



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:49 AM EST

PDB ID : 7TYS
EMDB ID : EMD-26193
Title : Cryo-EM structure of the pancreatic ATP-sensitive potassium channel bound to ATP and repaglinide with Kir6.2-CTD in the up conformation
Authors : Shyng, S.L.; Sung, M.W.; Driggers, C.M.
Deposited on : 2022-02-14
Resolution : 3.41 Å (reported)
Based on initial models : 6BAA, 6PZ9

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

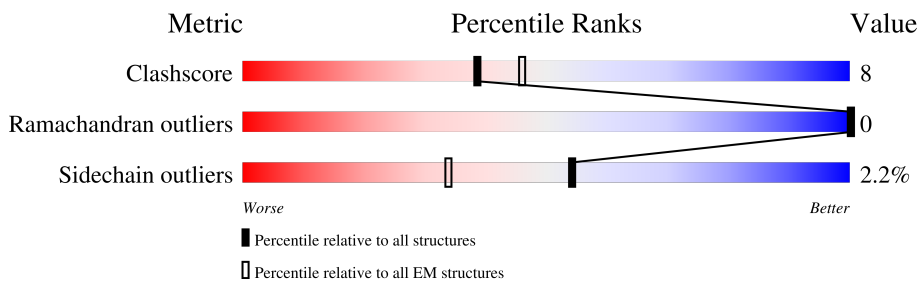
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	B	390	
1	C	390	
1	D	390	
2	E	1582	
3	F	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21286 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
			Total	C	N	O	S		
1	A	361	2660	1717	466	462	15	0	0
1	B	333	2531	1636	442	436	17	0	0
1	C	332	2515	1624	439	435	17	0	0
1	D	331	2511	1623	438	434	16	0	0

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

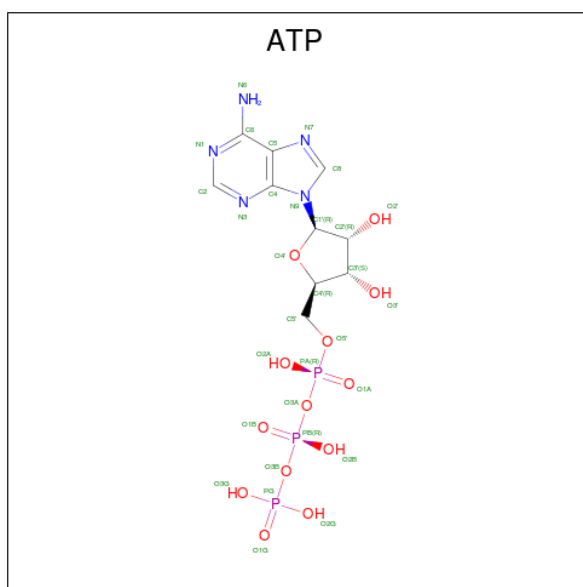
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	1431	10155	6570	1757	1784	44	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	2	28	16	2	10	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

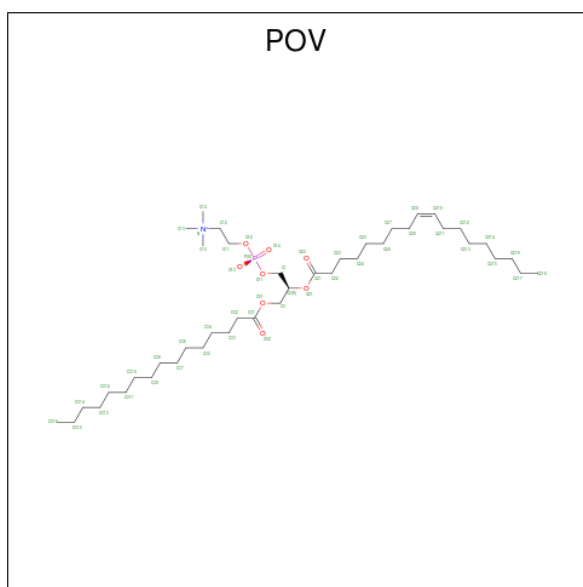


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

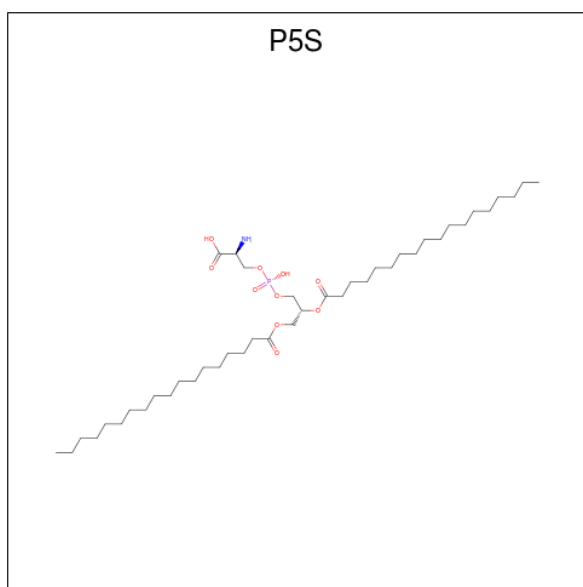
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	K	0
			2	2	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



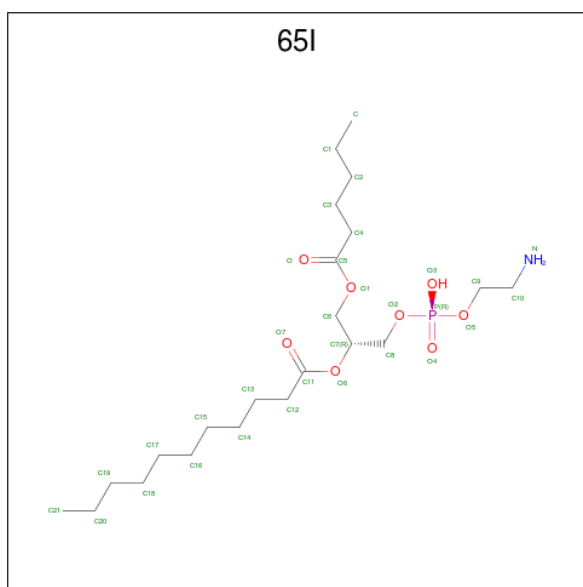
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total 36	C 26	N 1	O 8	P 1	0
6	B	1	Total 36	C 26	N 1	O 8	P 1	0
6	C	1	Total 36	C 26	N 1	O 8	P 1	0
6	D	1	Total 36	C 26	N 1	O 8	P 1	0
6	E	1	Total 36	C 26	N 1	O 8	P 1	0

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}](hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



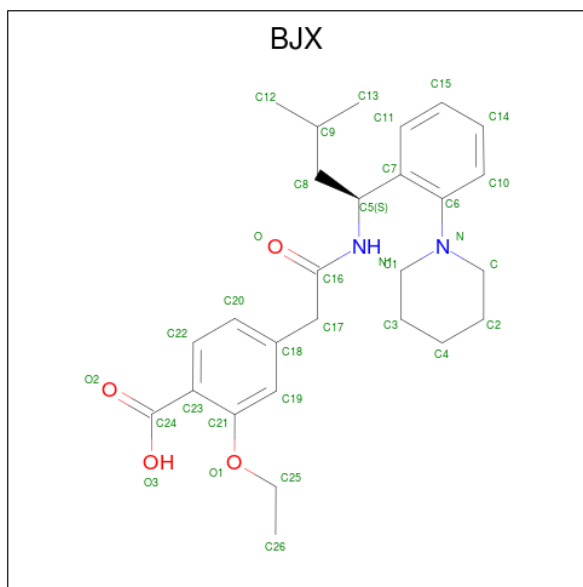
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	108	84	2	20	2	0
7	A	1	108	84	2	20	2	0
7	B	1	54	42	1	10	1	0
7	C	1	54	42	1	10	1	0
7	D	1	54	42	1	10	1	0
7	E	1	54	42	1	10	1	0

- Molecule 8 is (9R,12R)-15-amino-12-hydroxy-6,12-dioxo-7,11,13-trioxa-12lambda 5 -phosphapentadecan-9-yl undecanoate (three-letter code: 65I) (formula: C₂₂H₄₄NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	E	1	Total	C	N	O	P	0
			192	132	6	48	6	
8	E	1	Total	C	N	O	P	0
			192	132	6	48	6	
8	E	1	Total	C	N	O	P	0
			192	132	6	48	6	
8	E	1	Total	C	N	O	P	0
			192	132	6	48	6	
8	E	1	Total	C	N	O	P	0
			192	132	6	48	6	

- Molecule 9 is Repaglinide (three-letter code: BJX) (formula: $C_{27}H_{36}N_2O_4$) (labeled as "Ligand of Interest" by depositor).

