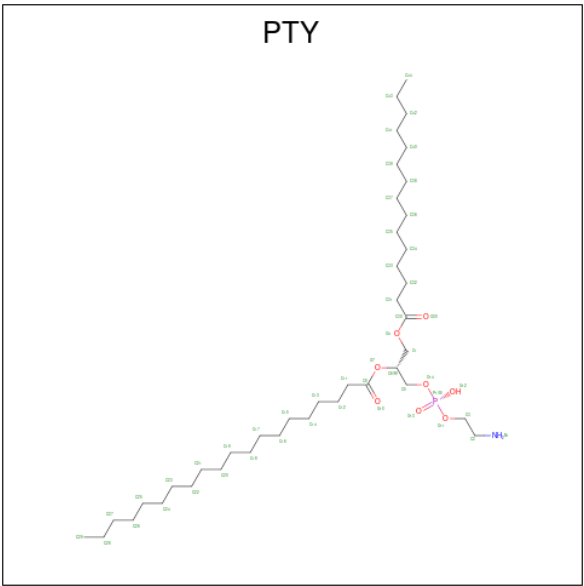
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	348	Total	C	N	O	S	0	0
			2381	1545	415	410	11		
1	B	326	Total	C	N	O	S	0	0
			2277	1483	401	380	13		
1	C	326	Total	C	N	O	S	0	0
			2282	1481	401	387	13		
1	D	326	Total	C	N	O	S	0	0
			2296	1494	400	389	13		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

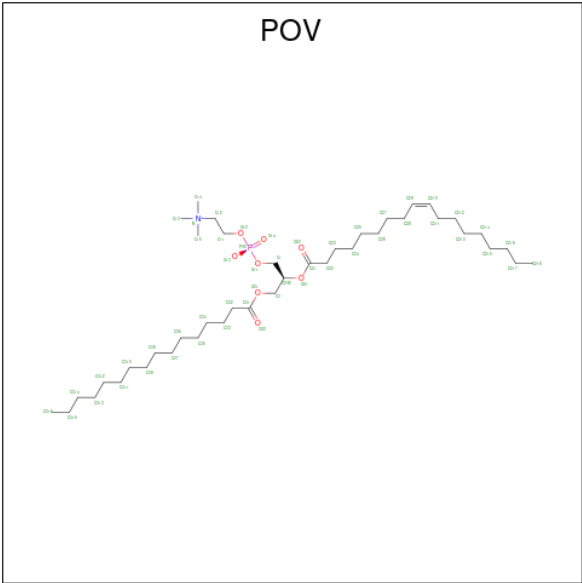
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1427	Total	C	N	O	S	0	0
			9709	6264	1708	1711	26		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	B	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	C	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



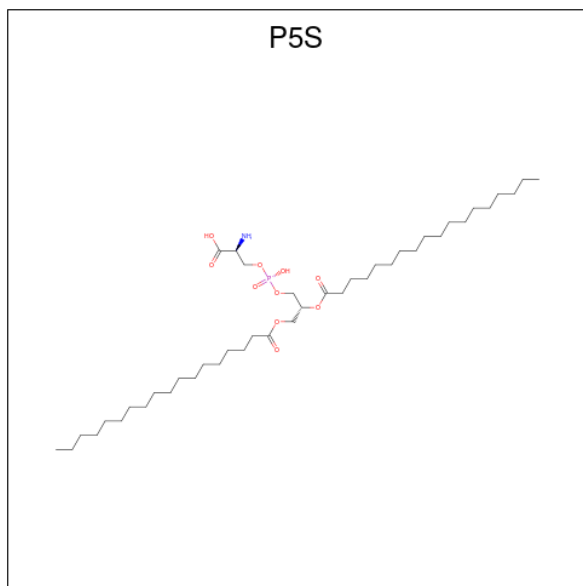
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	E	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	B	1	Total	C	N	O	P	0
			36	26	1	8	1	

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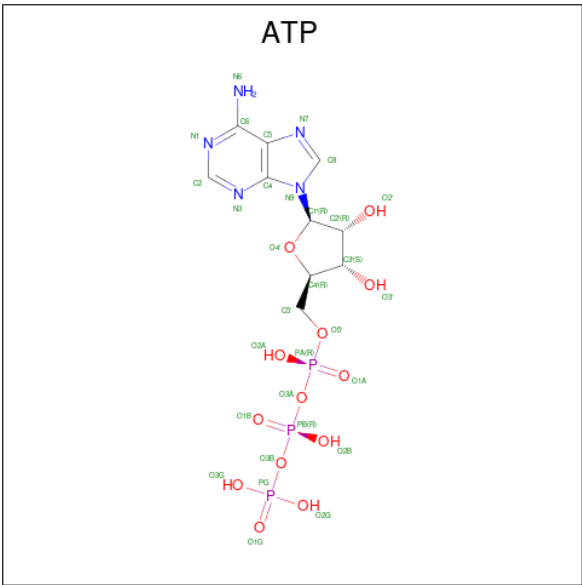
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	D	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 5 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



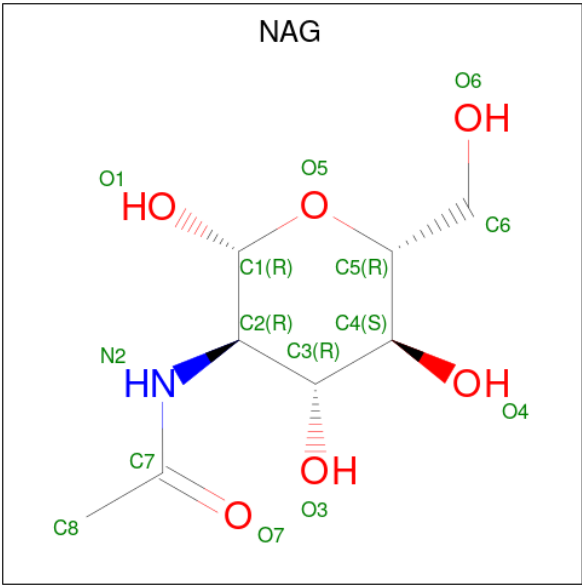
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

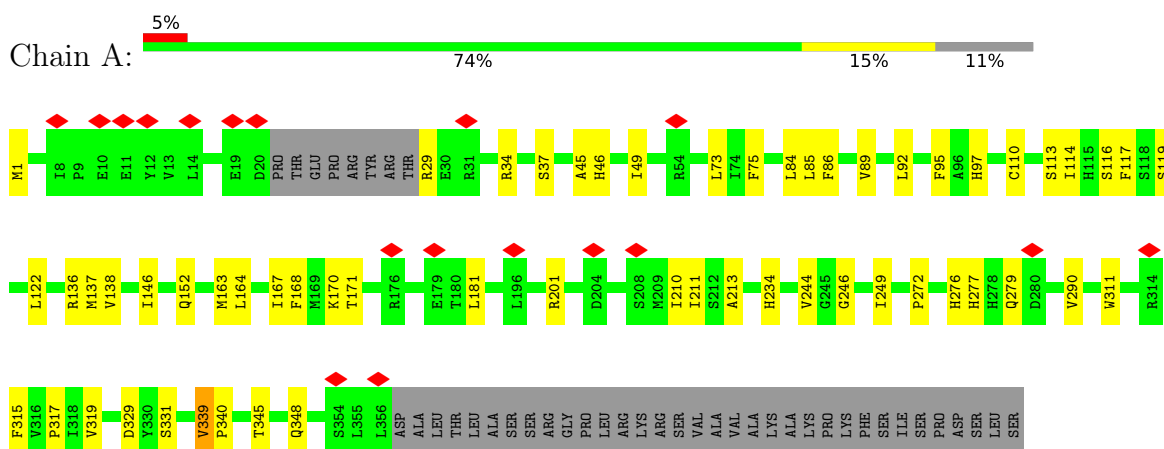


Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			14	8	1	5	

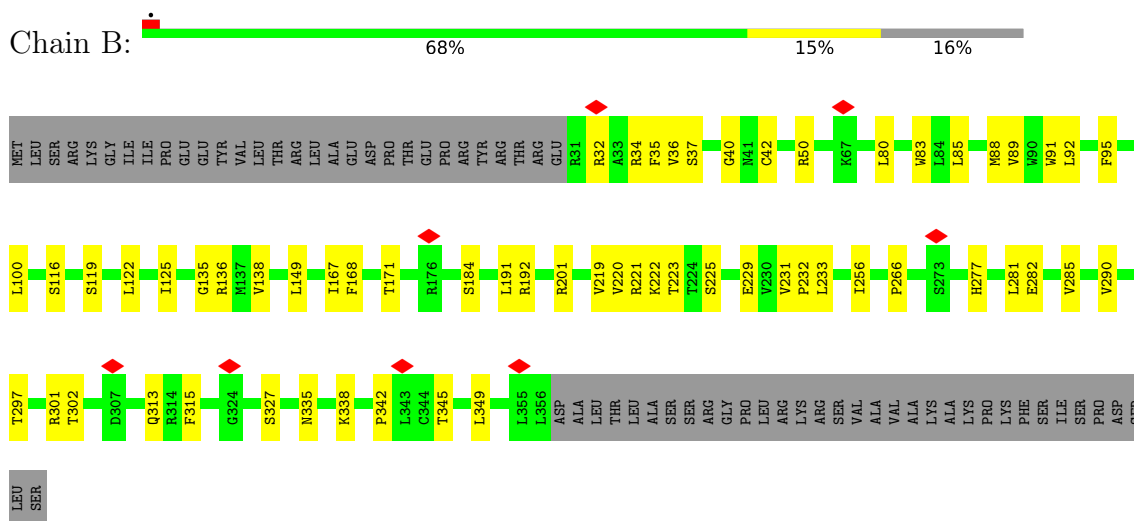
3 Residue-property plots

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: ATP-sensitive inward rectifier potassium channel 11

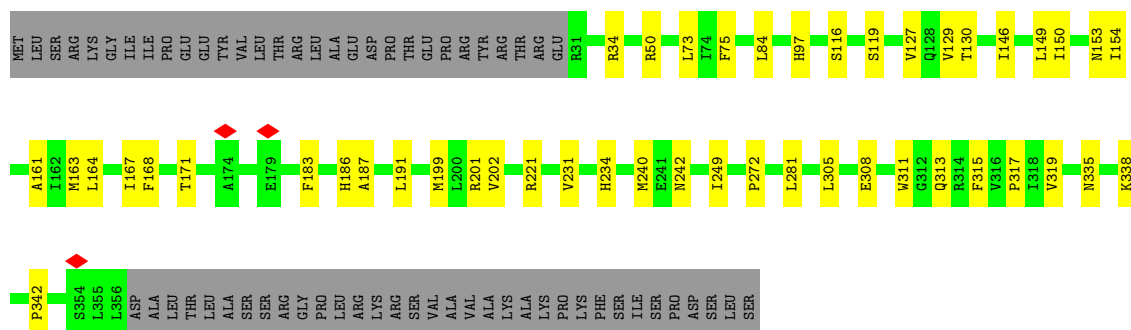


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



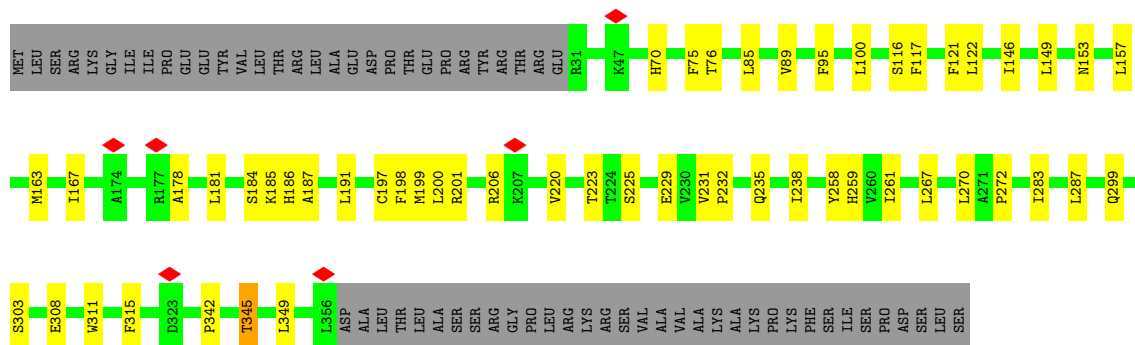
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





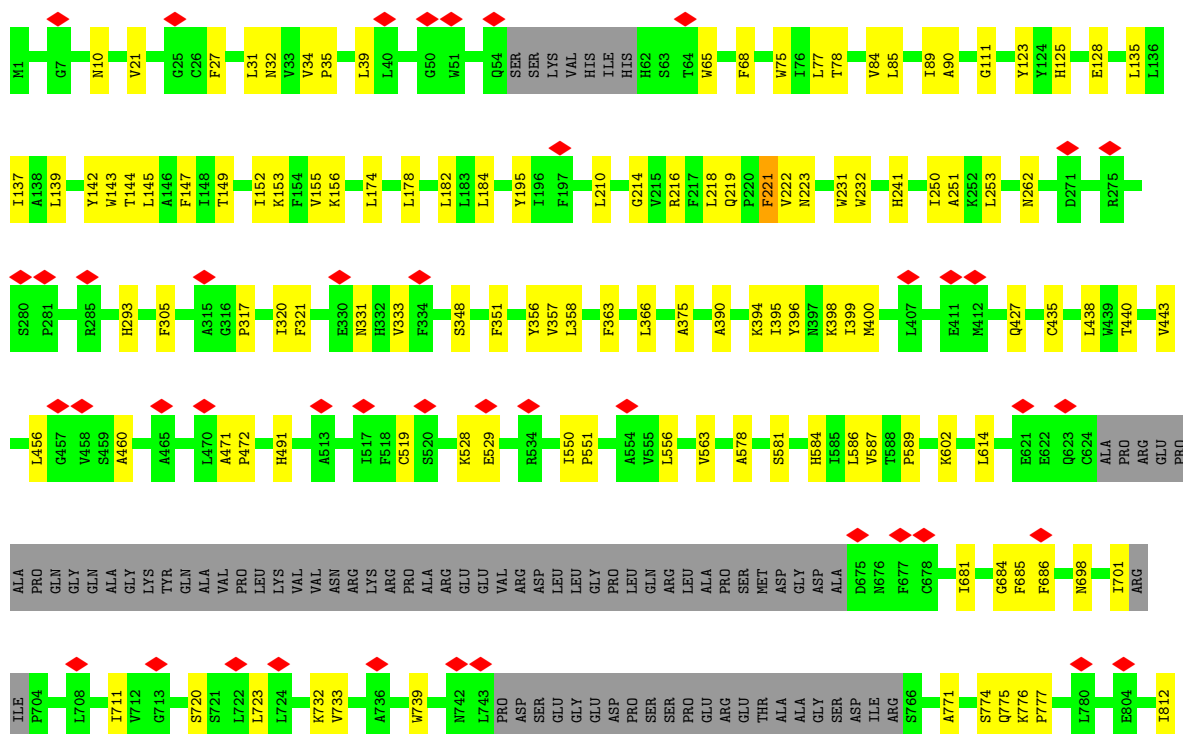
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