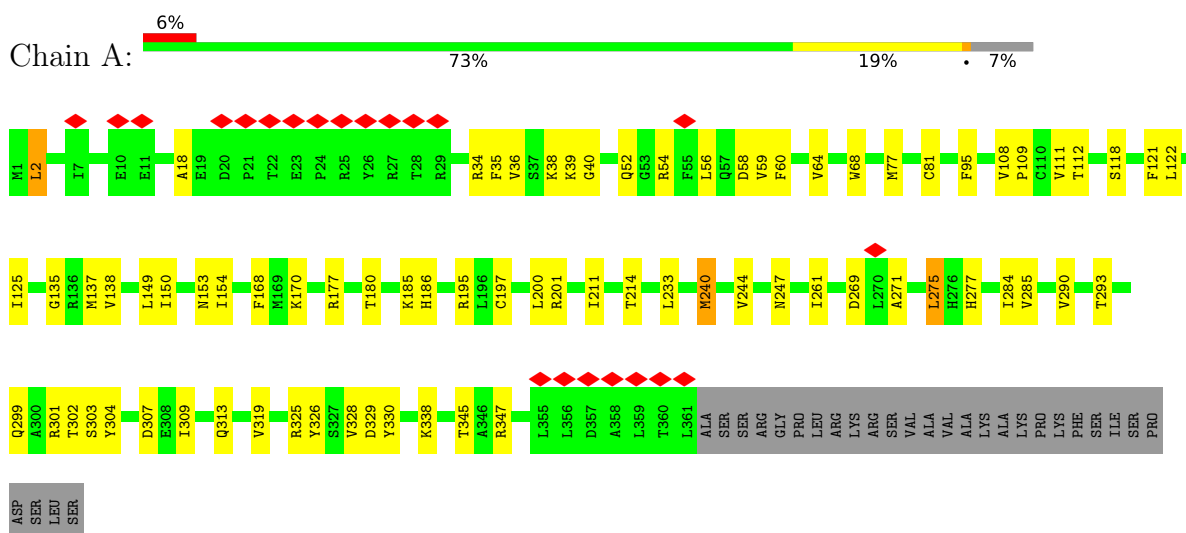


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	E	1	33	27	2	4	0

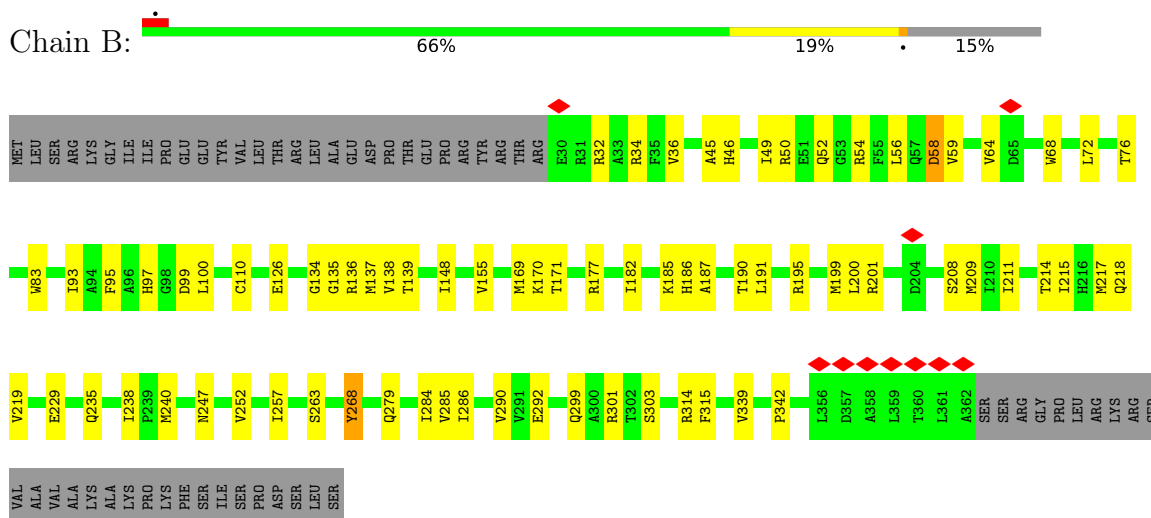
3 Residue-property plots

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: ATP-sensitive inward rectifier potassium channel 11

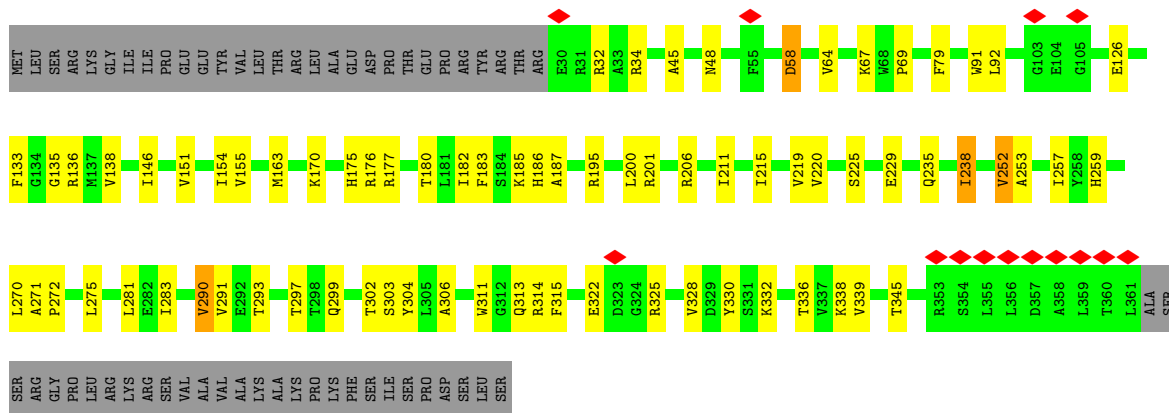


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

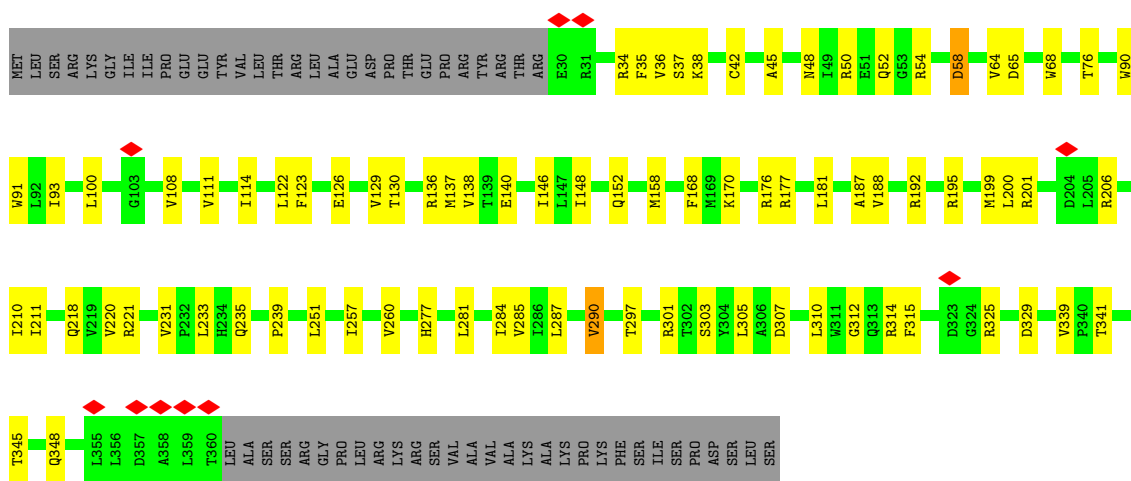


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

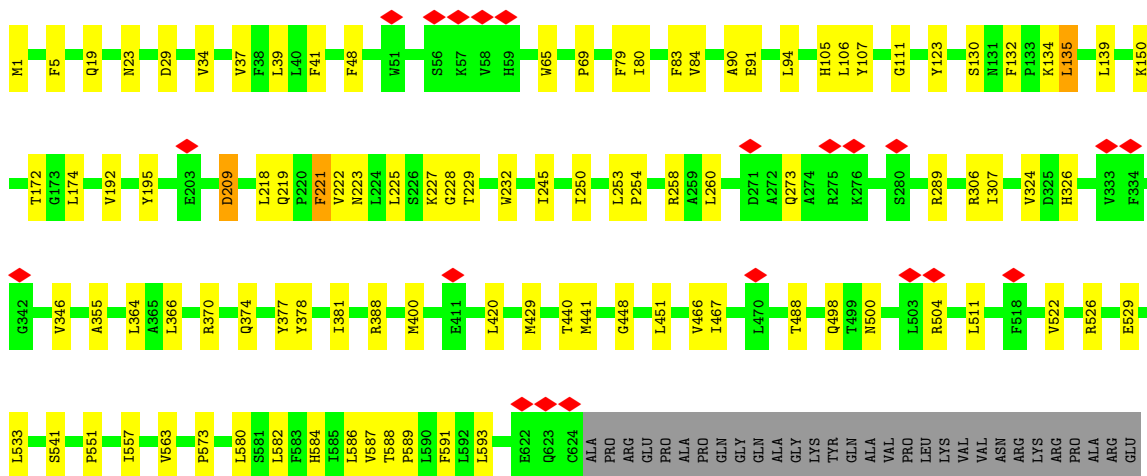
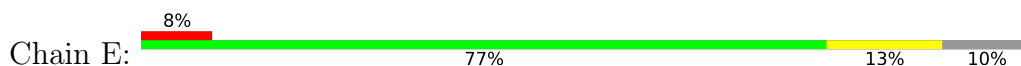


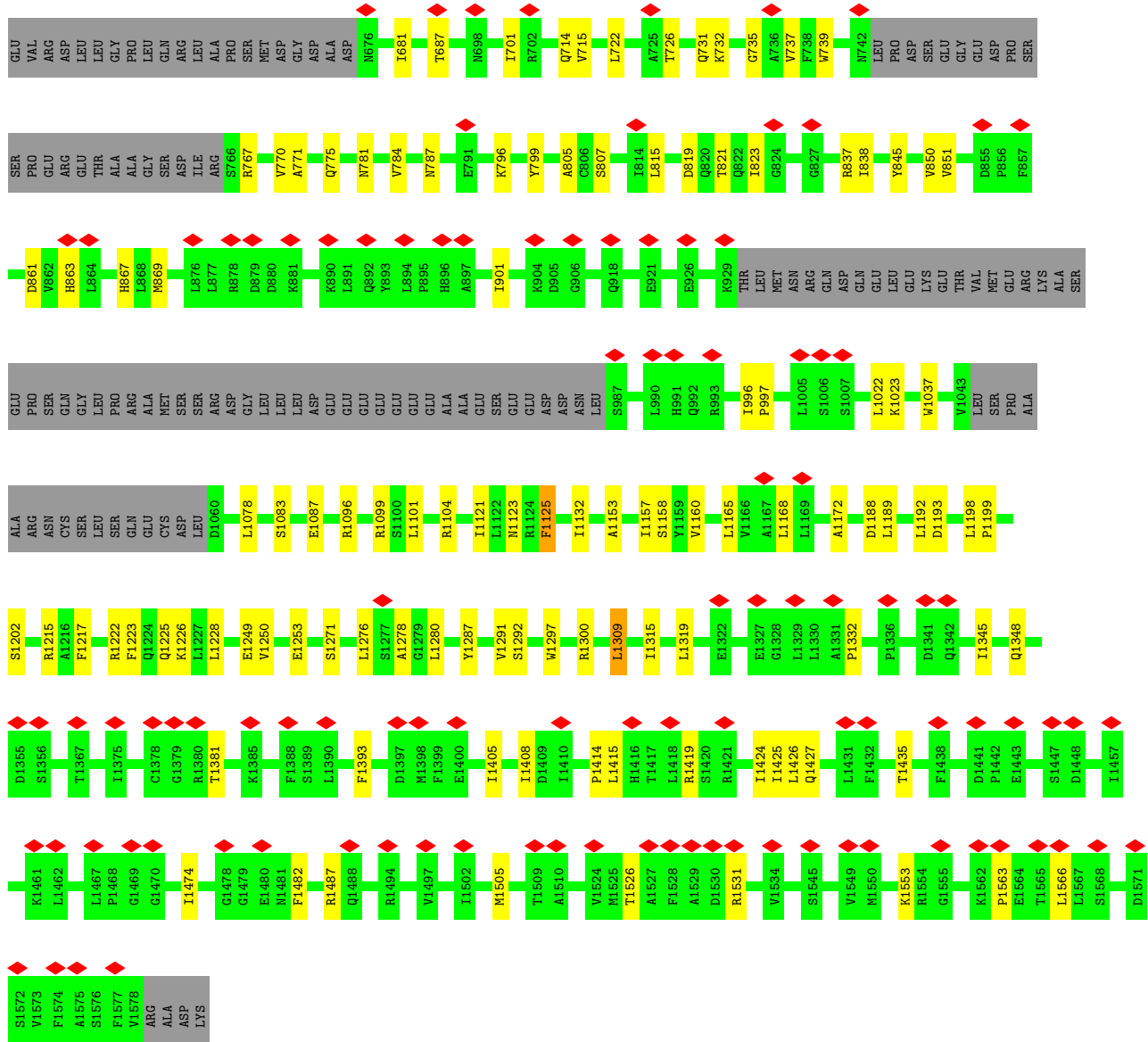


• Molecule 1: ATP-sensitive inward rectifier potassium channel 11



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





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64405	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	12.908	Depositor
Minimum map value	-9.470	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (\AA)	176.605, 112.85999, 146.29999	wwPDB
Map dimensions	169, 108, 140	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.045, 1.045, 1.045	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: 65I, NAG, POV, K, ATP, BJX, P5S

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	0.27	0/2720	0.48	0/3718
1	B	0.28	0/2588	0.48	0/3526
1	C	0.27	0/2571	0.47	0/3503
1	D	0.27	0/2568	0.47	0/3501
2	E	0.25	0/10371	0.43	0/14209
All	All	0.26	0/20818	0.46	0/28457