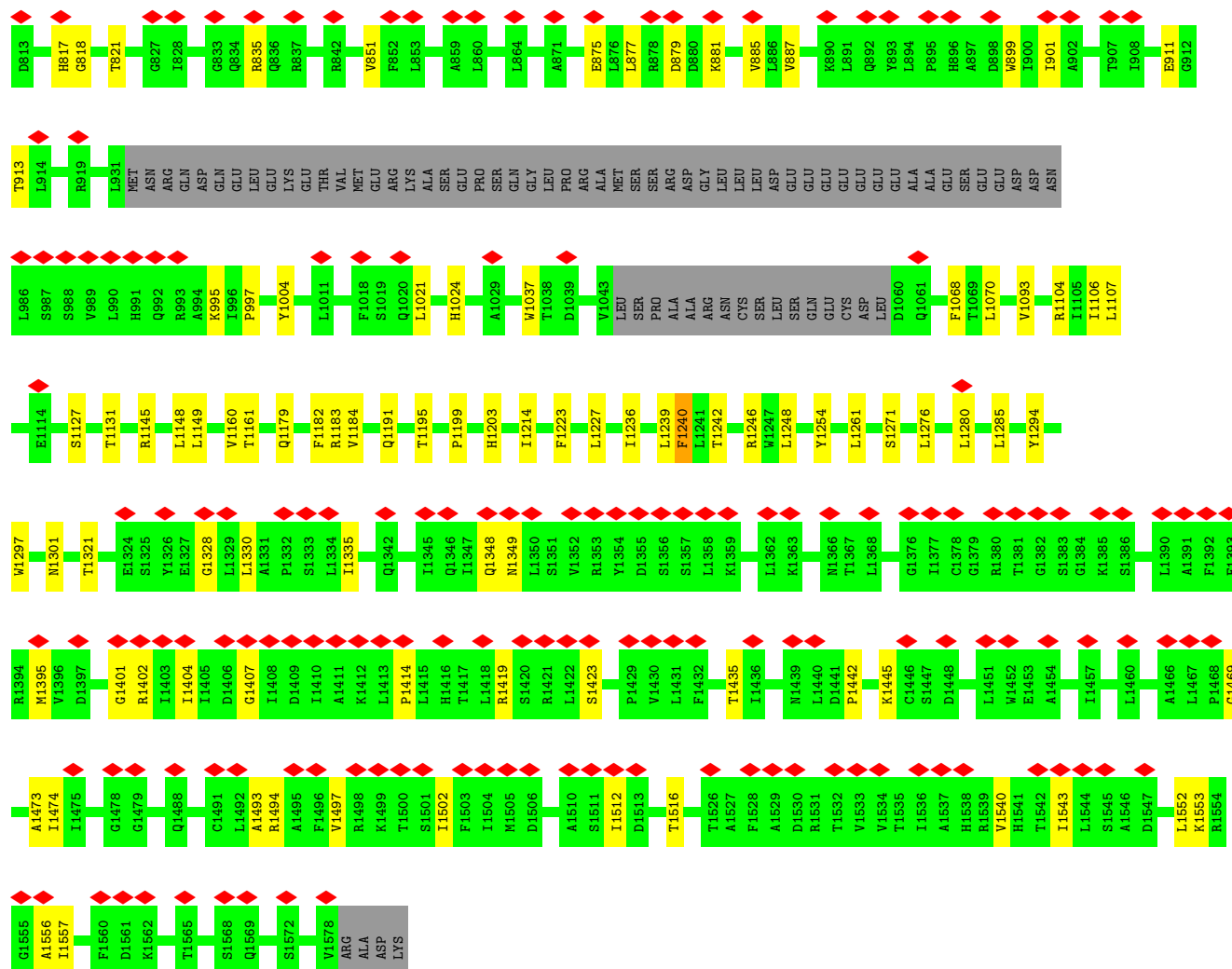
Chain D: 70% 14% 16%



- Molecule 2: ATP-binding cassette sub-family C member 8

Chain E: 13% 77% 13% 10%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.347	Depositor
Minimum map value	-12.322	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	196.65001, 128.25, 160.74	wwPDB
Map dimensions	94, 75, 115	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.71, 1.71, 1.71	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: PTY, P5S, NAG, ATP, POV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2434	0.40	0/3348
1	B	0.26	0/2329	0.37	0/3197
1	C	0.26	0/2334	0.37	0/3203
1	D	0.26	0/2349	0.39	0/3222
2	E	0.21	0/9915	0.39	0/13630
All	All	0.24	0/19361	0.39	0/26600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	0	2135	44	0
1	B	2277	0	2114	40	0
1	C	2282	0	2120	32	0
1	D	2296	0	2146	40	0
2	E	9709	0	8473	138	0
3	A	96	0	111	1	0
3	B	32	0	37	0	0
3	C	32	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	96	0	111	4	0
4	A	36	0	45	4	0
4	B	36	0	45	1	0
4	C	36	0	45	1	0
4	D	36	0	45	1	0
4	E	36	0	45	2	0
5	E	54	0	80	5	0
6	E	31	0	12	1	0
7	E	14	0	13	1	0
All	All	19480	0	17614	276	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 7.