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	2660	0	2570	54	0
1	B	2531	0	2533	55	0
1	C	2515	0	2499	62	0
1	D	2511	0	2496	64	0
2	E	10155	0	9372	127	0
3	F	28	0	25	0	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	31	0	12	4	0
4	D	31	0	12	0	0
4	E	31	0	12	1	0
5	A	2	0	0	0	0
6	A	36	0	45	1	0
6	B	36	0	45	0	0
6	C	36	0	45	1	0
6	D	36	0	45	1	0
6	E	36	0	45	1	0
7	A	108	0	160	7	0
7	B	54	0	80	4	0
7	C	54	0	80	6	0
7	D	54	0	80	5	0
7	E	54	0	80	5	0
8	E	192	0	0	0	0
9	E	33	0	0	1	0
All	All	21286	0	20260	330	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 (330) 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:370:ARG:HD3	2:E:1253:GLU:HB3	1.59	0.84
1:A:18:ALA:HA	2:E:1123:ASN:HD21	1.50	0.77
1:A:325:ARG:HE	1:D:45:ALA:HB2	1.53	0.73
1:B:229:GLU:HG3	1:C:314:ARG:HD2	1.72	0.72
1:C:271:ALA:HB2	1:C:345:THR:HG22	1.71	0.72
1:D:312:GLY:HA3	1:D:341:THR:HG21	1.75	0.69
7:A:406:P5S:H35	7:B:403:P5S:H52	1.74	0.69
1:D:111:VAL:HG12	1:D:138:VAL:HA	1.76	0.68
1:C:291:VAL:HG12	1:C:293:THR:H	1.58	0.68
2:E:771:ALA:HB3	2:E:851:VAL:HA	1.74	0.68
1:B:58:ASP:OD2	1:C:206:ARG:NH1	2.27	0.67
1:A:299:GLN:HG3	1:B:211:ILE:HG23	1.77	0.67
2:E:1132:ILE:HD12	2:E:1315:ILE:HD12	1.76	0.67
1:D:211:ILE:HB	1:D:290:VAL:HG22	1.77	0.67
2:E:726:THR:O	2:E:767:ARG:NH2	2.28	0.67
1:C:69:PRO:HG3	7:C:403:P5S:H40A	1.76	0.66
1:B:138:VAL:O	1:C:136:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:ASP:OD1	2:E:209:ASP:N	2.28	0.66
2:E:366:LEU:HD13	2:E:370:ARG:HH12	1.61	0.66
1:A:177:ARG:NH1	1:A:180:THR:OG1	2.28	0.66
1:D:90:TRP:HE1	1:D:152:GLN:HE22	1.44	0.66
2:E:526:ARG:NH1	2:E:529:GLU:OE2	2.29	0.65
1:A:68:TRP:HD1	7:A:405:P5S:HA	1.62	0.64
2:E:1381:THR:H	2:E:1553:LYS:HE3	1.62	0.64
1:C:229:GLU:HA	1:D:314:ARG:HH12	1.61	0.64
1:B:299:GLN:HG3	1:C:211:ILE:HG23	1.79	0.64
2:E:580:LEU:O	2:E:584:HIS:ND1	2.29	0.64
2:E:1435:THR:HA	2:E:1474:ILE:HA	1.79	0.63
7:E:1607:P5S:H40	7:E:1607:P5S:H20	1.81	0.63
1:C:299:GLN:HG3	1:D:211:ILE:HG23	1.79	0.63
1:A:138:VAL:O	1:B:136:ARG:NH2	2.31	0.63
1:D:58:ASP:N	1:D:58:ASP:OD1	2.31	0.63
1:A:185:LYS:HG3	4:A:401:ATP:H5'2	1.80	0.62
2:E:1415:LEU:HB3	2:E:1419:ARG:HH22	1.62	0.62
1:B:97:HIS:ND1	1:B:99:ASP:OD1	2.32	0.62
2:E:807:SER:HG	2:E:837:ARG:HH12	1.48	0.61
2:E:1104:ARG:NH1	2:E:1319:LEU:O	2.33	0.61
1:A:34:ARG:NH2	1:A:303:SER:OG	2.30	0.61
1:D:220:VAL:HG22	1:D:235:GLN:HG2	1.83	0.60
1:C:211:ILE:HB	1:C:290:VAL:HG22	1.83	0.60
2:E:19:GLN:O	2:E:23:ASN:ND2	2.34	0.60
1:B:190:THR:OG1	1:B:191:LEU:N	2.31	0.60
2:E:29:ASP:OD2	2:E:105:HIS:ND1	2.34	0.60
2:E:1426:LEU:O	2:E:1487:ARG:NH1	2.34	0.60
2:E:807:SER:OG	2:E:837:ARG:NH1	2.31	0.60
1:B:52:GLN:OE1	1:B:54:ARG:NH1	2.33	0.60
1:C:151:VAL:HG22	7:D:402:P5S:H35A	1.83	0.60
1:D:36:VAL:HG12	1:D:42:CYS:HA	1.84	0.59
1:C:313:GLN:NE2	1:C:336:THR:OG1	2.35	0.59
2:E:306:ARG:HG3	2:E:440:THR:HG21	1.84	0.59
1:A:36:VAL:HG22	1:A:284:ILE:HD12	1.84	0.59
1:C:176:ARG:NH1	7:C:403:P5S:OXT	2.36	0.58
2:E:805:ALA:HB1	2:E:869:MET:HA	1.85	0.58
1:B:34:ARG:NH2	1:B:303:SER:O	2.36	0.58
2:E:1023:LYS:HA	2:E:1078:LEU:HD23	1.84	0.58
1:C:34:ARG:NH2	1:C:303:SER:OG	2.32	0.58
1:B:34:ARG:NH2	1:B:303:SER:OG	2.36	0.58
1:A:329:ASP:OD1	1:D:48:ASN:ND2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:CYS:HB3	2:E:41:PHE:HB3	1.85	0.58
1:C:58:ASP:OD1	1:C:58:ASP:N	2.36	0.57
1:B:50:ARG:NH1	4:C:401:ATP:O3G	2.37	0.57
2:E:219:GLN:OE1	2:E:232:TRP:NE1	2.26	0.57
2:E:815:LEU:HB3	2:E:821:THR:HG21	1.86	0.57
1:A:277:HIS:HA	1:A:307:ASP:HB3	1.87	0.57
1:B:99:ASP:OD2	1:B:110:CYS:N	2.34	0.57
1:A:122:LEU:HD21	1:D:146:ILE:HG12	1.86	0.56
1:D:90:TRP:HE1	1:D:152:GLN:NE2	2.02	0.56
1:A:244:VAL:HG12	1:D:239:PRO:HG3	1.87	0.56
1:B:93:ILE:HD11	1:B:148:ILE:HG13	1.87	0.56
2:E:687:THR:N	2:E:731:GLN:O	2.39	0.56
2:E:541:SER:O	2:E:1083:SER:OG	2.24	0.56
1:A:154:ILE:HD13	1:B:76:THR:HG23	1.88	0.56
2:E:1158:SER:HB2	2:E:1165:LEU:HD23	1.87	0.56
1:C:185:LYS:NZ	4:C:401:ATP:O2G	2.39	0.55
1:A:40:GLY:HA2	1:A:301:ARG:HB2	1.89	0.55
2:E:1405:ILE:N	2:E:1408:ILE:O	2.40	0.55
2:E:448:GLY:HA3	2:E:586:LEU:HD21	1.86	0.55
2:E:787:ASN:HD22	2:E:823:ILE:HD13	1.72	0.55
1:D:111:VAL:HG23	1:D:114:ILE:HG13	1.88	0.55
2:E:1160:VAL:HG22	2:E:1280:LEU:HB3	1.88	0.55
2:E:861:ASP:OD1	2:E:861:ASP:N	2.39	0.55
1:B:177:ARG:NH1	1:B:208:SER:OG	2.40	0.55
1:B:110:CYS:O	1:B:139:THR:OG1	2.24	0.55
2:E:807:SER:HG	2:E:837:ARG:NH1	2.05	0.55
1:D:201:ARG:NH2	1:D:315:PHE:HB3	2.22	0.54
2:E:388:ARG:HB2	2:E:429:MET:HG3	1.89	0.54
1:D:34:ARG:NH2	1:D:303:SER:OG	2.35	0.54
2:E:781:ASN:HD21	2:E:1202:SER:HB3	1.70	0.54
1:C:146:ILE:HG12	1:D:122:LEU:HD21	1.89	0.54
1:B:218:GLN:OE1	1:B:235:GLN:NE2	2.38	0.54
1:D:210:ILE:HD11	1:D:251:LEU:HD23	1.89	0.54
1:D:345:THR:HG23	1:D:348:GLN:H	1.72	0.54
2:E:1253:GLU:HG2	2:E:1292:SER:HB2	1.88	0.54
1:D:188:VAL:HG12	1:D:310:LEU:HB2	1.90	0.53
1:C:91:TRP:NE1	6:C:402:POV:O14	2.39	0.53
1:B:155:VAL:HG22	7:C:403:P5S:H30	1.90	0.53
1:D:93:ILE:HD11	1:D:148:ILE:HG13	1.89	0.53
2:E:250:ILE:HD12	2:E:1192:LEU:HD13	1.90	0.53
1:B:219:VAL:HG23	1:B:238:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:HD13	1:D:287:LEU:HD23	1.91	0.53
1:D:314:ARG:HE	1:D:339:VAL:HG11	1.74	0.53
2:E:150:LYS:HE3	2:E:172:THR:HG23	1.91	0.53
1:C:138:VAL:O	1:D:136:ARG:NH2	2.38	0.53
2:E:551:PRO:HB3	2:E:587:VAL:HG21	1.89	0.52
2:E:726:THR:HG22	2:E:739:TRP:HZ3	1.74	0.52
1:B:211:ILE:HB	1:B:290:VAL:HG23	1.92	0.52
1:C:314:ARG:HG3	1:C:339:VAL:HG11	1.92	0.52
2:E:796:LYS:HA	2:E:799:TYR:HB3	1.92	0.52
2:E:587:VAL:HG13	2:E:591:PHE:HD2	1.75	0.52
1:C:272:PRO:HG3	1:C:311:TRP:CD2	2.45	0.52
1:D:64:VAL:HG13	1:D:170:LYS:HG2	1.90	0.52
1:B:201:ARG:NH2	1:B:315:PHE:HB3	2.25	0.52
2:E:221:PHE:HA	6:E:1608:POV:H13	1.92	0.52
1:A:36:VAL:HG23	1:A:303:SER:HB3	1.92	0.52
1:A:319:VAL:HG22	1:A:328:VAL:HG22	1.92	0.52
2:E:134:LYS:NZ	2:E:195:TYR:O	2.42	0.52
1:C:330:TYR:HB3	4:C:401:ATP:N6	2.24	0.52
2:E:223:ASN:N	2:E:223:ASN:OD1	2.43	0.51
1:D:277:HIS:HA	1:D:307:ASP:HB3	1.93	0.51
1:D:290:VAL:HA	1:D:297:THR:HA	1.91	0.51
1:B:286:ILE:HG23	1:B:301:ARG:HG2	1.92	0.51
1:B:215:ILE:HG21	1:B:257:ILE:HG21	1.92	0.51
1:C:155:VAL:HG22	7:D:402:P5S:H29A	1.92	0.51
1:D:91:TRP:NE1	6:D:403:POV:O14	2.44	0.51
1:D:221:ARG:HH12	1:D:281:LEU:HD13	1.76	0.51
1:A:211:ILE:HB	1:A:290:VAL:HG23	1.92	0.51
2:E:374:GLN:NE2	2:E:1249:GLU:OE2	2.42	0.50
6:A:404:POV:H3	2:E:5:PHE:HB2	1.94	0.50
1:C:58:ASP:OD2	1:D:206:ARG:NH2	2.44	0.50
1:D:36:VAL:HG22	1:D:284:ILE:HD12	1.93	0.50
2:E:563:VAL:HG21	2:E:1037:TRP:HZ2	1.77	0.50
1:B:32:ARG:NH1	1:B:279:GLN:O	2.44	0.50
2:E:80:ILE:O	2:E:84:VAL:HG23	2.11	0.50
2:E:400:MET:O	2:E:1215:ARG:NH1	2.45	0.50
2:E:306:ARG:HH21	2:E:377:TYR:HE1	1.60	0.50
2:E:1022:LEU:HG	2:E:1078:LEU:HD21	1.94	0.50
1:C:187:ALA:HB2	1:C:200:LEU:HD13	1.94	0.50
1:C:176:ARG:HH22	7:C:403:P5S:P12	2.34	0.50
1:A:39:LYS:NZ	4:A:401:ATP:O3'	2.32	0.49
1:A:109:PRO:HG2	1:A:112:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ALA:HB2	1:C:325:ARG:HH12	1.77	0.49
1:B:191:LEU:HD21	1:B:342:PRO:HD2	1.95	0.49
1:C:272:PRO:HG3	1:C:311:TRP:CG	2.47	0.49
7:A:405:P5S:H44A	1:D:158:MET:HG2	1.94	0.49
2:E:364:LEU:HD22	7:E:1607:P5S:H56A	1.93	0.49
1:C:175:HIS:CE1	1:C:176:ARG:HG3	2.48	0.49
1:C:220:VAL:HG22	1:C:235:GLN:HG2	1.94	0.49
1:A:64:VAL:HG13	1:A:170:LYS:HG2	1.94	0.49
1:B:209:MET:H	1:B:292:GLU:HG2	1.78	0.48
1:A:68:TRP:HB2	7:A:405:P5S:H3A	1.95	0.48
1:B:214:THR:HG23	1:B:247:ASN:HB3	1.96	0.48
2:E:1563:PRO:HG2	2:E:1566:LEU:HB2	1.94	0.48
2:E:722:LEU:O	2:E:726:THR:OG1	2.28	0.48
1:B:72:LEU:HD13	7:B:403:P5S:H31	1.95	0.48
2:E:228:GLY:HA3	7:E:1607:P5S:H45	1.96	0.48
1:B:185:LYS:HG3	4:B:401:ATP:H5'1	1.95	0.48
1:C:238:ILE:HD13	1:C:259:HIS:CD2	2.49	0.48
1:C:48:ASN:ND2	1:D:329:ASP:OD1	2.38	0.47
2:E:273:GLN:HE21	2:E:289:ARG:CZ	2.26	0.47
2:E:784:VAL:HG22	2:E:823:ILE:HB	1.96	0.47
1:A:121:PHE:O	1:A:125:ILE:HG12	2.14	0.47
1:D:200:LEU:O	1:D:257:ILE:N	2.46	0.47
2:E:130:SER:O	2:E:132:PHE:N	2.47	0.47
2:E:714:GLN:HG3	2:E:715:VAL:H	1.78	0.47
2:E:227:LYS:HB3	7:E:1607:P5S:H41A	1.95	0.47
1:C:126:GLU:OE2	1:C:136:ARG:NH1	2.48	0.47
1:D:177:ARG:NH2	1:D:206:ARG:HB2	2.30	0.47
1:B:64:VAL:HG21	1:B:169:MET:HE3	1.95	0.47
2:E:681:ILE:HA	2:E:737:VAL:HG22	1.95	0.47
2:E:1332:PRO:HB2	2:E:1414:PRO:HG3	1.95	0.47
2:E:1345:ILE:HG12	2:E:1405:ILE:HA	1.96	0.47
1:C:69:PRO:HB3	7:C:403:P5S:H45	1.95	0.47
1:C:225:SER:HB3	1:C:229:GLU:HB2	1.97	0.47
2:E:123:TYR:HD2	2:E:139:LEU:HD13	1.80	0.47
2:E:307:ILE:HD13	2:E:440:THR:HG23	1.95	0.47
2:E:1526:THR:O	2:E:1531:ARG:N	2.44	0.47
1:A:59:VAL:HG11	7:A:406:P5S:H42A	1.96	0.47
1:B:36:VAL:HG22	1:B:284:ILE:HD12	1.97	0.47
7:C:403:P5S:H45	7:C:403:P5S:H42	1.79	0.47
1:A:299:GLN:HB2	1:B:211:ILE:HD12	1.97	0.46
1:B:46:HIS:HB3	1:B:49:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:HD11	1:B:285:VAL:HG21	1.98	0.46
1:C:252:VAL:HG23	1:C:253:ALA:H	1.79	0.46
1:D:200:LEU:HD11	1:D:285:VAL:HG21	1.97	0.46
2:E:91:GLU:HG3	2:E:346:VAL:HG12	1.97	0.46
2:E:784:VAL:N	2:E:819:ASP:O	2.47	0.46
1:C:201:ARG:NH2	1:C:315:PHE:HB3	2.31	0.46
1:A:214:THR:HG23	1:A:247:ASN:HB2	1.98	0.46
1:C:290:VAL:HA	1:C:297:THR:HA	1.98	0.46
1:A:277:HIS:ND1	1:A:307:ASP:OD2	2.38	0.46
2:E:466:VAL:HG21	2:E:557:ILE:HD12	1.98	0.46
2:E:1271:SER:HA	2:E:1276:LEU:H	1.81	0.46
1:A:2:LEU:HD23	1:A:2:LEU:H	1.81	0.45
2:E:79:PHE:HZ	2:E:225:LEU:HD13	1.82	0.45
2:E:451:LEU:HD11	2:E:582:LEU:HD21	1.98	0.45
2:E:511:LEU:HD22	2:E:1393:PHE:HD2	1.80	0.45
2:E:1153:ALA:O	2:E:1157:ILE:HG12	2.16	0.45
1:C:270:LEU:HD11	1:C:281:LEU:HD11	1.98	0.45
2:E:229:THR:HA	2:E:1250:VAL:HG11	1.98	0.45
1:A:118:SER:HB2	1:D:140:GLU:HB2	1.97	0.45
1:B:137:MET:SD	1:C:135:GLY:HA3	2.56	0.45
1:B:314:ARG:HG3	1:B:339:VAL:HG21	1.97	0.45
2:E:1:MET:SD	2:E:1:MET:N	2.67	0.45
2:E:541:SER:HB3	2:E:1087:GLU:HG3	1.99	0.45
2:E:324:VAL:HG11	2:E:573:PRO:HB2	1.98	0.45
1:B:36:VAL:HG23	1:B:303:SER:HB3	1.97	0.45
2:E:1425:ILE:HG12	2:E:1505:MET:HA	1.98	0.45
2:E:1297:TRP:CZ3	2:E:1300:ARG:HG2	2.52	0.45
1:D:35:PHE:HD1	1:D:36:VAL:HG13	1.81	0.45
1:A:60:PHE:CD1	1:B:171:THR:HG23	2.52	0.45
1:C:182:ILE:HD12	4:C:401:ATP:H1'	1.99	0.45
1:C:215:ILE:HD13	1:C:257:ILE:HG21	1.99	0.45
2:E:260:LEU:HB3	2:E:1228:LEU:HD13	1.99	0.45
2:E:996:ILE:N	2:E:997:PRO:HD3	2.32	0.44
2:E:1393:PHE:HE2	2:E:1424:ILE:HD12	1.82	0.44
1:A:275:LEU:HD21	1:A:309:ILE:HB	1.99	0.44
1:C:79:PHE:HE1	1:C:163:MET:HG3	1.81	0.44
1:C:332:LYS:HB2	1:C:332:LYS:HE3	1.81	0.44
2:E:441:MET:HB3	2:E:593:LEU:HD12	1.99	0.44
1:B:182:ILE:HD12	4:B:401:ATP:H1'	1.99	0.44
1:C:64:VAL:HG13	1:C:170:LYS:HG2	1.98	0.44
1:C:313:GLN:HG2	1:C:338:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:VAL:HA	2:E:37:VAL:HG22	1.99	0.44
1:B:263:SER:HA	1:B:268:TYR:CE2	2.52	0.44
1:C:177:ARG:O	1:C:180:THR:HG22	2.18	0.44
1:D:35:PHE:HD2	1:D:233:LEU:HD23	1.81	0.44
1:D:301:ARG:HH11	1:D:301:ARG:HB2	1.82	0.44
2:E:219:GLN:HB2	2:E:232:TRP:CZ2	2.52	0.44
1:A:52:GLN:OE1	1:A:54:ARG:NH1	2.49	0.44
2:E:83:PHE:CD2	7:E:1607:P5S:H34A	2.52	0.44
1:D:195:ARG:HG2	1:D:260:VAL:HG13	1.99	0.44
1:C:229:GLU:HA	1:D:314:ARG:NH1	2.31	0.44
1:B:58:ASP:N	1:B:58:ASP:OD1	2.49	0.43
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.85	0.43
2:E:863:HIS:O	2:E:867:HIS:ND1	2.39	0.43
1:A:326:TYR:CZ	1:D:233:LEU:HD21	2.53	0.43
1:D:187:ALA:HB1	1:D:199:MET:O	2.18	0.43
2:E:1309:LEU:HD22	2:E:1309:LEU:HA	1.84	0.43
2:E:1427:GLN:O	2:E:1487:ARG:NH1	2.50	0.43
1:B:200:LEU:HD23	1:B:201:ARG:N	2.33	0.43
2:E:1189:LEU:O	2:E:1193:ASP:N	2.51	0.43
1:A:200:LEU:HD11	1:A:285:VAL:HG21	1.99	0.43
1:C:275:LEU:HD12	1:C:306:ALA:HB1	2.00	0.43
2:E:488:THR:HG21	2:E:533:LEU:HD13	2.00	0.43
2:E:79:PHE:CZ	2:E:225:LEU:HD13	2.54	0.43
2:E:83:PHE:HD1	2:E:364:LEU:HD13	1.83	0.43
1:A:56:LEU:O	1:A:59:VAL:HG22	2.18	0.43
2:E:701:ILE:HG21	2:E:901:ILE:HD12	2.00	0.43
1:B:217:MET:HG2	1:B:285:VAL:HG22	2.00	0.43
1:A:293:THR:OG1	1:D:65:ASP:OD1	2.29	0.43
1:B:134:GLY:HA3	1:C:133:PHE:O	2.19	0.43
1:D:129:VAL:O	1:D:130:THR:OG1	2.32	0.43
1:C:67:LYS:HB3	1:C:69:PRO:HD2	2.00	0.43
1:C:219:VAL:HG22	1:C:283:ILE:HD13	1.99	0.43
1:D:176:ARG:NH2	7:D:402:P5S:OG	2.52	0.43
2:E:1101:LEU:HA	2:E:1319:LEU:HD21	2.00	0.43
1:B:64:VAL:HA	1:B:170:LYS:HD3	2.01	0.42
2:E:732:LYS:HD2	2:E:735:GLY:HA3	2.01	0.42
1:A:137:MET:SD	1:B:135:GLY:HA3	2.59	0.42
1:C:229:GLU:HG3	1:D:192:ARG:HD3	2.01	0.42
2:E:69:PRO:HG2	2:E:192:VAL:HB	2.02	0.42
1:A:271:ALA:HB2	1:A:345:THR:HG22	2.00	0.42
7:D:402:P5S:H51	7:D:402:P5S:H48	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD11	1:A:304:TYR:HE2	1.84	0.42
1:C:200:LEU:HD11	1:C:304:TYR:OH	2.20	0.42
2:E:381:ILE:HD11	9:E:1602:BJX:C21	2.49	0.42
1:A:111:VAL:HG13	1:A:137:MET:O	2.20	0.42
1:A:168:PHE:CE2	1:D:168:PHE:HE2	2.38	0.42
1:C:322:GLU:N	1:C:325:ARG:O	2.43	0.42
2:E:1222:ARG:NH1	2:E:1225:GLN:OE1	2.53	0.42
1:D:50:ARG:HG2	1:D:52:GLN:HE22	1.84	0.42
2:E:1223:PHE:CD1	2:E:1226:LYS:HE2	2.55	0.42
2:E:90:ALA:O	2:E:94:LEU:HB2	2.20	0.42
2:E:135:LEU:HD13	2:E:135:LEU:HA	1.87	0.42
2:E:326:HIS:HD2	2:E:355:ALA:HB2	1.85	0.42
2:E:467:ILE:HG23	2:E:591:PHE:CZ	2.54	0.41
1:D:68:TRP:HB2	7:D:402:P5S:H2	2.02	0.41
2:E:254:PRO:O	2:E:258:ARG:HG3	2.20	0.41
1:A:135:GLY:HA3	1:D:137:MET:SD	2.59	0.41
1:B:209:MET:HE1	1:B:252:VAL:HG12	2.01	0.41
1:D:52:GLN:OE1	1:D:54:ARG:NH1	2.53	0.41
2:E:219:GLN:HG2	2:E:378:TYR:CZ	2.55	0.41
2:E:775:GLN:NE2	4:E:1603:ATP:O2B	2.53	0.41
1:A:313:GLN:HG2	1:A:338:LYS:HD2	2.01	0.41
2:E:588:THR:HB	2:E:589:PRO:HD3	2.01	0.41
1:A:35:PHE:CD1	1:A:233:LEU:HD13	2.56	0.41
1:A:38:LYS:O	1:A:302:THR:HG22	2.21	0.41
1:A:269:ASP:OD2	1:A:347:ARG:NH2	2.53	0.41
1:D:277:HIS:ND1	1:D:307:ASP:OD2	2.38	0.41
2:E:823:ILE:HD11	2:E:838:ILE:HG13	2.03	0.41
1:A:149:LEU:O	1:A:153:ASN:ND2	2.54	0.41
1:D:37:SER:OG	1:D:38:LYS:N	2.54	0.41
2:E:1096:ARG:HG2	2:E:1099:ARG:NH2	2.35	0.41
1:A:240:MET:HG2	1:A:240:MET:O	2.21	0.41
1:C:229:GLU:HG2	1:D:314:ARG:HH22	1.86	0.41
1:D:126:GLU:OE2	1:D:136:ARG:NH1	2.53	0.41
1:D:90:TRP:CE2	1:D:123:PHE:HE2	2.39	0.41
1:D:218:GLN:O	1:D:284:ILE:N	2.53	0.41
2:E:580:LEU:HD23	2:E:580:LEU:HA	1.83	0.41
1:B:68:TRP:HD1	7:B:403:P5S:H2	1.85	0.41
1:B:95:PHE:CD2	1:B:100:LEU:HD11	2.56	0.41
1:B:185:LYS:HE2	4:B:401:ATP:O3B	2.20	0.41
1:B:187:ALA:HB1	1:B:199:MET:O	2.20	0.41
1:C:45:ALA:HB2	1:D:325:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:LEU:HD23	2:E:106:LEU:HA	1.95	0.41
2:E:500:ASN:HD21	2:E:504:ARG:NH2	2.18	0.41
2:E:770:VAL:HA	2:E:850:VAL:HG23	2.03	0.41
2:E:1198:LEU:HB3	2:E:1199:PRO:HD3	2.02	0.41
1:A:77:MET:HG3	2:E:48:PHE:CD2	2.55	0.41
1:A:197:CYS:HA	1:A:261:ILE:HG13	2.02	0.41
2:E:1168:LEU:O	2:E:1172:ALA:N	2.44	0.41
1:A:330:TYR:HB3	4:A:401:ATP:N6	2.36	0.40
1:C:32:ARG:HA	1:C:32:ARG:HD2	1.92	0.40
2:E:324:VAL:HG13	2:E:1278:ALA:HB1	2.02	0.40
2:E:498:GLN:OE1	2:E:522:VAL:HG22	2.21	0.40
2:E:771:ALA:HA	2:E:1217:PHE:CE1	2.56	0.40
1:A:200:LEU:HD23	1:A:201:ARG:N	2.36	0.40
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.55	0.40
1:D:34:ARG:CZ	1:D:305:LEU:HD23	2.51	0.40
2:E:107:TYR:O	2:E:111:GLY:N	2.45	0.40
2:E:273:GLN:HE21	2:E:289:ARG:NH2	2.19	0.40
7:A:406:P5S:O13	7:B:403:P5S:H3	2.21	0.40
1:C:154:ILE:HD13	1:D:76:THR:HG23	2.02	0.40
2:E:245:ILE:HB	2:E:1188:ASP:HB3	2.04	0.40
1:A:150:ILE:HG23	1:B:83:TRP:HZ3	1.86	0.40
7:A:405:P5S:H23A	7:A:405:P5S:H20A	1.83	0.40
2:E:1121:ILE:O	2:E:1125:PHE:HB2	2.21	0.40
2:E:1287:TYR:O	2:E:1291:VAL:HG23	2.21	0.40
1:C:58:ASP:CG	1:D:206:ARG:HH22	2.25	0.40
1:C:183:PHE:HB2	1:C:302:THR:HG21	2.03	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	359/390 (92%)	344 (96%)	15 (4%)	0	100	100
1	B	331/390 (85%)	322 (97%)	9 (3%)	0	100	100
1	C	330/390 (85%)	313 (95%)	17 (5%)	0	100	100
1	D	329/390 (84%)	313 (95%)	16 (5%)	0	100	100
2	E	1421/1582 (90%)	1375 (97%)	46 (3%)	0	100	100
All	All	2770/3142 (88%)	2667 (96%)	103 (4%)	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	264/341 (77%)	256 (97%)	8 (3%)	41	71
1	B	267/341 (78%)	260 (97%)	7 (3%)	46	74
1	C	263/341 (77%)	255 (97%)	8 (3%)	41	71
1	D	263/341 (77%)	258 (98%)	5 (2%)	57	80
2	E	910/1373 (66%)	895 (98%)	15 (2%)	62	82
All	All	1967/2737 (72%)	1924 (98%)	43 (2%)	54	78