All (276) 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)
2:E:1160:VAL:HG22	2:E:1280:LEU:HG	1.71	0.73
1:A:339:VAL:HG22	1:A:340:PRO:HD2	1.71	0.72
2:E:1328:GLY:H	2:E:1414:PRO:HG3	1.54	0.71
1:A:201:ARG:HH11	1:A:315:PHE:HD2	1.39	0.70
2:E:1512:ILE:O	2:E:1516:THR:N	2.22	0.69
1:B:40:GLY:O	1:B:301:ARG:NH2	2.24	0.69
1:A:45:ALA:HB3	1:B:327:SER:HA	1.72	0.69
1:B:138:VAL:HG21	1:B:149:LEU:HD22	1.75	0.68
1:C:201:ARG:HB2	1:C:315:PHE:HE2	1.57	0.68
1:B:290:VAL:HA	1:B:297:THR:HA	1.77	0.66
1:C:116:SER:O	1:C:119:SER:OG	2.12	0.66
2:E:995:LYS:HB2	2:E:997:PRO:HD3	1.77	0.66
2:E:1404:ILE:HD12	2:E:1407:GLY:HA2	1.78	0.66
1:A:113:SER:HB2	1:A:136:ARG:HG2	1.77	0.65
4:A:402:POV:H37	4:A:402:POV:H26	1.79	0.65
1:C:154:ILE:HD13	1:D:76:THR:HG23	1.76	0.65
1:B:32:ARG:NH1	1:B:277:HIS:O	2.30	0.65
1:B:345:THR:O	1:B:349:LEU:N	2.28	0.64
1:A:117:PHE:N	4:A:402:POV:O13	2.29	0.64
5:E:1604:P5S:HA	4:E:1606:POV:H12	1.80	0.63
1:D:178:ALA:O	1:D:206:ARG:NH2	2.31	0.63
2:E:1423:SER:OG	2:E:1502:ILE:O	2.17	0.62
2:E:875:GLU:O	2:E:879:ASP:N	2.27	0.62
2:E:1195:THR:O	2:E:1199:PRO:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LEU:HD11	1:C:342:PRO:HD2	1.81	0.61
2:E:877:LEU:HD12	2:E:881:LYS:HA	1.81	0.61
1:A:92:LEU:HD22	3:A:403:PTY:H162	1.83	0.61
1:D:267:LEU:HD22	1:D:270:LEU:HD11	1.83	0.61
1:A:116:SER:O	1:A:119:SER:OG	2.18	0.60
1:C:201:ARG:HH21	1:C:315:PHE:HB3	1.65	0.60
1:C:146:ILE:HG12	1:D:122:LEU:HD21	1.83	0.60
1:D:116:SER:OG	1:D:117:PHE:N	2.34	0.60
2:E:253:LEU:HB3	2:E:1236:ILE:HD12	1.83	0.60
1:D:117:PHE:N	4:D:401:POV:O14	2.34	0.59
2:E:262:ASN:HB3	2:E:390:ALA:HB2	1.84	0.59
2:E:1469:GLY:HA3	2:E:1473:ALA:HA	1.83	0.59
2:E:1104:ARG:NH1	2:E:1321:THR:O	2.35	0.59
1:B:191:LEU:HD11	1:B:342:PRO:HD2	1.84	0.59
2:E:348:SER:HA	2:E:351:PHE:HB3	1.85	0.58
1:D:149:LEU:O	1:D:153:ASN:ND2	2.36	0.58
2:E:65:TRP:CD1	2:E:210:LEU:HD21	2.39	0.58
1:D:181:LEU:HD13	1:D:287:LEU:HD23	1.86	0.57
2:E:1160:VAL:HG12	2:E:1161:THR:HG23	1.84	0.57
2:E:90:ALA:HB1	2:E:357:VAL:HG22	1.86	0.57
1:C:34:ARG:HG2	1:C:305:LEU:HD21	1.85	0.57
2:E:686:PHE:HA	2:E:732:LYS:HA	1.86	0.57
2:E:774:SER:OG	2:E:776:LYS:O	2.23	0.57
1:D:200:LEU:HD23	1:D:201:ARG:H	1.69	0.56
1:C:272:PRO:HG3	1:C:311:TRP:CE2	2.40	0.56
1:D:187:ALA:HB1	1:D:198:PHE:HE1	1.70	0.56
1:B:34:ARG:HE	1:B:37:SER:HA	1.70	0.56
1:C:149:LEU:O	1:C:153:ASN:ND2	2.39	0.56
2:E:1442:PRO:HD3	2:E:1497:VAL:HG22	1.87	0.55
2:E:219:GLN:HG2	2:E:232:TRP:HE1	1.71	0.55
2:E:321:PHE:HB2	2:E:578:ALA:HB2	1.89	0.55
1:C:97:HIS:O	1:C:97:HIS:ND1	2.39	0.55
1:A:122:LEU:HD21	1:D:146:ILE:HG12	1.88	0.54
1:A:46:HIS:HB3	1:A:49:ILE:HD12	1.89	0.54
1:D:201:ARG:HB2	1:D:315:PHE:CE2	2.42	0.54
2:E:137:ILE:HG13	2:E:195:TYR:HE1	1.72	0.54
2:E:214:GLY:O	2:E:216:ARG:NH1	2.39	0.54
1:B:50:ARG:H	1:B:50:ARG:HD2	1.73	0.54
2:E:396:TYR:CG	2:E:1227:LEU:HD22	2.43	0.54
1:D:184:SER:HB3	1:D:201:ARG:HB3	1.87	0.54
1:C:240:MET:HE2	1:C:242:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:HA	1:D:299:GLN:NE2	2.23	0.54
1:B:232:PRO:HD3	1:C:317:PRO:HB3	1.90	0.53
2:E:1149:LEU:HD23	2:E:1294:TYR:CZ	2.43	0.53
2:E:125:HIS:NE2	3:E:1601:PTY:O12	2.38	0.53
2:E:1004:TYR:CE2	2:E:1093:VAL:HG11	2.43	0.53
2:E:125:HIS:HE2	3:E:1601:PTY:P1	2.32	0.53
1:C:129:VAL:O	1:C:130:THR:OG1	2.24	0.53
1:C:75:PHE:CZ	1:C:163:MET:HA	2.44	0.53
1:A:272:PRO:HG3	1:A:311:TRP:CD2	2.44	0.53
1:C:50:ARG:HH22	1:D:185:LYS:NZ	2.07	0.53
2:E:35:PRO:HG3	2:E:145:LEU:HG	1.90	0.53
1:B:91:TRP:HE1	1:B:100:LEU:HD21	1.73	0.52
1:B:167:ILE:O	1:B:171:THR:HG23	2.08	0.52
1:D:220:VAL:HG22	1:D:235:GLN:HG2	1.91	0.52
1:D:199:MET:HG2	1:D:258:TYR:HB3	1.91	0.52
2:E:1540:VAL:HG13	2:E:1543:ILE:HD11	1.92	0.52
1:C:161:ALA:HB1	1:D:167:ILE:HG13	1.91	0.52
1:D:200:LEU:HD23	1:D:201:ARG:N	2.25	0.52
2:E:491:HIS:HB3	2:E:529:GLU:HB2	1.92	0.51
2:E:817:HIS:HB2	2:E:821:THR:HG22	1.91	0.51
2:E:363:PHE:CG	2:E:1261:LEU:HD12	2.44	0.51
2:E:143:TRP:O	2:E:147:PHE:N	2.40	0.51
1:D:85:LEU:O	1:D:89:VAL:HG23	2.11	0.51
2:E:684:GLY:O	2:E:698:ASN:N	2.44	0.51
2:E:812:ILE:O	2:E:818:GLY:HA2	2.10	0.51
2:E:771:ALA:HB3	2:E:851:VAL:HA	1.93	0.51
1:B:223:THR:O	1:B:231:VAL:N	2.44	0.51
1:B:95:PHE:HA	1:B:100:LEU:HD13	1.93	0.51
2:E:685:PHE:O	2:E:733:VAL:N	2.42	0.50
2:E:1348:GLN:O	2:E:1402:ARG:HB3	2.11	0.50
1:B:116:SER:O	1:B:119:SER:OG	2.24	0.50
1:A:1:MET:HA	2:E:1297:TRP:CH2	2.47	0.50
2:E:775:GLN:NE2	6:E:1605:ATP:O2B	2.23	0.50
1:C:183:PHE:HE1	1:C:202:VAL:HG23	1.75	0.50
2:E:395:ILE:O	2:E:399:ILE:HG13	2.11	0.50
1:C:186:HIS:HB2	1:C:308:GLU:O	2.11	0.50
2:E:184:LEU:HD22	4:E:1606:POV:H36A	1.94	0.50
2:E:331:ASN:O	2:E:333:VAL:HG23	2.12	0.49
1:C:221:ARG:HD3	1:C:281:LEU:HD21	1.94	0.49
2:E:400:MET:HE2	2:E:400:MET:HA	1.95	0.49
2:E:550:ILE:N	2:E:551:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD21	1:A:210:ILE:HD11	1.95	0.49
2:E:720:SER:HB3	2:E:775:GLN:NE2	2.28	0.49
1:D:197:CYS:HA	1:D:261:ILE:HG13	1.93	0.49
1:D:198:PHE:HZ	1:D:200:LEU:HD12	1.78	0.49
1:A:201:ARG:HB2	1:A:315:PHE:HE2	1.78	0.49
2:E:84:VAL:HG11	2:E:174:LEU:HD22	1.94	0.49
2:E:39:LEU:HD12	2:E:142:TYR:CG	2.48	0.49
1:A:276:HIS:NE2	1:A:279:GLN:OE1	2.43	0.49
1:C:84:LEU:HD21	4:C:401:POV:H35A	1.95	0.49
1:A:146:ILE:HG12	1:B:122:LEU:HD21	1.94	0.48
2:E:139:LEU:O	2:E:142:TYR:HB3	2.12	0.48
1:D:223:THR:HB	1:D:231:VAL:HB	1.94	0.48
1:A:92:LEU:HD12	2:E:34:VAL:HG21	1.94	0.48
2:E:293:HIS:O	2:E:293:HIS:ND1	2.45	0.48
1:A:317:PRO:HB3	1:D:232:PRO:HD3	1.95	0.48
1:A:84:LEU:HD21	4:A:402:POV:H36A	1.94	0.48
2:E:375:ALA:HB1	5:E:1604:P5S:H41A	1.95	0.48
2:E:39:LEU:HD12	2:E:142:TYR:CD1	2.48	0.48
1:A:29:ARG:N	1:A:277:HIS:HE2	2.12	0.48
2:E:427:GLN:NE2	2:E:602:LYS:HD3	2.29	0.48
2:E:456:LEU:HB2	2:E:460:ALA:HB2	1.96	0.47
1:A:211:ILE:HB	1:A:290:VAL:HG13	1.95	0.47
2:E:231:TRP:CE3	3:E:1601:PTY:H311	2.50	0.47
2:E:1021:LEU:HA	2:E:1148:LEU:HD21	1.96	0.47
1:B:221:ARG:HG2	1:B:222:LYS:N	2.29	0.47
1:B:313:GLN:HG2	1:B:338:LYS:HA	1.95	0.47
1:A:319:VAL:HB	1:D:232:PRO:HB2	1.96	0.47
1:A:234:HIS:CE1	1:B:192:ARG:HH21	2.32	0.47
1:A:329:ASP:OD1	1:A:331:SER:OG	2.21	0.47
1:A:345:THR:HG23	1:A:348:GLN:H	1.79	0.47
2:E:144:THR:O	2:E:147:PHE:HB3	2.15	0.47
2:E:305:PHE:HE1	5:E:1604:P5S:H22A	1.80	0.47
1:D:75:PHE:CZ	1:D:163:MET:HA	2.50	0.47
1:A:211:ILE:HA	1:D:299:GLN:HE21	1.81	0.46
2:E:241:HIS:CE1	2:E:1184:VAL:HG21	2.50	0.46
1:B:36:VAL:HG12	1:B:42:CYS:HA	1.97	0.46
2:E:32:ASN:ND2	2:E:153:LYS:HD2	2.30	0.46
1:A:85:LEU:O	1:A:89:VAL:HG23	2.15	0.46
2:E:320:ILE:HG23	2:E:1285:LEU:HD23	1.98	0.46
2:E:1330:LEU:HD22	2:E:1335:ILE:HG21	1.98	0.46
1:D:191:LEU:HD11	1:D:342:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1271:SER:HA	2:E:1276:LEU:H	1.81	0.46
1:B:201:ARG:HB2	1:B:315:PHE:CE2	2.51	0.46
2:E:1349:ASN:O	2:E:1401:GLY:HA2	2.16	0.46
1:B:88:MET:HE1	4:B:402:POV:H33A	1.98	0.46
2:E:68:PHE:HE1	2:E:128:GLU:HA	1.81	0.46
2:E:435:CYS:HA	2:E:438:LEU:HD23	1.98	0.46
1:B:232:PRO:HB2	1:C:319:VAL:HB	1.98	0.46
1:A:138:VAL:O	1:B:136:ARG:NH2	2.48	0.45
2:E:75:TRP:HA	2:E:78:THR:HG22	1.98	0.45
1:C:183:PHE:CE1	1:C:202:VAL:HG23	2.51	0.45
1:A:34:ARG:HH21	1:A:37:SER:HA	1.81	0.45
2:E:89:ILE:HD11	2:E:111:GLY:N	2.31	0.45
1:B:95:PHE:HD1	1:B:100:LEU:HD22	1.81	0.45
1:B:184:SER:HB3	1:B:201:ARG:HB3	1.99	0.45
2:E:210:LEU:HD22	2:E:221:PHE:CE2	2.50	0.45
1:B:83:TRP:CE3	1:B:125:ILE:HD11	2.51	0.45
2:E:1493:ALA:O	2:E:1497:VAL:HG23	2.17	0.45
2:E:10:ASN:ND2	7:E:1607:NAG:O5	2.50	0.45
2:E:556:LEU:HA	2:E:1068:PHE:HE1	1.82	0.45
1:D:272:PRO:HB3	1:D:311:TRP:CE2	2.52	0.45
1:A:84:LEU:HD11	4:A:402:POV:H28A	1.99	0.45
2:E:1552:LEU:HA	2:E:1557:ILE:HA	1.98	0.45
1:D:225:SER:HB3	1:D:229:GLU:HB2	1.99	0.45
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.79	0.44
2:E:440:THR:O	2:E:443:VAL:N	2.50	0.44
1:B:219:VAL:HG21	1:B:266:PRO:HG2	1.99	0.44
1:D:201:ARG:HB2	1:D:315:PHE:HE2	1.81	0.44
2:E:471:ALA:HB3	2:E:472:PRO:HD3	2.00	0.44
1:B:85:LEU:O	1:B:89:VAL:HG23	2.18	0.44
1:B:168:PHE:HB3	1:C:168:PHE:CZ	2.52	0.44
1:C:313:GLN:HG2	1:C:338:LYS:HG2	1.98	0.44
2:E:398:LYS:HG2	2:E:614:LEU:HD12	1.98	0.44
2:E:885:VAL:HG12	2:E:887:VAL:HG23	1.99	0.44
1:A:167:ILE:O	1:A:171:THR:HG23	2.17	0.44
2:E:1214:ILE:HG12	2:E:1223:PHE:HE2	1.81	0.44
2:E:1246:ARG:HA	2:E:1246:ARG:NE	2.33	0.44
1:B:221:ARG:HG2	1:B:222:LYS:H	1.83	0.44
1:D:198:PHE:CZ	1:D:200:LEU:HD12	2.53	0.44
2:E:777:PRO:HG2	2:E:835:ARG:CZ	2.47	0.44
1:B:225:SER:OG	1:B:229:GLU:N	2.51	0.44
2:E:1070:LEU:HD23	2:E:1070:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PHE:HA	1:D:100:LEU:HD13	2.00	0.44
2:E:681:ILE:HB	2:E:701:ILE:H	1.82	0.43
2:E:394:LYS:NZ	2:E:614:LEU:HD21	2.33	0.43
2:E:1442:PRO:HG2	2:E:1445:LYS:HA	2.01	0.43
1:B:35:PHE:HE2	1:B:233:LEU:HD13	1.83	0.43
2:E:899:TRP:CD1	2:E:913:THR:HG22	2.53	0.43
2:E:1553:LYS:N	2:E:1556:ALA:O	2.46	0.43
1:C:168:PHE:HD1	1:C:168:PHE:O	2.01	0.43
2:E:901:ILE:HB	2:E:911:GLU:HA	1.99	0.43
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.83	0.43
1:B:285:VAL:HB	1:B:302:THR:HG23	2.01	0.43
2:E:178:LEU:O	2:E:182:LEU:HG	2.19	0.43
2:E:1254:TYR:OH	5:E:1604:P5S:H52	2.18	0.43
1:C:249:ILE:HD12	1:C:249:ILE:HA	1.92	0.43
1:D:225:SER:OG	1:D:229:GLU:N	2.49	0.43
2:E:586:LEU:O	2:E:589:PRO:HD2	2.19	0.43
2:E:1024:HIS:ND1	2:E:1148:LEU:HD23	2.34	0.43
2:E:1179:GLN:NE2	2:E:1183:ARG:HE	2.17	0.43
2:E:1435:THR:HA	2:E:1474:ILE:HA	2.00	0.43
2:E:219:GLN:HB2	2:E:232:TRP:CZ2	2.53	0.43
2:E:711:ILE:HB	2:E:887:VAL:HG13	2.00	0.43
2:E:1191:GLN:O	2:E:1195:THR:HG23	2.18	0.43
3:C:402:PTY:H162	3:C:402:PTY:H191	1.86	0.43
1:D:238:ILE:HG23	1:D:259:HIS:CE1	2.54	0.43
2:E:305:PHE:HZ	5:E:1604:P5S:H20	1.84	0.43
1:B:201:ARG:HG3	1:B:256:ILE:HD13	2.00	0.43
1:C:150:ILE:HD11	1:D:121:PHE:HE2	1.84	0.43
2:E:358:LEU:HD12	2:E:358:LEU:HA	1.81	0.42
2:E:519:CYS:SG	2:E:1106:ILE:HD11	2.59	0.42
2:E:1024:HIS:HE1	2:E:1145:ARG:HA	1.84	0.42
2:E:1179:GLN:HE22	2:E:1183:ARG:HH21	1.66	0.42
2:E:1239:LEU:HA	2:E:1239:LEU:HD23	1.82	0.42
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.81	0.42
2:E:85:LEU:O	2:E:89:ILE:HG12	2.19	0.42
1:D:167:ILE:HD13	1:D:167:ILE:HA	1.88	0.42
2:E:77:LEU:HD23	2:E:77:LEU:HA	1.85	0.42
2:E:123:TYR:OH	2:E:135:LEU:HG	2.19	0.42
2:E:366:LEU:HD23	2:E:366:LEU:HA	1.80	0.42
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.79	0.42
1:B:335:ASN:OD1	1:B:335:ASN:N	2.52	0.42
2:E:1179:GLN:NE2	2:E:1183:ARG:HH21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:563:VAL:HG21	2:E:1037:TRP:CH2	2.55	0.42
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.79	0.42
2:E:356:TYR:HD2	3:E:1602:PTY:HC6	1.85	0.42
2:E:152:ILE:O	2:E:155:VAL:HG22	2.19	0.42
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.77	0.42
2:E:250:ILE:HG23	2:E:1240:PHE:CE2	2.55	0.42
2:E:251:ALA:O	2:E:1236:ILE:HD13	2.19	0.42
2:E:1024:HIS:ND1	2:E:1148:LEU:HB3	2.35	0.42
2:E:1301:ASN:HD22	2:E:1301:ASN:HA	1.61	0.42
1:B:220:VAL:HB	1:B:282:GLU:HB3	2.02	0.42
2:E:21:VAL:HB	2:E:27:PHE:CD2	2.55	0.41
2:E:214:GLY:O	2:E:216:ARG:HD2	2.20	0.41
2:E:317:PRO:HB3	2:E:581:SER:OG	2.20	0.41
1:C:167:ILE:O	1:C:171:THR:HG23	2.20	0.41
1:D:345:THR:O	1:D:349:LEU:N	2.39	0.41
2:E:1240:PHE:HD1	2:E:1240:PHE:HA	1.64	0.41
1:D:186:HIS:HB2	1:D:308:GLU:O	2.19	0.41
1:D:283:ILE:O	1:D:303:SER:HA	2.20	0.41
2:E:149:THR:O	2:E:152:ILE:HB	2.20	0.41
2:E:1127:SER:O	2:E:1131:THR:HG23	2.20	0.41
2:E:1494:ARG:O	2:E:1497:VAL:HB	2.20	0.41
1:A:86:PHE:CD2	1:A:152:GLN:HG3	2.55	0.41
1:A:97:HIS:ND1	1:A:110:CYS:SG	2.94	0.41
2:E:1106:ILE:HG22	2:E:1107:LEU:HD23	2.03	0.41
1:A:137:MET:SD	1:B:135:GLY:HA3	2.61	0.41
2:E:156:LYS:HD3	2:E:156:LYS:HA	1.73	0.41
2:E:427:GLN:OE1	2:E:602:LYS:HB3	2.21	0.41
2:E:1395:MET:HE3	2:E:1419:ARG:HD3	2.02	0.41
1:C:231:VAL:HG11	1:C:234:HIS:ND1	2.36	0.41
2:E:305:PHE:HD1	2:E:305:PHE:HA	1.78	0.41
2:E:1203:HIS:CD2	2:E:1203:HIS:C	2.99	0.41
1:A:97:HIS:O	1:A:97:HIS:CG	2.74	0.40
1:A:213:ALA:HB3	1:A:249:ILE:O	2.21	0.40
1:A:114:ILE:HD13	1:A:114:ILE:HA	1.91	0.40
2:E:491:HIS:CE1	2:E:528:LYS:HB3	2.56	0.40
2:E:584:HIS:O	2:E:587:VAL:HG12	2.20	0.40
2:E:1182:PHE:CD2	2:E:1248:LEU:HD22	2.57	0.40
1:C:187:ALA:HB1	1:C:199:MET:O	2.20	0.40
1:C:335:ASN:OD1	1:C:335:ASN:N	2.54	0.40
1:A:75:PHE:CZ	1:A:163:MET:HA	2.56	0.40
1:A:95:PHE:HE2	2:E:27:PHE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:723:LEU:HD21	2:E:887:VAL:HG21	2.03	0.40
2:E:1223:PHE:HD1	2:E:1223:PHE:HA	1.77	0.40
2:E:1242:THR:O	2:E:1246:ARG:HG2	2.21	0.40
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.90	0.40
1:A:244:VAL:HG23	1:A:246:GLY:H	1.87	0.40
2:E:222:VAL:HG12	2:E:223:ASN:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/390 (88%)	321 (93%)	23 (7%)	0	100	100
1	B	324/390 (83%)	310 (96%)	14 (4%)	0	100	100
1	C	324/390 (83%)	307 (95%)	17 (5%)	0	100	100
1	D	324/390 (83%)	308 (95%)	16 (5%)	0	100	100
2	E	1413/1582 (89%)	1358 (96%)	55 (4%)	0	100	100
All	All	2729/3142 (87%)	2604 (95%)	125 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/341 (60%)	202 (99%)	2 (1%)	68	76
1	B	202/341 (59%)	201 (100%)	1 (0%)	81	82
1	C	206/341 (60%)	204 (99%)	2 (1%)	68	76
1	D	209/341 (61%)	206 (99%)	3 (1%)	59	71
2	E	776/1373 (56%)	771 (99%)	5 (1%)	78	80
All	All	1597/2737 (58%)	1584 (99%)	13 (1%)	70	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	PHE
1	A	339	VAL
2	E	31	LEU
2	E	218	LEU
2	E	221	PHE
2	E	739	TRP
2	E	1240	PHE
1	B	92	LEU
1	C	73	LEU
1	C	127	VAL
1	D	70	HIS
1	D	157	LEU
1	D	345	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
2	E	10	ASN
2	E	493	ASN
2	E	584	HIS
2	E	870	GLN
2	E	896	HIS
1	B	46	HIS
1	D	160	ASN
1	D	299	GLN
1	D	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PTY	A	404	-	31,31,49	0.57	0	34,36,54	0.45	0
3	PTY	B	401	-	31,31,49	0.56	0	34,36,54	0.48	0
3	PTY	C	402	-	31,31,49	0.58	0	34,36,54	0.49	0
4	POV	B	402	-	35,35,51	0.61	0	41,43,59	0.52	0
4	POV	C	401	-	35,35,51	0.63	0	41,43,59	0.56	0
4	POV	D	401	-	35,35,51	0.63	0	41,43,59	0.53	0
4	POV	A	402	-	35,35,51	0.63	0	41,43,59	0.66	0
4	POV	E	1606	-	35,35,51	0.61	0	41,43,59	0.57	1 (2%)
6	ATP	E	1605	-	32,33,33	0.48	1 (3%)	48,52,52	0.29	0
3	PTY	E	1601	-	31,31,49	0.58	0	34,36,54	0.57	0
7	NAG	E	1607	-	14,14,15	0.22	0	17,19,21	0.44	0
3	PTY	A	403	-	31,31,49	0.57	0	34,36,54	0.52	0
3	PTY	E	1603	-	31,31,49	0.59	0	34,36,54	0.46	0
3	PTY	E	1602	-	31,31,49	0.57	0	34,36,54	0.45	0
3	PTY	A	401	-	31,31,49	0.56	0	34,36,54	0.46	0
5	P5S	E	1604	-	52,53,53	0.53	0	54,60,60	0.83	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PTY	A	404	-	-	15/35/35/53	-
3	PTY	B	401	-	-	13/35/35/53	-
3	PTY	C	402	-	-	9/35/35/53	-
4	POV	B	402	-	-	22/39/39/55	-
4	POV	C	401	-	-	20/39/39/55	-
4	POV	D	401	-	-	13/39/39/55	-
4	POV	A	402	-	-	15/39/39/55	-
4	POV	E	1606	-	-	13/39/39/55	-
6	ATP	E	1605	-	-	3/22/38/38	0/3/3/3
3	PTY	E	1601	-	-	11/35/35/53	-
7	NAG	E	1607	-	-	2/6/23/26	0/1/1/1
3	PTY	A	403	-	-	16/35/35/53	-
3	PTY	E	1603	-	-	18/35/35/53	-
3	PTY	E	1602	-	-	9/35/35/53	-
3	PTY	A	401	-	-	6/35/35/53	-
5	P5S	E	1604	-	-	33/59/59/59	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1605	ATP	PB-O3B	-2.02	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1604	P5S	OG-CB-CA	4.59	112.06	108.06
4	E	1606	POV	O13-P-O14	2.01	121.81	112.44

There are no chirality outliers.