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	58	ASP
1	A	95	PHE
1	A	108	VAL
1	A	186	HIS
1	A	195	ARG
1	A	240	MET
1	A	275	LEU
1	B	56	LEU
1	B	58	ASP

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Mol	Chain	Res	Type
1	B	59	VAL
1	B	186	HIS
1	B	195	ARG
1	B	240	MET
1	B	268	TYR
1	C	58	ASP
1	C	92	LEU
1	C	186	HIS
1	C	195	ARG
1	C	238	ILE
1	C	252	VAL
1	C	290	VAL
1	C	328	VAL
1	D	58	ASP
1	D	100	LEU
1	D	108	VAL
1	D	231	VAL
1	D	290	VAL
2	E	39	LEU
2	E	65	TRP
2	E	135	LEU
2	E	174	LEU
2	E	209	ASP
2	E	218	LEU
2	E	221	PHE
2	E	222	VAL
2	E	253	LEU
2	E	420	LEU
2	E	845	TYR
2	E	1125	PHE
2	E	1309	LEU
2	E	1348	GLN
2	E	1482	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	B	46	HIS
1	B	173	GLN
1	B	175	HIS
1	B	277	HIS

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Mol	Chain	Res	Type
1	B	278	HIS
1	B	348	GLN
1	C	128	GLN
1	C	313	GLN
1	D	46	HIS
1	D	128	GLN
1	D	152	GLN
1	D	218	GLN
1	D	235	GLN
1	D	313	GLN
2	E	126	ASN
2	E	273	GLN
2	E	293	HIS
2	E	326	HIS
2	E	349	GLN
2	E	500	ASN
2	E	775	GLN
2	E	787	ASN
2	E	846	GLN
2	E	1123	ASN
2	E	1488	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

2 monosaccharides 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	NAG	F	1	2,3	14,14,15	0.47	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

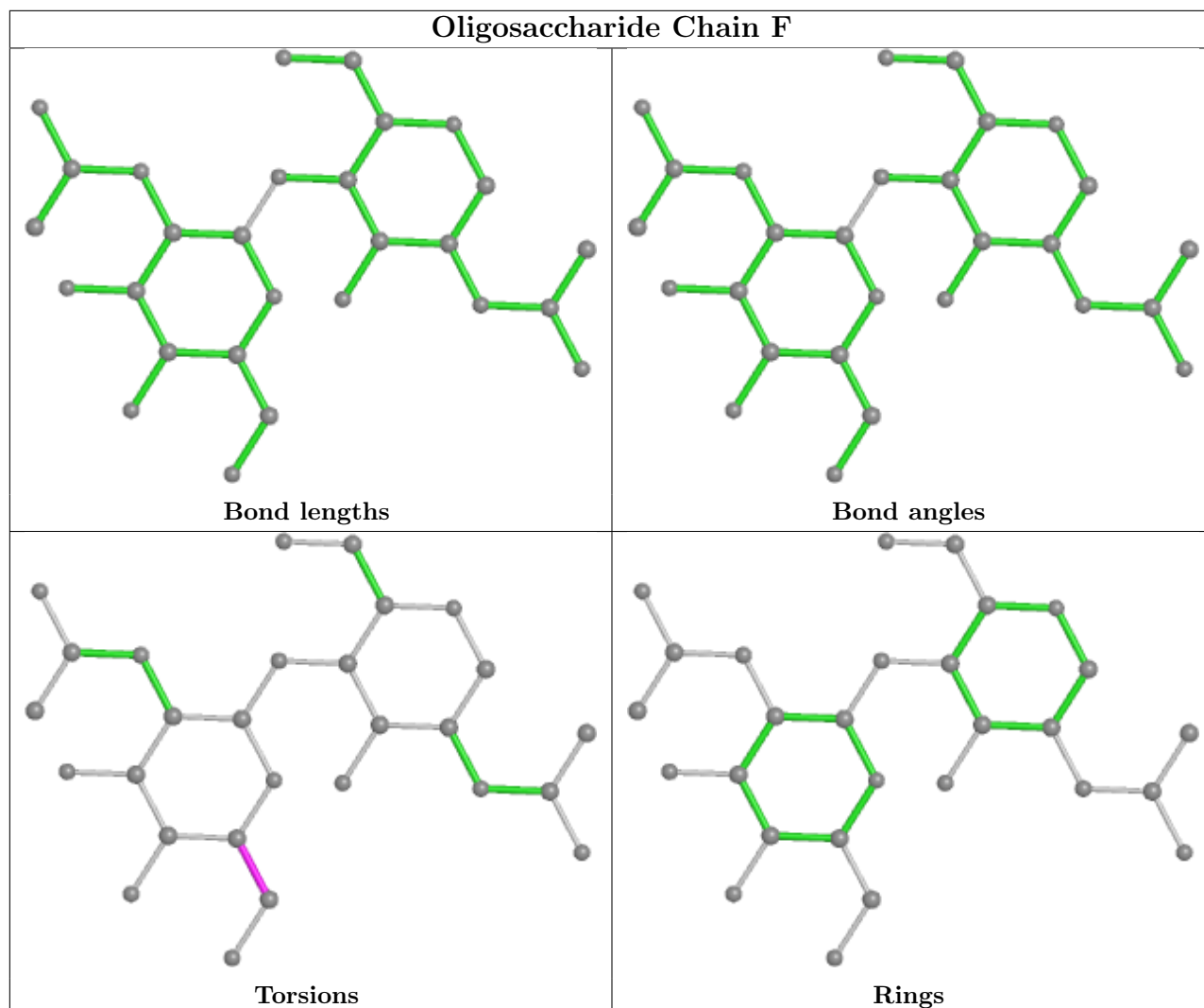
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
8	65I	E	1604	-	31,31,31	0.55	0	34,36,36	0.52	0
4	ATP	C	401	-	26,33,33	0.62	0	31,52,52	0.74	2 (6%)
4	ATP	B	401	-	26,33,33	0.61	0	31,52,52	0.74	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	POV	E	1608	-	35,35,51	0.59	0	41,43,59	0.58	0
6	POV	D	403	-	35,35,51	0.59	0	41,43,59	0.49	0
7	P5S	B	403	-	52,53,53	0.52	0	56,60,60	0.81	1 (1%)
7	P5S	C	403	-	52,53,53	0.52	0	56,60,60	0.78	1 (1%)
6	POV	B	402	-	35,35,51	0.59	0	41,43,59	0.54	0
6	POV	A	404	-	35,35,51	0.61	0	41,43,59	0.49	0
7	P5S	E	1607	-	52,53,53	0.53	0	56,60,60	0.83	1 (1%)
8	65I	E	1605	-	31,31,31	0.55	0	34,36,36	0.45	0
6	POV	C	402	-	35,35,51	0.59	0	41,43,59	0.51	0
4	ATP	D	401	-	26,33,33	0.62	0	31,52,52	0.74	2 (6%)
7	P5S	A	406	-	52,53,53	0.54	0	56,60,60	0.78	1 (1%)
9	BJX	E	1602	-	35,35,35	2.55	12 (34%)	47,47,47	1.50	3 (6%)
4	ATP	A	401	-	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
7	P5S	D	402	-	52,53,53	0.53	0	56,60,60	1.05	1 (1%)
8	65I	E	1601	-	31,31,31	0.56	0	34,36,36	0.43	0
7	P5S	A	405	-	52,53,53	0.53	0	56,60,60	0.70	1 (1%)
8	65I	E	1606	-	31,31,31	0.56	0	34,36,36	0.47	0
4	ATP	E	1603	-	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
8	65I	E	1609	-	31,31,31	0.56	0	34,36,36	0.46	0
8	65I	E	1610	-	31,31,31	0.56	0	34,36,36	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	65I	E	1604	-	-	19/35/35/35	-
4	ATP	C	401	-	-	3/18/38/38	0/3/3/3
4	ATP	B	401	-	-	8/18/38/38	0/3/3/3
6	POV	E	1608	-	-	19/39/39/55	-
6	POV	D	403	-	-	15/39/39/55	-
7	P5S	B	403	-	-	26/59/59/59	-
7	P5S	C	403	-	-	32/59/59/59	-
6	POV	B	402	-	-	14/39/39/55	-
6	POV	A	404	-	-	13/39/39/55	-
7	P5S	E	1607	-	-	26/59/59/59	-
8	65I	E	1605	-	-	10/35/35/35	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	C	402	-	-	7/39/39/55	-
4	ATP	D	401	-	-	7/18/38/38	0/3/3/3
7	P5S	A	406	-	-	22/59/59/59	-
9	BJX	E	1602	-	-	17/27/35/35	0/3/3/3
4	ATP	A	401	-	-	7/18/38/38	0/3/3/3
7	P5S	D	402	-	-	17/59/59/59	-
8	65I	E	1601	-	-	16/35/35/35	-
7	P5S	A	405	-	-	19/59/59/59	-
8	65I	E	1606	-	-	21/35/35/35	-
4	ATP	E	1603	-	-	3/18/38/38	0/3/3/3
8	65I	E	1609	-	-	11/35/35/35	-
8	65I	E	1610	-	-	21/35/35/35	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1602	BJX	C8-C5	7.33	1.60	1.53
9	E	1602	BJX	C16-N1	5.86	1.46	1.34
9	E	1602	BJX	C6-N	4.87	1.51	1.41
9	E	1602	BJX	C7-C5	4.51	1.58	1.52
9	E	1602	BJX	C6-C7	4.15	1.44	1.40
9	E	1602	BJX	C5-N1	4.13	1.52	1.46
9	E	1602	BJX	C-N	2.58	1.50	1.46
9	E	1602	BJX	O1-C21	2.54	1.42	1.37
9	E	1602	BJX	C23-C24	2.53	1.55	1.49
9	E	1602	BJX	O2-C24	2.10	1.29	1.22
9	E	1602	BJX	C1-N	2.09	1.50	1.46
9	E	1602	BJX	C17-C18	2.00	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	P5S	OG-CB-CA	6.70	113.90	108.06
9	E	1602	BJX	C5-N1-C16	6.54	133.75	123.33
7	E	1607	P5S	OG-CB-CA	4.54	112.02	108.06
7	A	406	P5S	OG-CB-CA	4.17	111.70	108.06
7	C	403	P5S	OG-CB-CA	3.96	111.52	108.06
7	B	403	P5S	OG-CB-CA	3.79	111.36	108.06
7	A	405	P5S	OG-CB-CA	3.29	110.92	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1602	BJX	C8-C5-N1	2.79	114.77	109.80
9	E	1602	BJX	C17-C16-N1	2.54	119.96	115.88
4	B	401	ATP	C5-C6-N6	2.31	123.86	120.35
4	A	401	ATP	C5-C6-N6	2.29	123.84	120.35
4	C	401	ATP	C5-C6-N6	2.29	123.83	120.35
4	D	401	ATP	C5-C6-N6	2.28	123.82	120.35
4	E	1603	ATP	C5-C6-N6	2.28	123.81	120.35
4	A	401	ATP	PB-O3B-PG	2.07	139.94	132.83
4	D	401	ATP	PB-O3B-PG	2.07	139.92	132.83
4	C	401	ATP	PB-O3B-PG	2.05	139.85	132.83
4	B	401	ATP	PB-O3B-PG	2.05	139.85	132.83
4	E	1603	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (353) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	C5'-O5'-PA-O3A
4	B	401	ATP	C5'-O5'-PA-O3A
4	B	401	ATP	O4'-C4'-C5'-O5'
4	B	401	ATP	C3'-C4'-C5'-O5'
4	D	401	ATP	PB-O3B-PG-O3G
4	D	401	ATP	O4'-C4'-C5'-O5'
6	A	404	POV	C1-O11-P-O14
6	A	404	POV	C11-O12-P-O14
6	A	404	POV	O12-C11-C12-N
6	B	402	POV	C1-O11-P-O14
6	B	402	POV	C11-O12-P-O11
6	B	402	POV	C11-O12-P-O14
6	B	402	POV	C12-C11-O12-P
6	D	403	POV	C1-O11-P-O14
6	D	403	POV	C11-O12-P-O14
6	E	1608	POV	C1-O11-P-O14
6	E	1608	POV	C11-O12-P-O11
6	E	1608	POV	O12-C11-C12-N
7	A	405	P5S	O-C-CA-N
7	A	406	P5S	O-C-CA-N
7	A	406	P5S	C-CA-CB-OG
7	A	406	P5S	N-CA-CB-OG
7	A	406	P5S	CB-OG-P12-O13
7	B	403	P5S	N-CA-CB-OG
7	B	403	P5S	CB-OG-P12-O13

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Mol	Chain	Res	Type	Atoms
7	B	403	P5S	C3-O16-P12-OG
7	B	403	P5S	C3-O16-P12-O13
7	B	403	P5S	O18-C17-O19-C1
7	B	403	P5S	C39-C38-O37-C2
7	C	403	P5S	O-C-CA-N
7	C	403	P5S	O-C-CA-CB
7	C	403	P5S	OXT-C-CA-CB
7	C	403	P5S	C-CA-CB-OG
7	C	403	P5S	N-CA-CB-OG
7	C	403	P5S	CB-OG-P12-O16
7	D	402	P5S	CB-OG-P12-O15
7	D	402	P5S	C3-O16-P12-O13
7	E	1607	P5S	O-C-CA-N
7	E	1607	P5S	CB-OG-P12-O16
7	E	1607	P5S	C3-O16-P12-O13
8	E	1601	65I	C12-C11-O6-C7
8	E	1601	65I	C10-C9-O5-P
8	E	1601	65I	C8-O2-P-O4
8	E	1601	65I	C9-O5-P-O2
8	E	1604	65I	C9-O5-P-O2
8	E	1604	65I	C9-O5-P-O3
8	E	1604	65I	C9-O5-P-O4
8	E	1606	65I	C8-O2-P-O4
8	E	1606	65I	C9-O5-P-O4
8	E	1609	65I	N-C10-C9-O5
8	E	1609	65I	C10-C9-O5-P
8	E	1609	65I	C8-O2-P-O4
8	E	1609	65I	C8-O2-P-O5
8	E	1609	65I	C9-O5-P-O3
8	E	1610	65I	C12-C11-O6-C7
8	E	1610	65I	C8-O2-P-O3
8	E	1610	65I	C9-O5-P-O2
8	E	1610	65I	C9-O5-P-O4
9	E	1602	BJX	C7-C5-C8-C9
9	E	1602	BJX	C8-C5-N1-C16
9	E	1602	BJX	C21-C23-C24-O2
9	E	1602	BJX	C21-C23-C24-O3
7	C	403	P5S	O18-C17-O19-C1
7	E	1607	P5S	O18-C17-O19-C1
8	E	1604	65I	O-C5-O1-C6
7	C	403	P5S	C20-C17-O19-C1
7	A	405	P5S	O18-C17-O19-C1