All (218) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	PTY	C3-O11-P1-O13
3	A	404	PTY	C3-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
3	A	404	PTY	C3-O11-P1-O14
3	E	1601	PTY	C2-C3-O11-P1
3	E	1602	PTY	C5-O14-P1-O11
3	E	1602	PTY	C5-O14-P1-O12
3	E	1603	PTY	C3-O11-P1-O12
3	E	1603	PTY	C5-O14-P1-O13
3	B	401	PTY	C11-C8-O7-C6
3	B	401	PTY	C3-O11-P1-O13
3	B	401	PTY	C5-O14-P1-O13
3	C	402	PTY	C3-O11-P1-O13
3	C	402	PTY	C5-O14-P1-O11
4	A	402	POV	C1-O11-P-O12
4	A	402	POV	C1-O11-P-O13
4	A	402	POV	C1-O11-P-O14
4	A	402	POV	O12-C11-C12-N
4	E	1606	POV	C1-O11-P-O14
4	B	402	POV	C1-O11-P-O12
4	B	402	POV	C11-O12-P-O11
4	B	402	POV	C11-O12-P-O14
4	B	402	POV	O21-C2-C3-O31
4	B	402	POV	C12-C11-O12-P
4	C	401	POV	C1-O11-P-O12
4	C	401	POV	C1-O11-P-O13
4	C	401	POV	C1-O11-P-O14
4	C	401	POV	C11-O12-P-O11
4	C	401	POV	C11-O12-P-O13
4	C	401	POV	C11-O12-P-O14
4	D	401	POV	C1-O11-P-O14
4	D	401	POV	C11-O12-P-O14
5	E	1604	P5S	O-C-CA-CB
5	E	1604	P5S	C3-O16-P12-OG
5	E	1604	P5S	C3-O16-P12-O15
6	E	1605	ATP	C5'-O5'-PA-O1A
3	B	401	PTY	O10-C8-O7-C6
3	E	1602	PTY	C31-C30-O4-C1
3	E	1602	PTY	O30-C30-O4-C1
4	C	401	POV	C32-C31-O31-C3
4	C	401	POV	O32-C31-O31-C3
5	E	1604	P5S	C39-C38-O37-C2
4	B	402	POV	C11-C12-N-C15
7	E	1607	NAG	C8-C7-N2-C2
7	E	1607	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	402	POV	C34-C35-C36-C37
3	E	1603	PTY	C8-C11-C12-C13
3	A	404	PTY	C30-C31-C32-C33
3	E	1603	PTY	C30-C31-C32-C33
4	D	401	POV	C21-C22-C23-C24
4	E	1606	POV	C32-C31-O31-C3
4	C	401	POV	C33-C34-C35-C36
5	E	1604	P5S	O47-C38-O37-C2
4	B	402	POV	C11-C12-N-C13
4	B	402	POV	C11-C12-N-C14
4	B	402	POV	C23-C24-C25-C26
3	C	402	PTY	C8-C11-C12-C13
4	E	1606	POV	O32-C31-O31-C3
5	E	1604	P5S	C20-C17-O19-C1
3	E	1601	PTY	C12-C13-C14-C15
4	A	402	POV	C22-C21-O21-C2
4	E	1606	POV	C22-C21-O21-C2
5	E	1604	P5S	C21-C22-C23-C24
5	E	1604	P5S	C23-C24-C25-C26
5	E	1604	P5S	C22-C23-C24-C25
4	D	401	POV	C32-C31-O31-C3
4	B	402	POV	C24-C25-C26-C27
4	C	401	POV	C25-C26-C27-C28
3	A	404	PTY	C12-C13-C14-C15
5	E	1604	P5S	C44-C45-C46-C48
3	E	1603	PTY	C31-C30-O4-C1
4	E	1606	POV	C24-C25-C26-C27
3	A	403	PTY	C30-C31-C32-C33
5	E	1604	P5S	O18-C17-O19-C1
4	A	402	POV	O22-C21-O21-C2
4	E	1606	POV	O22-C21-O21-C2
5	E	1604	P5S	C27-C28-C29-C30
5	E	1604	P5S	C25-C26-C27-C28
5	E	1604	P5S	C43-C44-C45-C46
3	E	1603	PTY	C32-C33-C34-C35
3	A	401	PTY	C15-C16-C17-C18
3	A	403	PTY	C11-C8-O7-C6
3	A	403	PTY	C14-C15-C16-C17
3	A	403	PTY	O10-C8-O7-C6
4	B	402	POV	C34-C35-C36-C37
6	E	1605	ATP	O4'-C4'-C5'-O5'
4	D	401	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	A	401	PTY	C31-C32-C33-C34
5	E	1604	P5S	C-CA-CB-OG
3	E	1603	PTY	C17-C18-C19-C20
4	C	401	POV	C22-C23-C24-C25
3	E	1603	PTY	O30-C30-O4-C1
4	B	402	POV	O11-C1-C2-C3
6	E	1605	ATP	C3'-C4'-C5'-O5'
3	E	1603	PTY	C11-C8-O7-C6
3	A	403	PTY	O4-C1-C6-C5
3	B	401	PTY	O4-C1-C6-C5
4	E	1606	POV	C1-C2-C3-O31
4	B	402	POV	C1-C2-C3-O31
5	E	1604	P5S	O19-C1-C2-C3
4	A	402	POV	C26-C27-C28-C29
5	E	1604	P5S	C39-C40-C41-C42
4	E	1606	POV	C34-C35-C36-C37
4	B	402	POV	C33-C34-C35-C36
3	A	403	PTY	O14-C5-C6-O7
5	E	1604	P5S	O37-C2-C3-O16
3	A	404	PTY	C11-C12-C13-C14
4	D	401	POV	O21-C2-C3-O31
3	A	403	PTY	C15-C16-C17-C18
4	D	401	POV	C33-C34-C35-C36
5	E	1604	P5S	C1-C2-C3-O16
3	A	401	PTY	C17-C18-C19-C20
5	E	1604	P5S	C40-C41-C42-C43
3	B	401	PTY	C13-C14-C15-C16
3	E	1601	PTY	O4-C1-C6-C5
4	C	401	POV	C1-C2-C3-O31
3	E	1603	PTY	C13-C14-C15-C16
4	B	402	POV	O11-C1-C2-O21
4	A	402	POV	C24-C25-C26-C27
4	E	1606	POV	C31-C32-C33-C34
4	C	401	POV	O21-C2-C3-O31
5	E	1604	P5S	C50-C51-C52-C53
3	A	403	PTY	C31-C30-O4-C1
4	A	402	POV	O11-C1-C2-C3
3	E	1603	PTY	O10-C8-O7-C6
3	E	1601	PTY	C14-C15-C16-C17
3	A	403	PTY	O30-C30-O4-C1
3	E	1603	PTY	C12-C13-C14-C15
3	B	401	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
3	C	402	PTY	O14-C5-C6-O7
4	D	401	POV	O11-C1-C2-O21
3	A	404	PTY	O4-C1-C6-C5
3	E	1603	PTY	O4-C1-C6-C5
3	A	404	PTY	C2-C3-O11-P1
3	E	1603	PTY	C2-C3-O11-P1
4	E	1606	POV	O12-C11-C12-N
4	B	402	POV	O12-C11-C12-N
4	C	401	POV	O12-C11-C12-N
3	C	402	PTY	C14-C15-C16-C17
3	C	402	PTY	O14-C5-C6-C1
4	D	401	POV	O11-C1-C2-C3
3	A	404	PTY	C31-C32-C33-C34
4	A	402	POV	O11-C1-C2-O21
3	A	403	PTY	O4-C1-C6-O7
3	E	1601	PTY	O4-C1-C6-O7
3	E	1603	PTY	O4-C1-C6-O7
3	B	401	PTY	O4-C1-C6-O7
4	E	1606	POV	O21-C2-C3-O31
4	D	401	POV	C1-C2-C3-O31
3	A	404	PTY	C5-O14-P1-O13
3	E	1602	PTY	C3-O11-P1-O13
3	E	1602	PTY	C5-O14-P1-O13
3	C	402	PTY	C5-O14-P1-O13
4	A	402	POV	C11-C12-N-C15
4	B	402	POV	C1-O11-P-O14
5	E	1604	P5S	OXT-C-CA-CB
5	E	1604	P5S	C3-O16-P12-O13
4	E	1606	POV	C33-C34-C35-C36
3	E	1601	PTY	C17-C18-C19-C20
5	E	1604	P5S	C49-C50-C51-C52
3	E	1602	PTY	C8-C11-C12-C13
3	A	404	PTY	O14-C5-C6-C1
3	A	401	PTY	C14-C15-C16-C17
5	E	1604	P5S	C24-C25-C26-C27
3	E	1601	PTY	C13-C14-C15-C16
4	B	402	POV	C21-C22-C23-C24
3	E	1602	PTY	C30-C31-C32-C33
4	D	401	POV	C22-C21-O21-C2
4	D	401	POV	O22-C21-O21-C2
4	B	402	POV	O21-C21-C22-C23
5	E	1604	P5S	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
4	D	401	POV	C24-C25-C26-C27
3	A	401	PTY	C13-C14-C15-C16
4	B	402	POV	C25-C26-C27-C28
3	E	1603	PTY	C31-C32-C33-C34
3	B	401	PTY	O4-C30-C31-C32
4	C	401	POV	C24-C25-C26-C27
3	A	404	PTY	O14-C5-C6-O7
4	C	401	POV	O11-C1-C2-O21
4	C	401	POV	C2-C1-O11-P
3	A	404	PTY	O4-C1-C6-O7
4	B	402	POV	C22-C23-C24-C25
3	E	1601	PTY	C31-C30-O4-C1
5	E	1604	P5S	C2-C3-O16-P12
3	E	1601	PTY	O30-C30-O4-C1
3	A	403	PTY	O14-C5-C6-C1
3	B	401	PTY	O14-C5-C6-C1
3	E	1601	PTY	C6-C5-O14-P1
3	A	403	PTY	C17-C18-C19-C20
5	E	1604	P5S	C30-C31-C32-C33
5	E	1604	P5S	C1-C2-O37-C38
5	E	1604	P5S	C48-C49-C50-C51
3	C	402	PTY	C6-C5-O14-P1
3	B	401	PTY	C31-C32-C33-C34
4	E	1606	POV	C35-C36-C37-C38
3	E	1602	PTY	C32-C33-C34-C35
4	A	402	POV	C32-C33-C34-C35
3	E	1603	PTY	C12-C11-C8-O7
3	A	403	PTY	C31-C32-C33-C34
5	E	1604	P5S	C32-C33-C34-C35
3	E	1601	PTY	C31-C32-C33-C34
3	A	403	PTY	C12-C11-C8-O7
3	A	404	PTY	O4-C30-C31-C32
3	E	1603	PTY	C6-C5-O14-P1
4	B	402	POV	C32-C33-C34-C35
3	A	401	PTY	C12-C13-C14-C15
3	C	402	PTY	C16-C17-C18-C19
4	A	402	POV	C11-C12-N-C13
4	A	402	POV	C11-C12-N-C14
4	C	401	POV	C11-C12-N-C13
4	C	401	POV	C11-C12-N-C14
4	C	401	POV	C11-C12-N-C15
3	B	401	PTY	C12-C11-C8-O7

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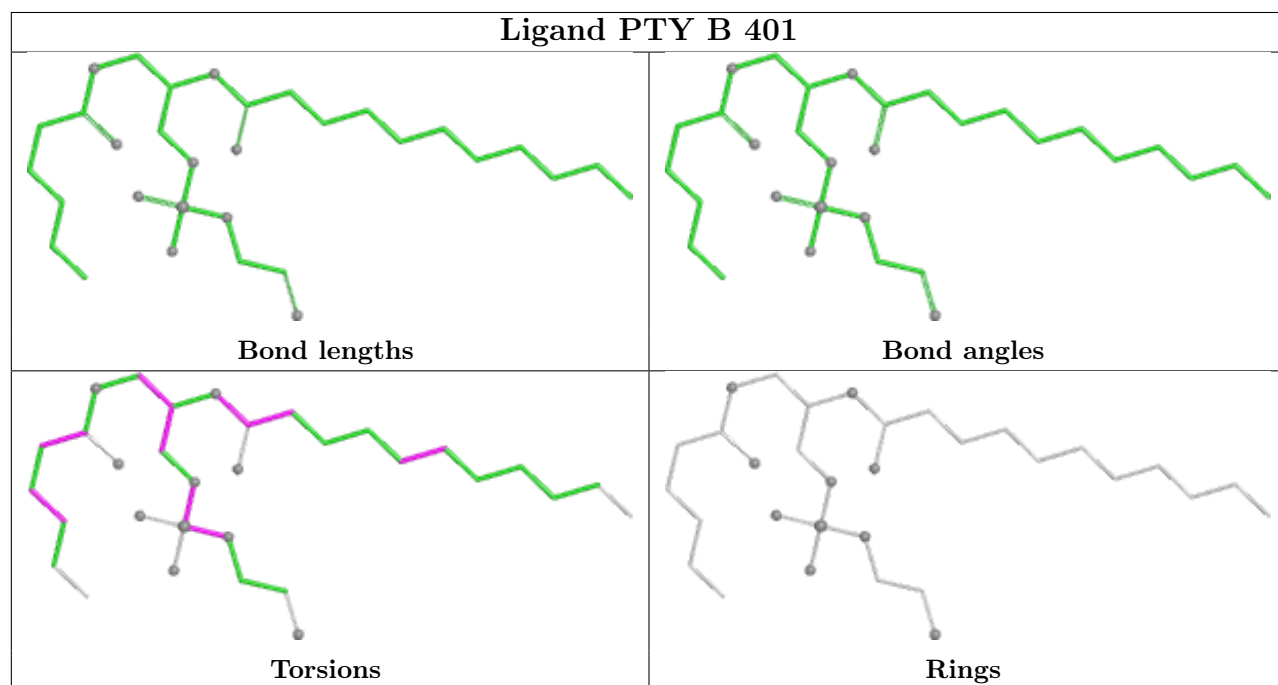
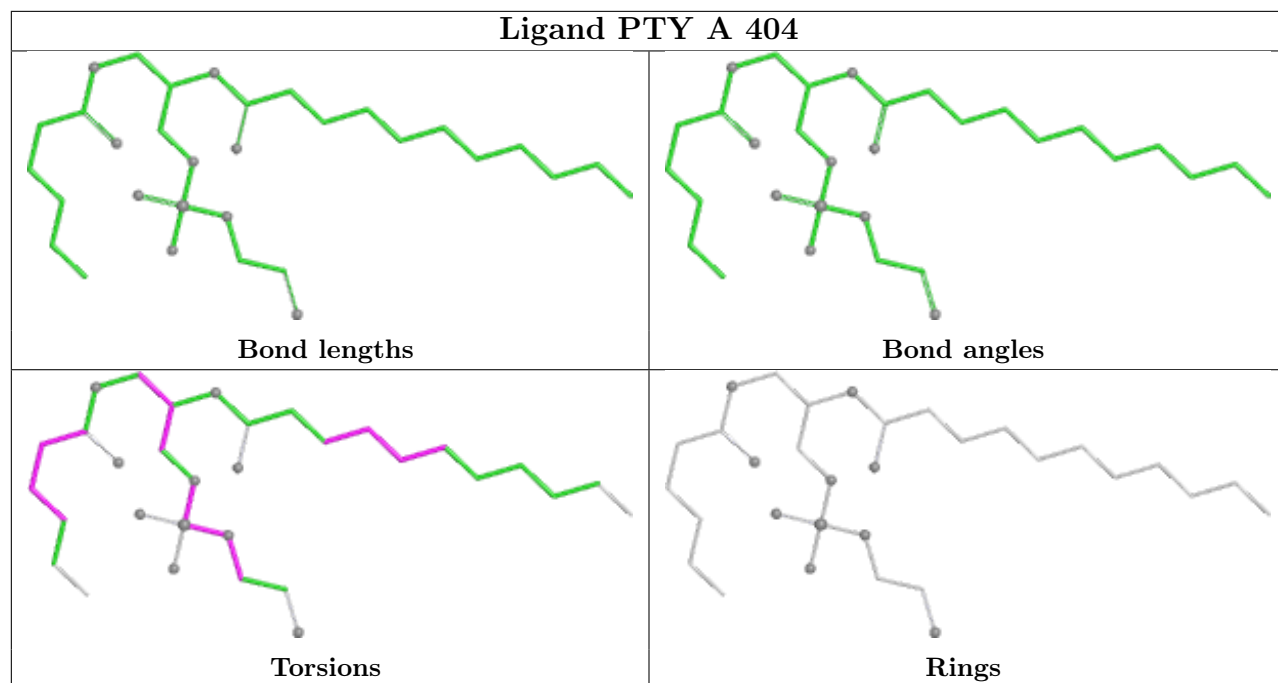
Mol	Chain	Res	Type	Atoms
5	E	1604	P5S	O19-C1-C2-O37
3	A	404	PTY	O30-C30-C31-C32
5	E	1604	P5S	C29-C30-C31-C32
3	A	404	PTY	C13-C14-C15-C16
3	A	403	PTY	C12-C11-C8-O10
3	B	401	PTY	C12-C11-C8-O10

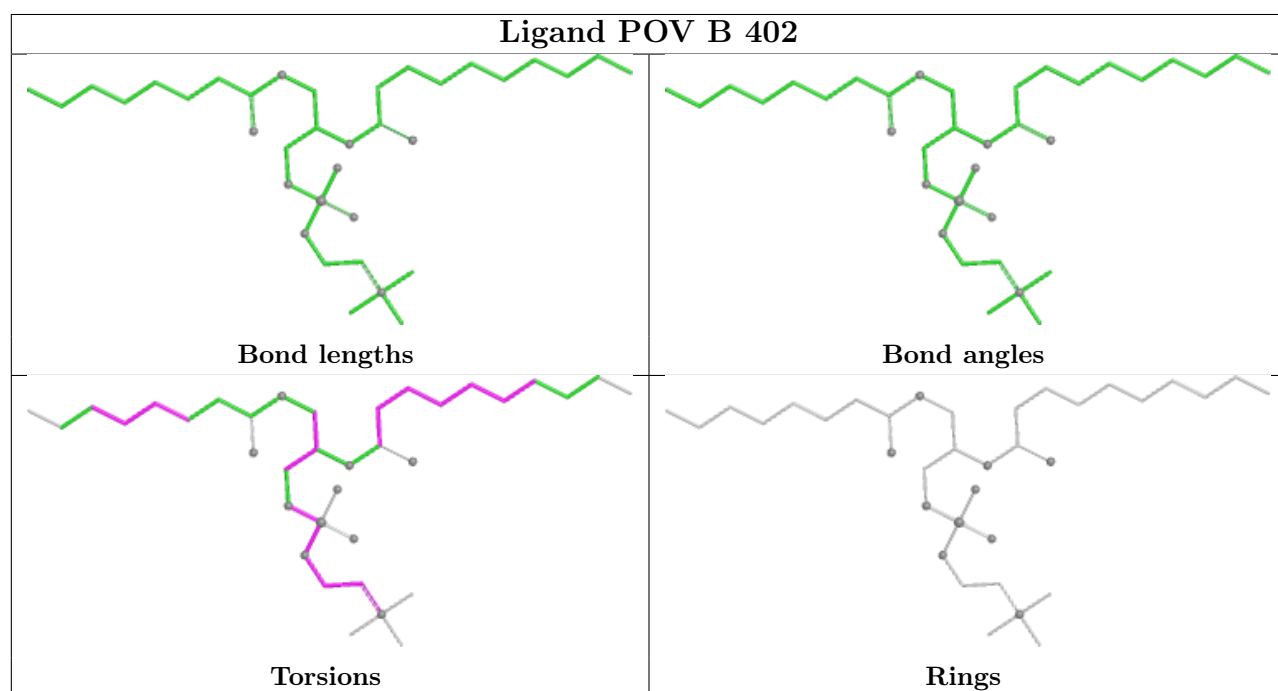
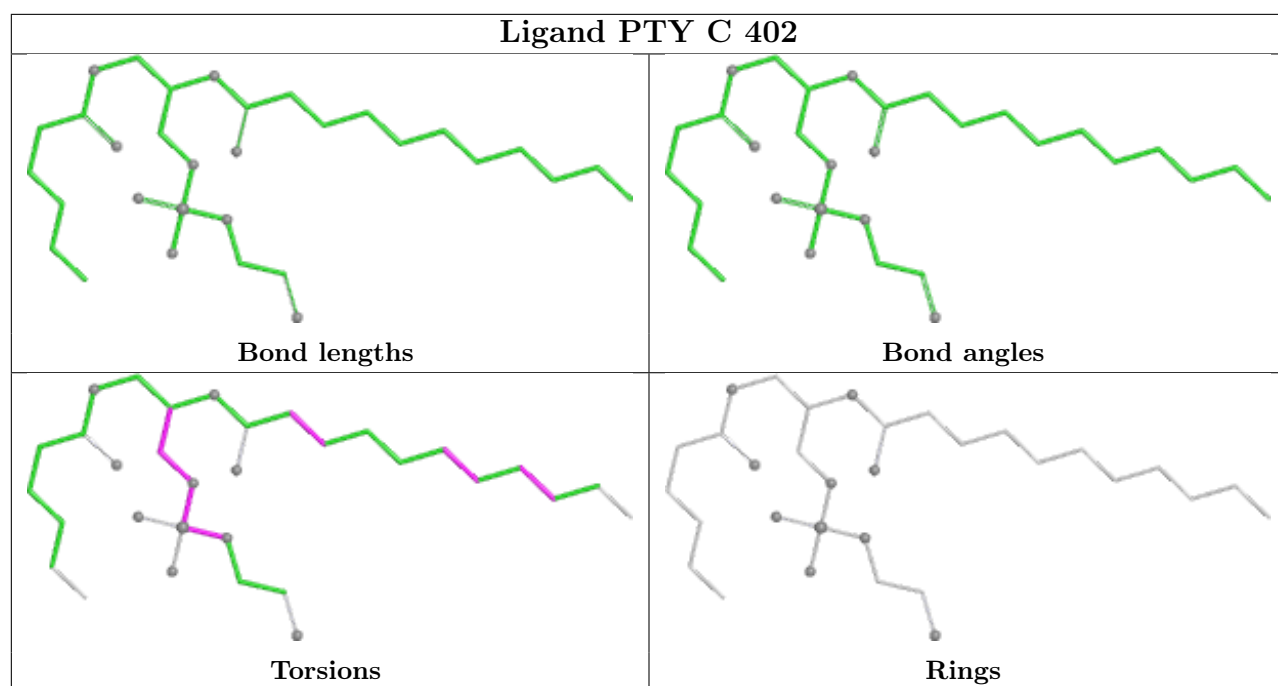
There are no ring outliers.

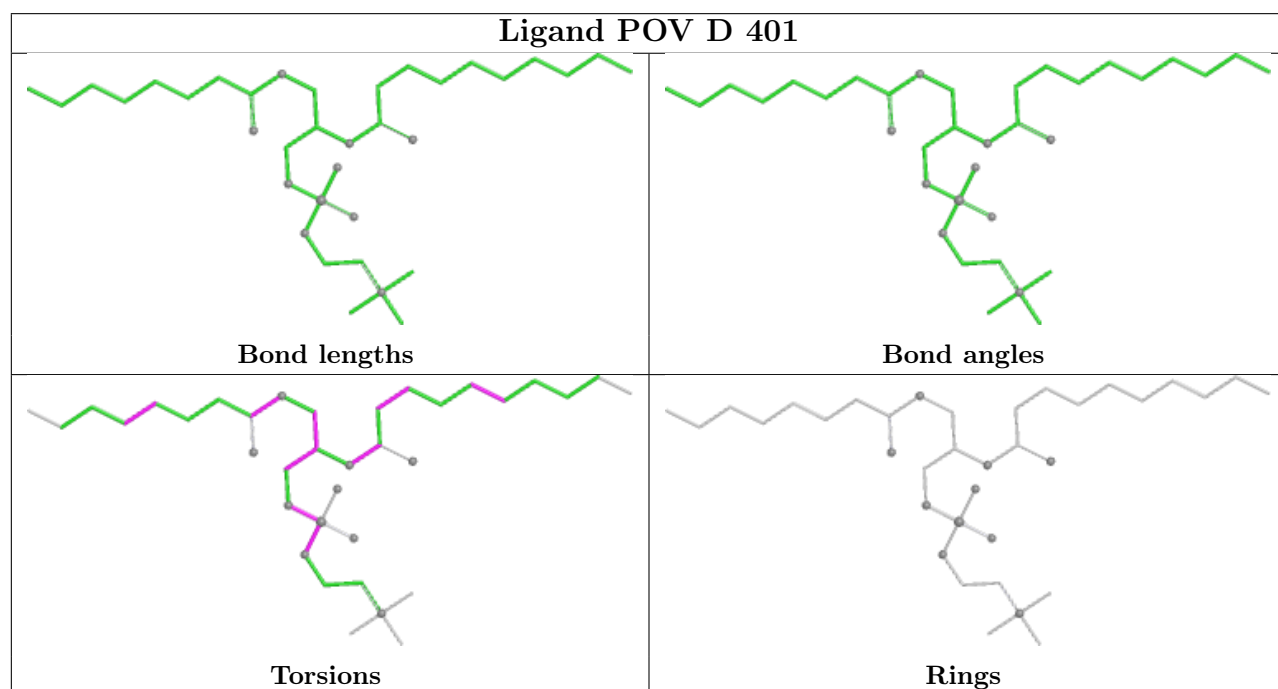
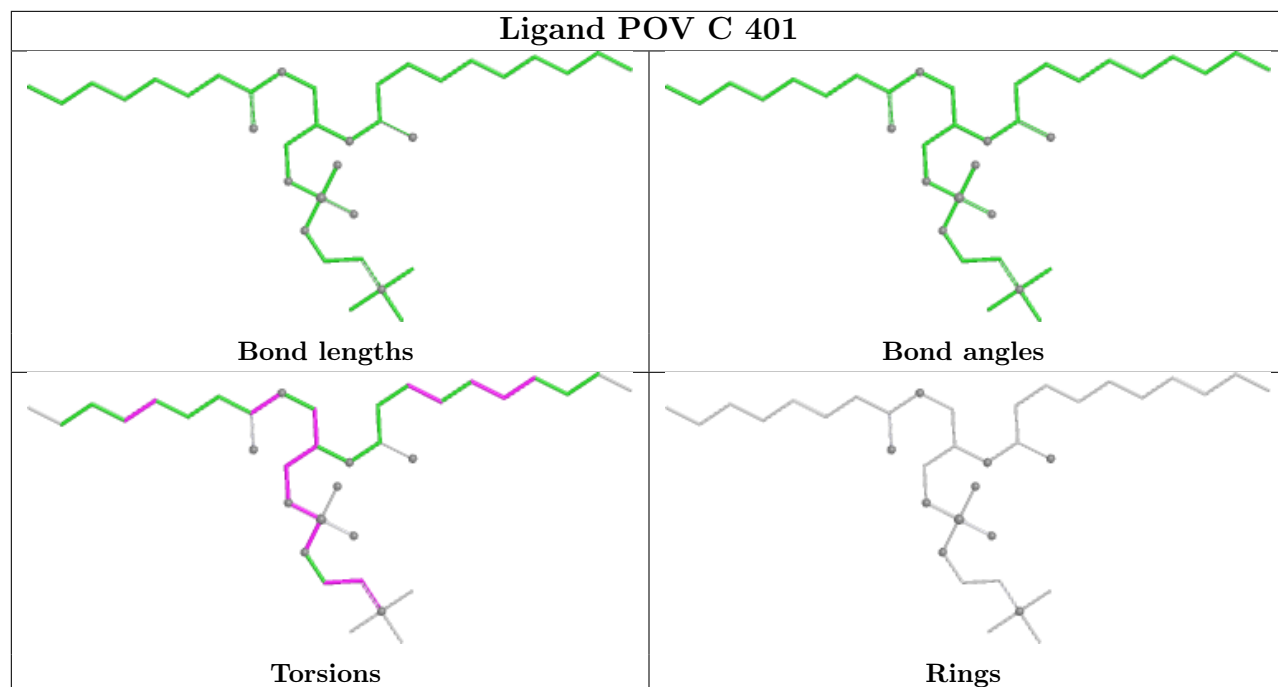
12 monomers are involved in 21 short contacts:

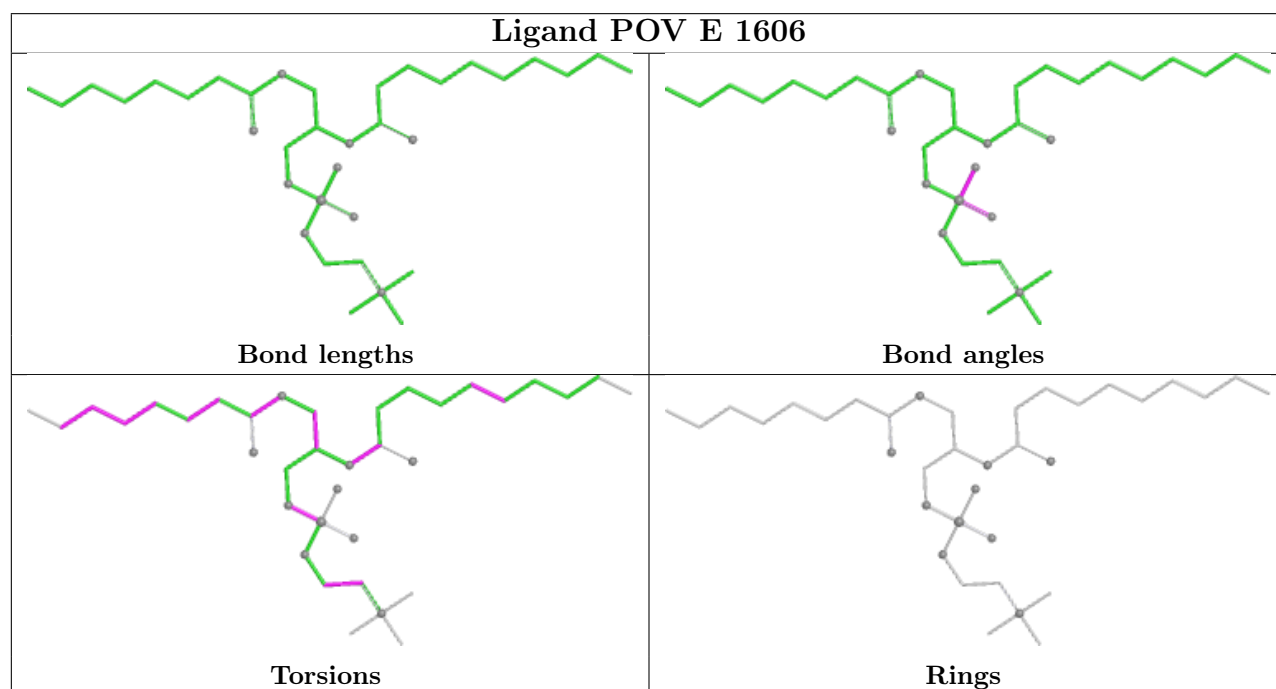
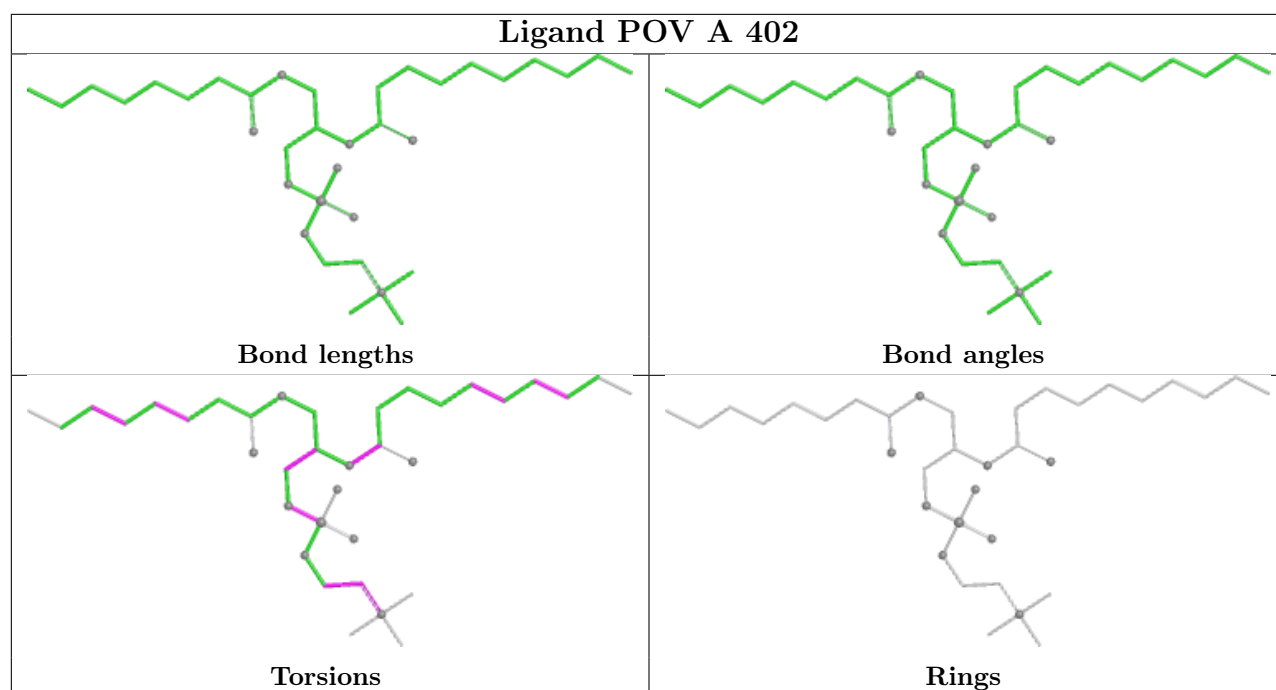
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	PTY	1	0
4	B	402	POV	1	0
4	C	401	POV	1	0
4	D	401	POV	1	0
4	A	402	POV	4	0
4	E	1606	POV	2	0
6	E	1605	ATP	1	0
3	E	1601	PTY	3	0
7	E	1607	NAG	1	0
3	A	403	PTY	1	0
3	E	1602	PTY	1	0
5	E	1604	P5S	5	0

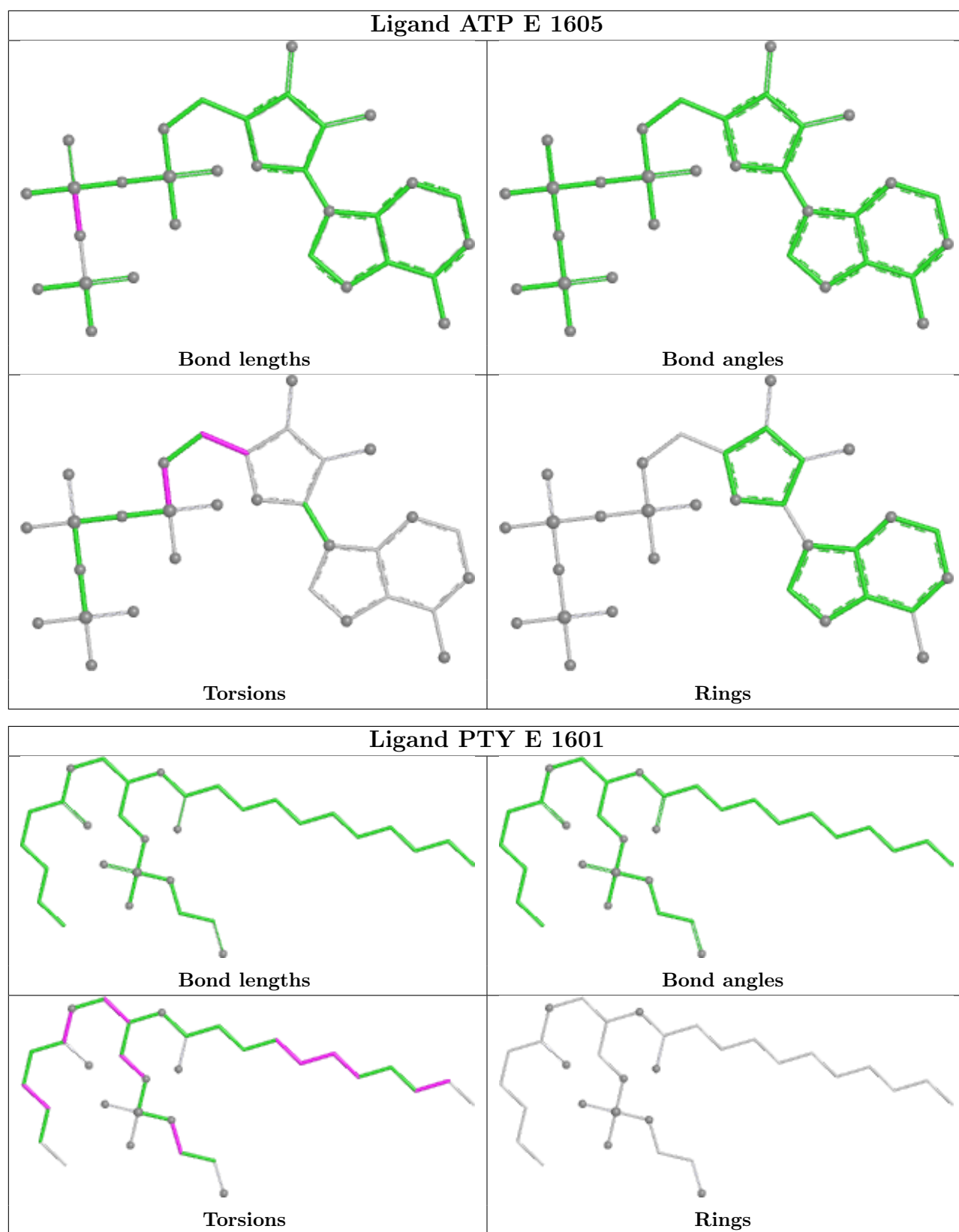
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

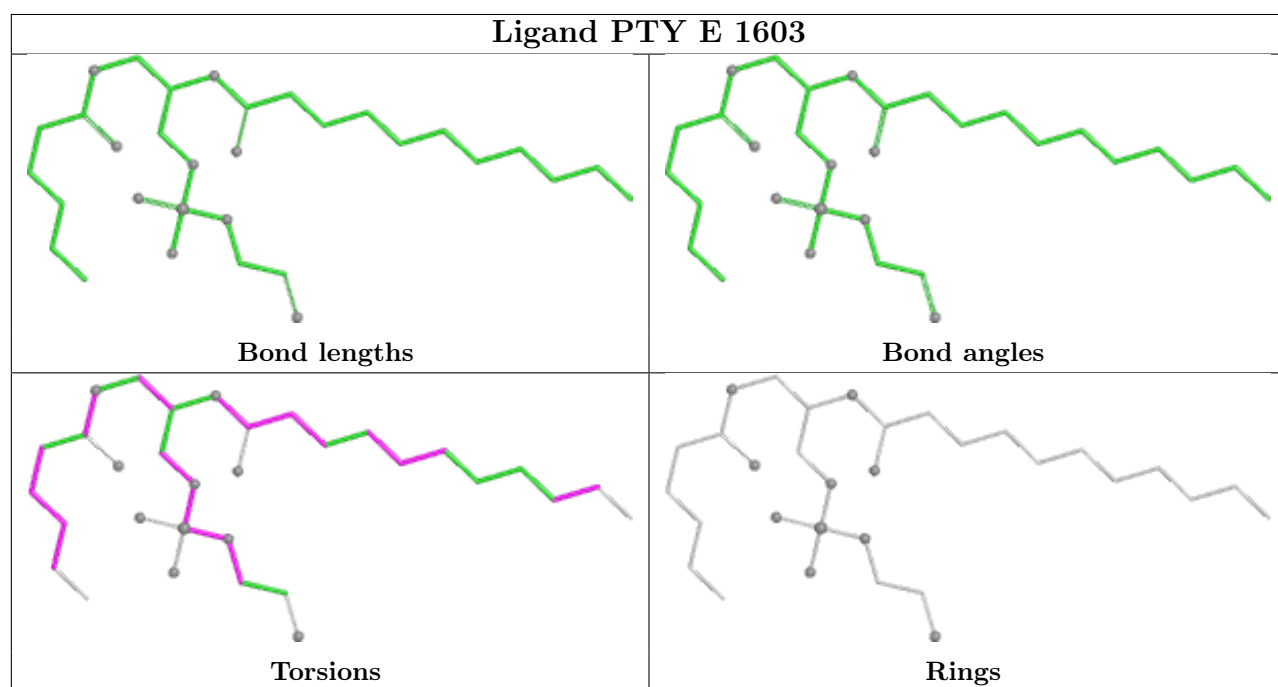
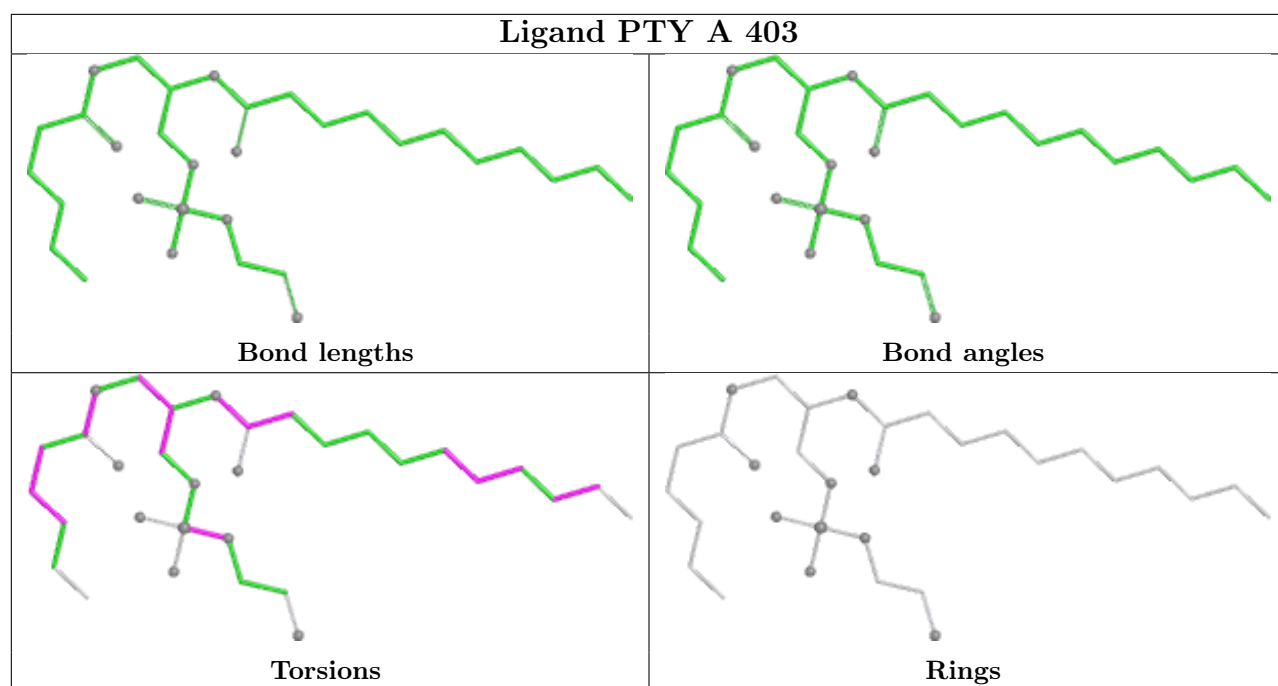


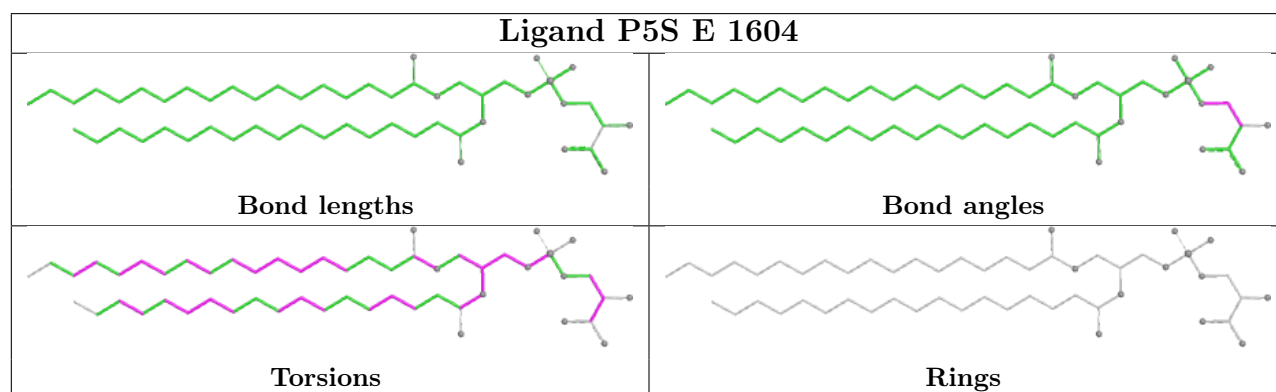
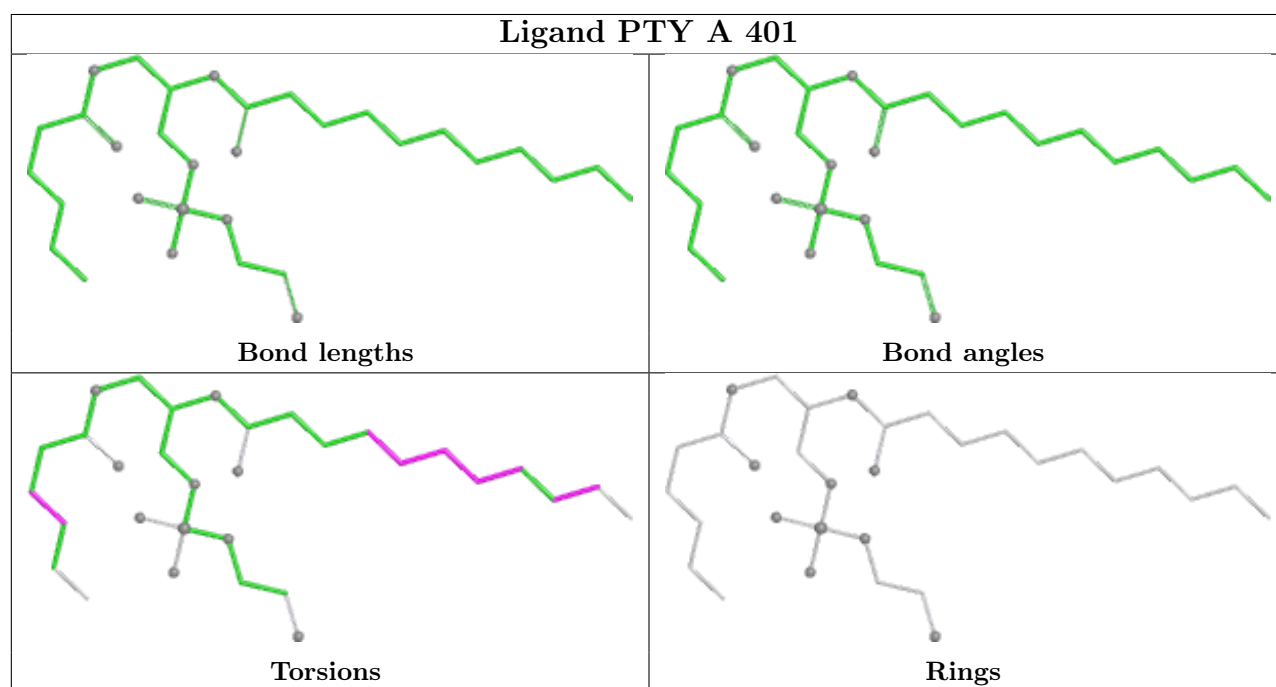
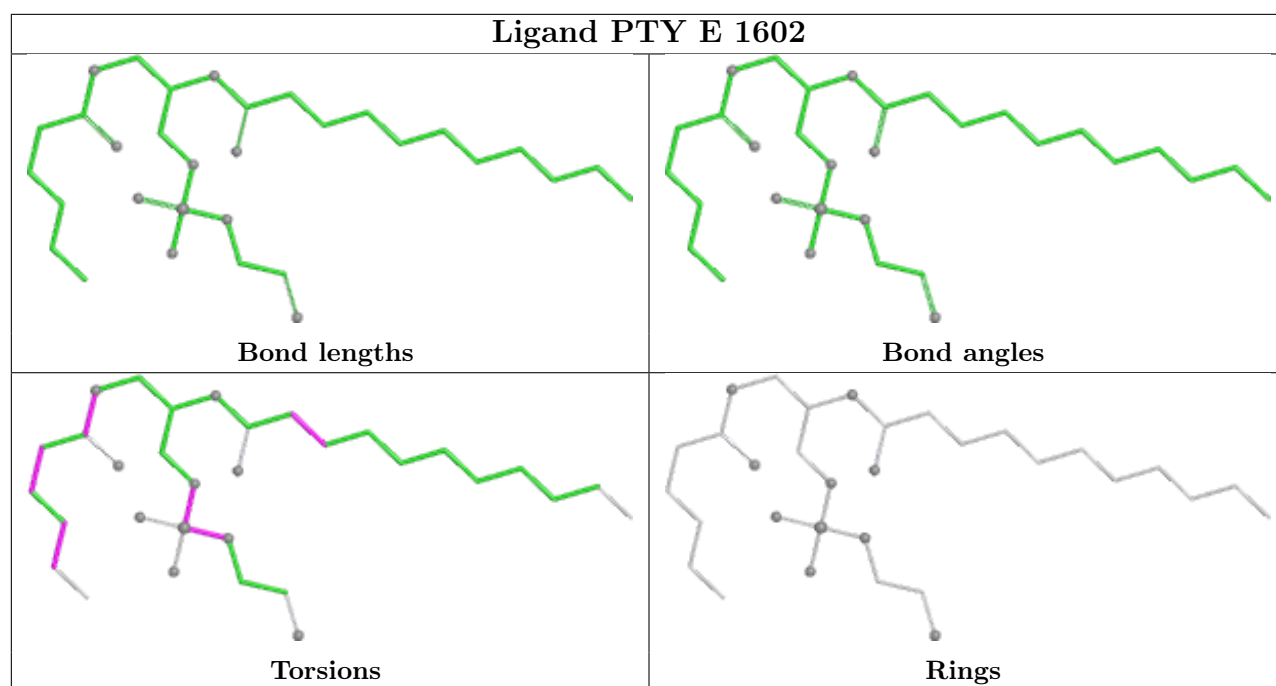












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

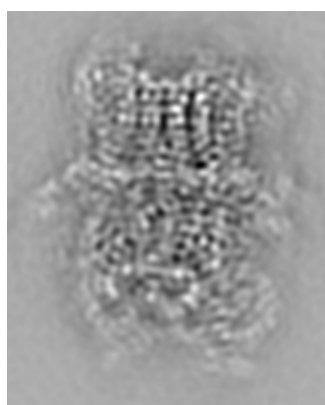
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26321. These allow visual inspection of the internal detail of the map and identification of artifacts.

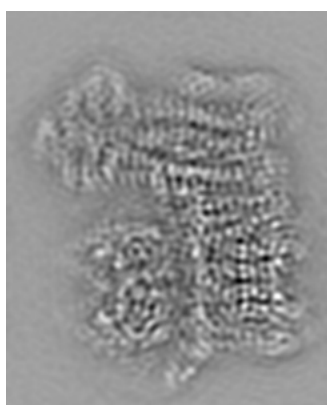
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

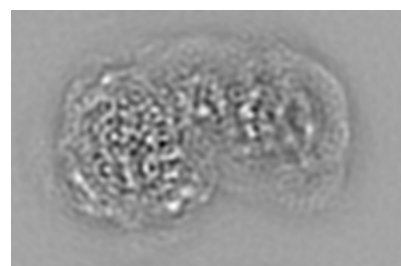
6.1.1 Primary map



X



Y

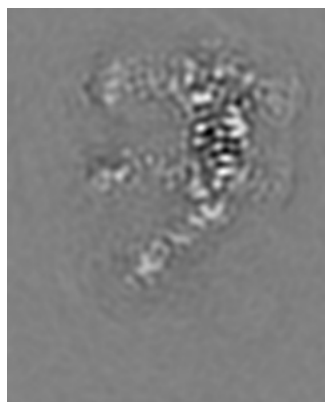


Z

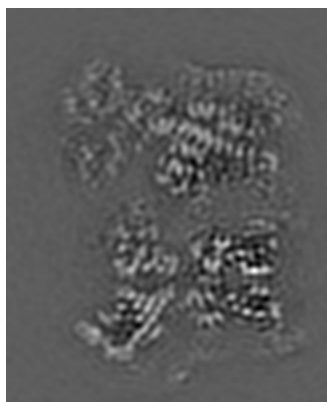
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

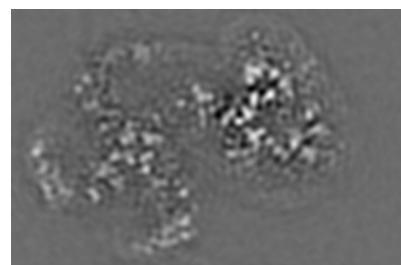
6.2.1 Primary map



X Index: 57



Y Index: 37

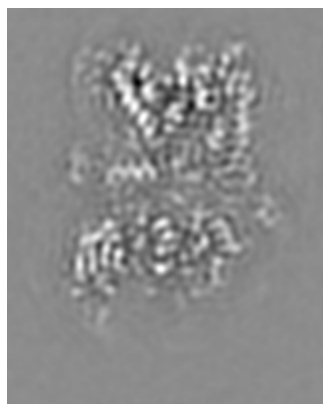


Z Index: 47

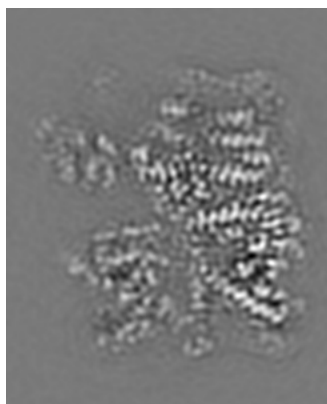
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

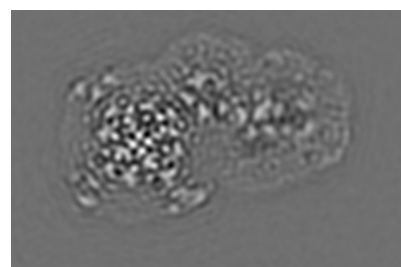
6.3.1 Primary map



X Index: 28



Y Index: 45

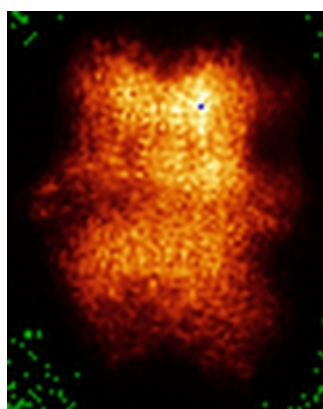


Z Index: 71

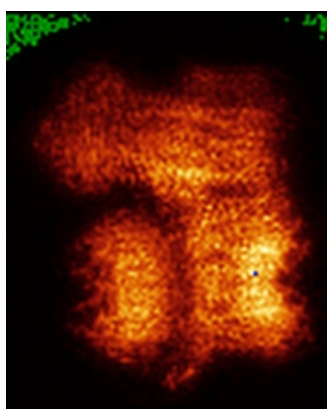
The images above show the largest variance slices of the map in three orthogonal directions.

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

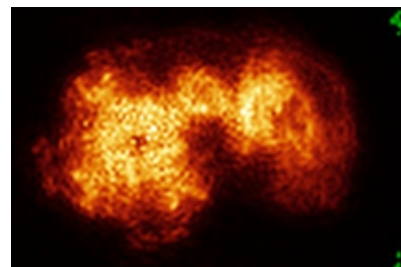
6.4.1 Primary map



X



Y

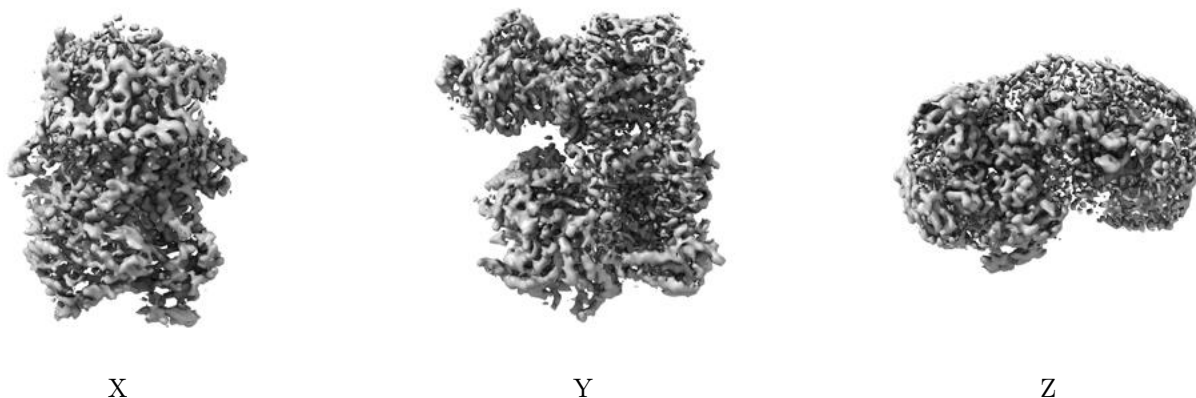


Z

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

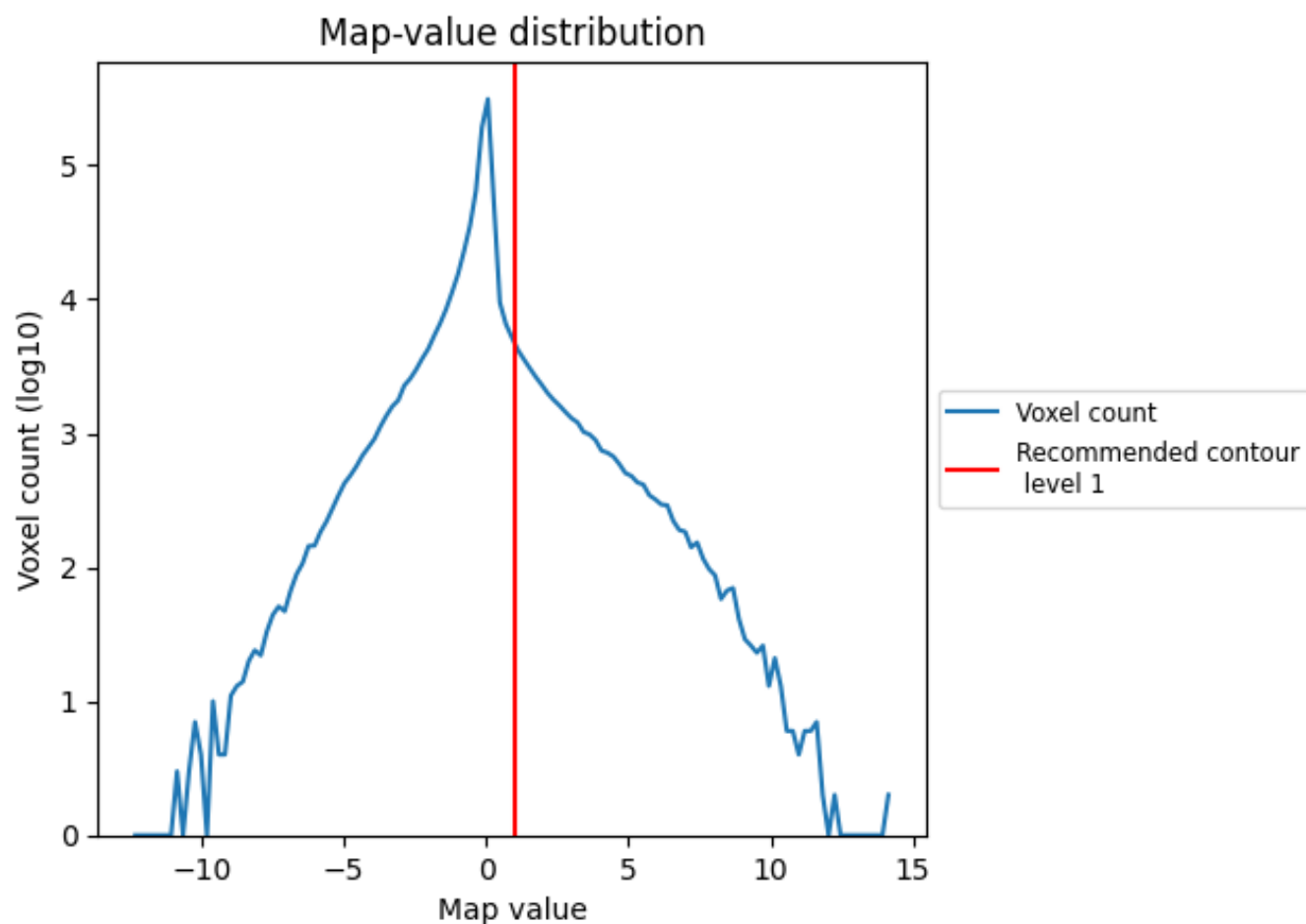
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

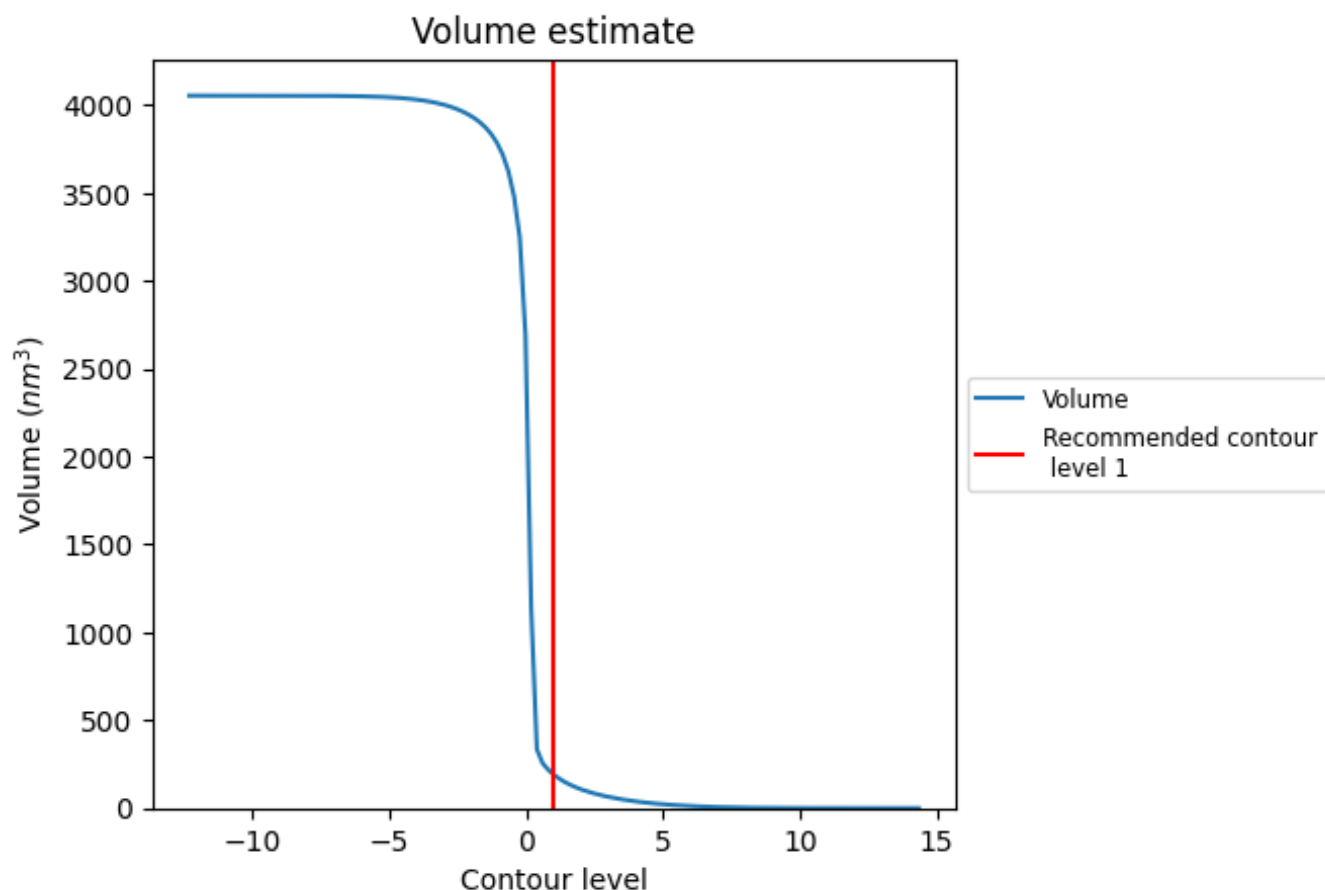
This section contains the results of statistical analysis of the map.

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 191 nm³; this corresponds to an approximate mass of 172 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation ⓘ

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

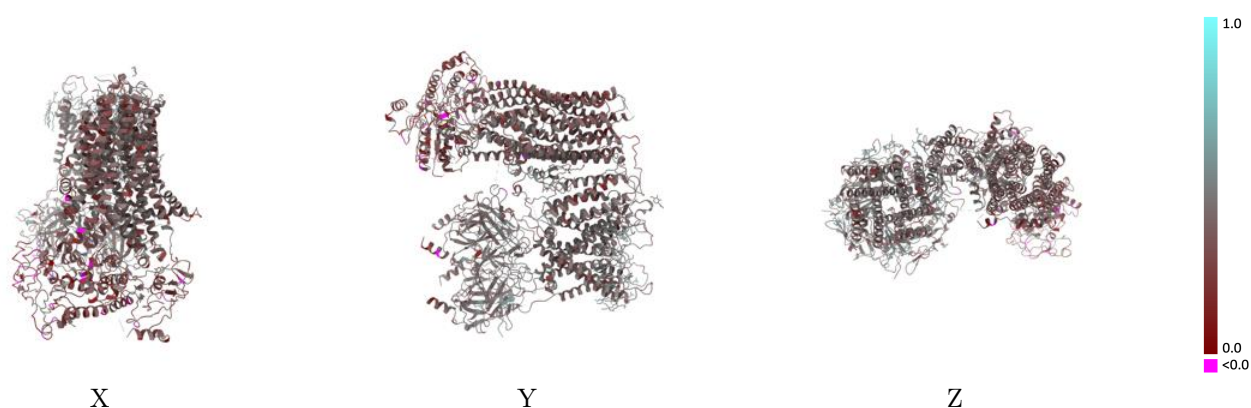
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26321 and PDB model 7U2X. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

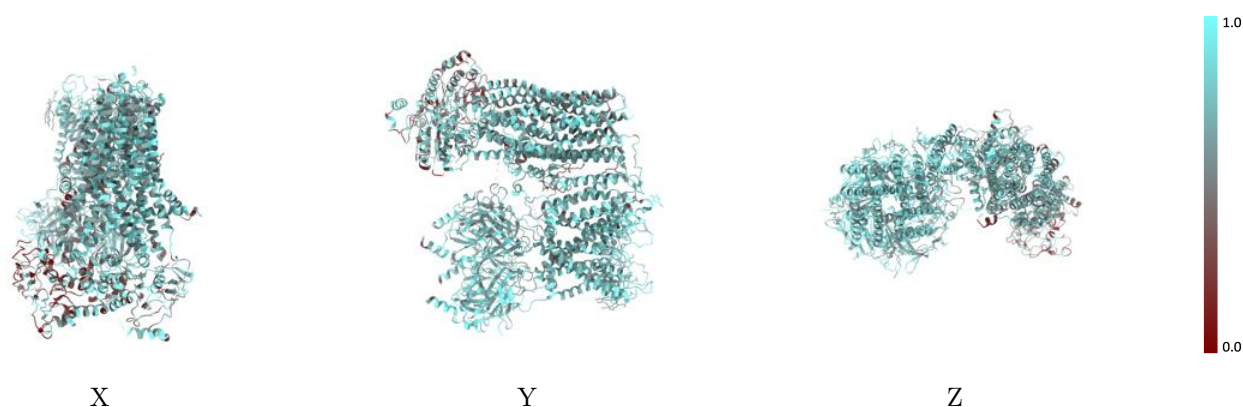
This section was not generated.

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



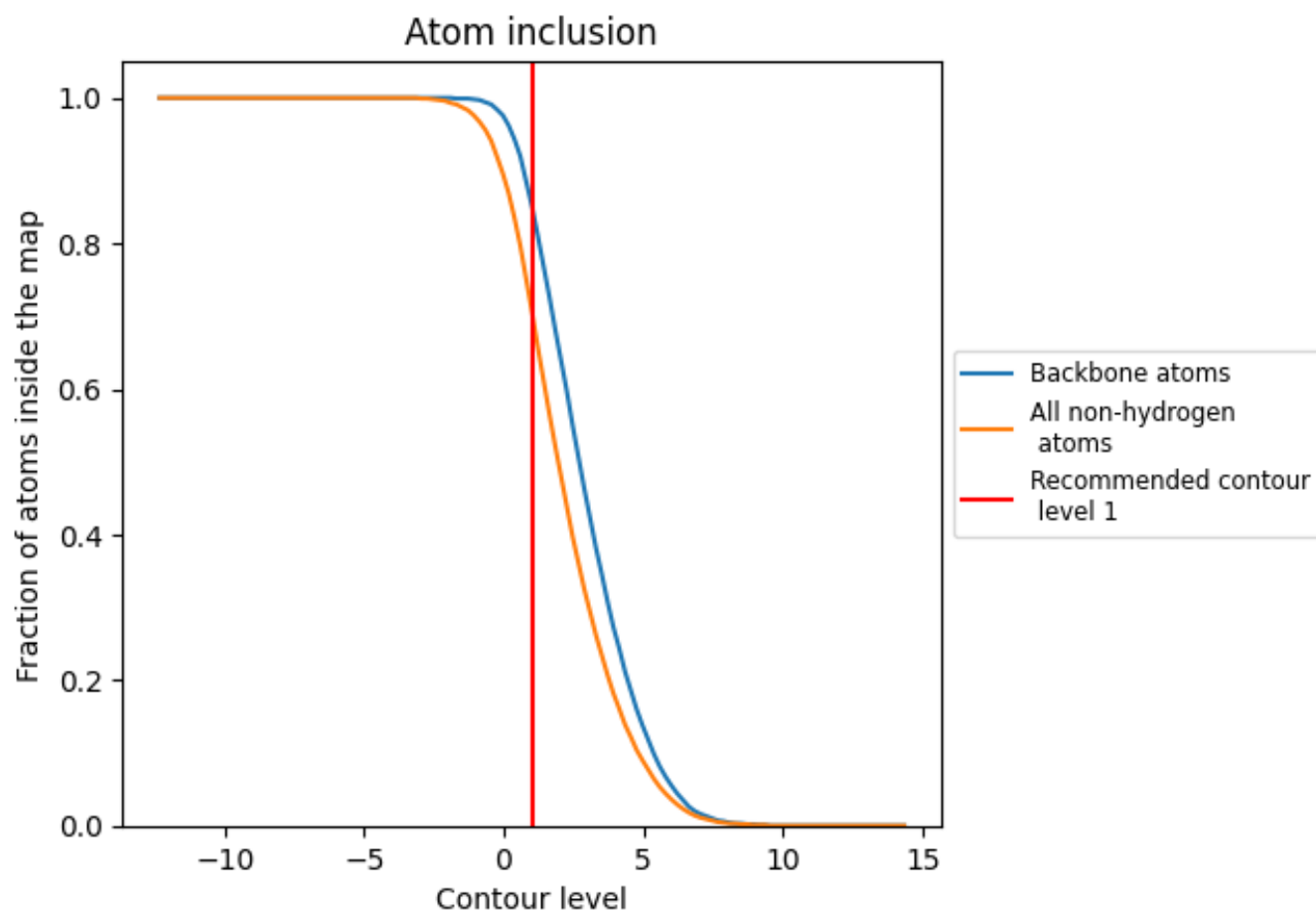
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.3890
A	0.7460	0.4280
B	0.7590	0.4180
C	0.7700	0.4240
D	0.7550	0.4160
E	0.6630	0.3590