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Mol	Chain	Res	Type	Atoms
8	E	1605	65I	O-C5-O1-C6
7	B	403	P5S	O47-C38-O37-C2
8	E	1601	65I	O7-C11-O6-C7
8	E	1610	65I	O7-C11-O6-C7
7	B	403	P5S	C20-C17-O19-C1
7	E	1607	P5S	C20-C17-O19-C1
8	E	1604	65I	C4-C5-O1-C6
9	E	1602	BJX	N1-C5-C8-C9
7	A	405	P5S	C20-C17-O19-C1
8	E	1605	65I	C4-C5-O1-C6
8	E	1606	65I	C4-C5-O1-C6
8	E	1606	65I	O-C5-O1-C6
8	E	1606	65I	C12-C11-O6-C7
4	D	401	ATP	C3'-C4'-C5'-O5'
8	E	1606	65I	O7-C11-O6-C7
6	B	402	POV	C11-C12-N-C15
6	E	1608	POV	C11-C12-N-C13
7	A	405	P5S	C38-C39-C40-C41
7	D	402	P5S	C48-C49-C50-C51
6	A	404	POV	C21-C22-C23-C24
7	C	403	P5S	OXT-C-CA-N
6	B	402	POV	C11-C12-N-C14
6	D	403	POV	C21-C22-C23-C24
7	A	406	P5S	C38-C39-C40-C41
8	E	1604	65I	C12-C11-O6-C7
6	A	404	POV	C1-O11-P-O12
6	D	403	POV	C1-O11-P-O12
6	E	1608	POV	C1-O11-P-O12
7	A	406	P5S	CB-OG-P12-O16
7	D	402	P5S	CB-OG-P12-O16
8	E	1601	65I	C8-O2-P-O5
8	E	1604	65I	C8-O2-P-O5
8	E	1609	65I	C9-O5-P-O2
8	E	1610	65I	C8-O2-P-O5
7	A	405	P5S	OXT-C-CA-N
7	A	406	P5S	OXT-C-CA-N
7	E	1607	P5S	OXT-C-CA-N
8	E	1604	65I	O7-C11-O6-C7
7	C	403	P5S	C27-C28-C29-C30
7	C	403	P5S	C42-C43-C44-C45
7	C	403	P5S	C43-C44-C45-C46
7	E	1607	P5S	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	A	406	P5S	C24-C25-C26-C27
7	C	403	P5S	C45-C46-C48-C49
9	E	1602	BJX	C26-C25-O1-C21
6	B	402	POV	C22-C23-C24-C25
7	A	405	P5S	C41-C42-C43-C44
7	B	403	P5S	C40-C41-C42-C43
7	C	403	P5S	C23-C24-C25-C26
7	A	405	P5S	C40-C41-C42-C43
7	E	1607	P5S	C51-C52-C53-C54
6	E	1608	POV	C21-C22-C23-C24
6	B	402	POV	O21-C2-C3-O31
6	A	404	POV	C33-C34-C35-C36
7	A	406	P5S	C49-C50-C51-C52
7	C	403	P5S	C20-C21-C22-C23
7	C	403	P5S	C52-C53-C54-C55
7	D	402	P5S	C49-C50-C51-C52
7	E	1607	P5S	C28-C29-C30-C31
6	E	1608	POV	O22-C21-O21-C2
6	E	1608	POV	C22-C21-O21-C2
8	E	1609	65I	C2-C3-C4-C5
6	D	403	POV	C22-C23-C24-C25
7	A	406	P5S	C26-C27-C28-C29
7	D	402	P5S	C42-C43-C44-C45
7	E	1607	P5S	C48-C49-C50-C51
6	B	402	POV	C11-C12-N-C13
6	E	1608	POV	C11-C12-N-C14
6	E	1608	POV	C11-C12-N-C15
6	D	403	POV	C24-C25-C26-C27
7	B	403	P5S	C21-C22-C23-C24
7	C	403	P5S	C22-C23-C24-C25
7	C	403	P5S	C25-C26-C27-C28
7	A	406	P5S	C43-C44-C45-C46
8	E	1601	65I	C12-C13-C14-C15
8	E	1610	65I	C15-C16-C17-C18
8	E	1604	65I	C11-C12-C13-C14
7	D	402	P5S	C24-C25-C26-C27
7	B	403	P5S	C41-C42-C43-C44
4	A	401	ATP	O4'-C4'-C5'-O5'
4	A	401	ATP	C3'-C4'-C5'-O5'
7	B	403	P5S	C26-C27-C28-C29
9	E	1602	BJX	C5-C8-C9-C13
7	A	406	P5S	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	B	403	P5S	C22-C23-C24-C25
7	E	1607	P5S	C21-C22-C23-C24
7	A	406	P5S	C51-C52-C53-C54
6	D	403	POV	C32-C31-O31-C3
8	E	1610	65I	C4-C5-O1-C6
7	A	405	P5S	C26-C27-C28-C29
7	D	402	P5S	C51-C52-C53-C54
7	E	1607	P5S	C39-C38-O37-C2
7	A	405	P5S	C42-C43-C44-C45
7	E	1607	P5S	O47-C38-O37-C2
4	E	1603	ATP	O4'-C4'-C5'-O5'
6	C	402	POV	C11-O12-P-O11
8	E	1609	65I	C6-C7-C8-O2
7	C	403	P5S	C24-C25-C26-C27
7	D	402	P5S	C22-C23-C24-C25
8	E	1606	65I	C14-C15-C16-C17
6	A	404	POV	C32-C33-C34-C35
6	E	1608	POV	C1-C2-C3-O31
7	B	403	P5S	O19-C1-C2-C3
6	D	403	POV	O32-C31-O31-C3
8	E	1610	65I	O-C5-O1-C6
9	E	1602	BJX	C23-C21-O1-C25
8	E	1604	65I	C18-C19-C20-C21
7	B	403	P5S	C3-C2-O37-C38
8	E	1601	65I	C14-C15-C16-C17
7	B	403	P5S	O37-C2-C3-O16
7	B	403	P5S	C38-C39-C40-C41
7	D	402	P5S	C38-C39-C40-C41
6	A	404	POV	C24-C25-C26-C27
8	E	1604	65I	O1-C6-C7-O6
6	C	402	POV	C32-C33-C34-C35
6	B	402	POV	O11-C1-C2-C3
6	D	403	POV	O11-C1-C2-C3
6	E	1608	POV	O11-C1-C2-C3
8	E	1604	65I	C6-C7-C8-O2
8	E	1610	65I	N-C10-C9-O5
8	E	1610	65I	C16-C17-C18-C19
9	E	1602	BJX	C19-C21-O1-C25
6	C	402	POV	C23-C24-C25-C26
7	B	403	P5S	C2-C3-O16-P12
8	E	1605	65I	C18-C19-C20-C21
6	D	403	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
6	B	402	POV	C1-C2-C3-O31
7	E	1607	P5S	O19-C1-C2-C3
8	E	1604	65I	O1-C6-C7-C8
7	C	403	P5S	C21-C22-C23-C24
7	A	405	P5S	C43-C44-C45-C46
6	A	404	POV	C11-O12-P-O11
8	E	1606	65I	C11-C12-C13-C14
8	E	1609	65I	O6-C7-C8-O2
8	E	1610	65I	O6-C7-C8-O2
7	C	403	P5S	C39-C40-C41-C42
6	A	404	POV	O21-C2-C3-O31
7	A	406	P5S	O19-C1-C2-O37
8	E	1604	65I	C12-C13-C14-C15
6	A	404	POV	C2-C1-O11-P
7	E	1607	P5S	C2-C3-O16-P12
8	E	1605	65I	C7-C8-O2-P
7	E	1607	P5S	C27-C28-C29-C30
7	B	403	P5S	C43-C44-C45-C46
9	E	1602	BJX	C8-C5-C7-C11
6	C	402	POV	O11-C1-C2-C3
7	A	406	P5S	C1-C2-C3-O16
8	E	1601	65I	C6-C7-C8-O2
9	E	1602	BJX	C22-C23-C24-O2
4	E	1603	ATP	C3'-C4'-C5'-O5'
9	E	1602	BJX	C22-C23-C24-O3
8	E	1604	65I	C6-C7-O6-C11
8	E	1601	65I	C15-C16-C17-C18
6	B	402	POV	O11-C1-C2-O21
6	D	403	POV	O11-C1-C2-O21
6	E	1608	POV	O11-C1-C2-O21
8	E	1601	65I	O6-C7-C8-O2
8	E	1604	65I	O6-C7-C8-O2
4	C	401	ATP	PB-O3B-PG-O2G
7	A	405	P5S	O19-C1-C2-O37
7	B	403	P5S	O19-C1-C2-O37
7	C	403	P5S	O19-C1-C2-O37
8	E	1606	65I	O1-C6-C7-O6
7	E	1607	P5S	CA-CB-OG-P12
9	E	1602	BJX	C8-C5-C7-C6
7	B	403	P5S	C20-C21-C22-C23
4	A	401	ATP	PB-O3A-PA-O1A
4	B	401	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	C	401	ATP	PA-O3A-PB-O2B
4	E	1603	ATP	PA-O3A-PB-O1B
7	C	403	P5S	C51-C52-C53-C54
7	D	402	P5S	N-CA-CB-OG
6	D	403	POV	C11-O12-P-O11
7	A	405	P5S	CB-OG-P12-O16
7	B	403	P5S	CB-OG-P12-O16
7	D	402	P5S	C3-O16-P12-OG
7	E	1607	P5S	C3-O16-P12-OG
8	E	1606	65I	C8-O2-P-O5
9	E	1602	BJX	O-C16-C17-C18
6	E	1608	POV	C2-C1-O11-P
8	E	1610	65I	C7-C8-O2-P
7	D	402	P5S	C46-C48-C49-C50
4	A	401	ATP	C5'-O5'-PA-O1A
4	A	401	ATP	C5'-O5'-PA-O2A
4	B	401	ATP	C5'-O5'-PA-O1A
4	B	401	ATP	C5'-O5'-PA-O2A
6	A	404	POV	C1-O11-P-O13
6	C	402	POV	C11-O12-P-O13
6	D	403	POV	C1-O11-P-O13
6	E	1608	POV	C1-O11-P-O13
6	E	1608	POV	C11-O12-P-O13
7	A	406	P5S	CB-OG-P12-O15
7	C	403	P5S	CB-OG-P12-O13
7	D	402	P5S	CB-OG-P12-O13
7	E	1607	P5S	CB-OG-P12-O15
8	E	1601	65I	C8-O2-P-O3
8	E	1601	65I	C9-O5-P-O3
8	E	1604	65I	C8-O2-P-O4
8	E	1610	65I	C8-O2-P-O4
7	B	403	P5S	C1-C2-C3-O16
8	E	1606	65I	C16-C17-C18-C19
7	E	1607	P5S	C53-C54-C55-C56
9	E	1602	BJX	N1-C5-C7-C6
6	C	402	POV	O11-C1-C2-O21
7	A	406	P5S	O37-C2-C3-O16
7	B	403	P5S	C25-C26-C27-C28
8	E	1606	65I	C-C1-C2-C3
7	A	405	P5S	O19-C1-C2-C3
8	E	1606	65I	C15-C16-C17-C18
7	D	402	P5S	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
8	E	1609	65I	C14-C15-C16-C17
8	E	1610	65I	C13-C14-C15-C16
6	E	1608	POV	C1-C2-O21-C21
7	A	405	P5S	C24-C25-C26-C27
6	B	402	POV	C1-O11-P-O12
7	A	406	P5S	C3-O16-P12-OG
8	E	1606	65I	C9-O5-P-O2
6	A	404	POV	C1-C2-C3-O31
8	E	1606	65I	O1-C6-C7-C8
7	E	1607	P5S	C46-C48-C49-C50
4	A	401	ATP	PB-O3A-PA-O2A
4	D	401	ATP	PB-O3A-PA-O2A
7	A	405	P5S	C27-C28-C29-C30
7	E	1607	P5S	C42-C43-C44-C45
8	E	1609	65I	C15-C16-C17-C18
7	E	1607	P5S	C23-C24-C25-C26
8	E	1606	65I	C18-C19-C20-C21
7	A	406	P5S	C22-C23-C24-C25
6	E	1608	POV	O21-C2-C3-O31
7	A	406	P5S	O19-C1-C2-C3
8	E	1606	65I	C12-C13-C14-C15
6	E	1608	POV	C23-C24-C25-C26
7	A	405	P5S	C17-C20-C21-C22
8	E	1605	65I	O7-C11-O6-C7
7	B	403	P5S	C24-C25-C26-C27
4	B	401	ATP	PB-O3A-PA-O1A
4	D	401	ATP	PB-O3A-PA-O1A
7	C	403	P5S	C30-C31-C32-C33
8	E	1601	65I	C16-C17-C18-C19
7	A	406	P5S	C25-C26-C27-C28
7	C	403	P5S	C40-C41-C42-C43
8	E	1605	65I	C17-C18-C19-C20
7	C	403	P5S	O37-C38-C39-C40
4	D	401	ATP	PB-O3B-PG-O1G
8	E	1610	65I	C3-C4-C5-O1
8	E	1610	65I	C-C1-C2-C3
7	A	406	P5S	C21-C22-C23-C24
7	E	1607	P5S	C-CA-CB-OG
7	C	403	P5S	O19-C1-C2-C3
9	E	1602	BJX	N1-C5-C7-C11
7	E	1607	P5S	C50-C51-C52-C53
7	C	403	P5S	O37-C2-C3-O16

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Mol	Chain	Res	Type	Atoms
8	E	1606	65I	C3-C4-C5-O1
8	E	1605	65I	C3-C4-C5-O1
8	E	1610	65I	C6-C7-C8-O2
7	D	402	P5S	CA-CB-OG-P12
8	E	1606	65I	O6-C11-C12-C13
7	C	403	P5S	O47-C38-C39-C40
8	E	1601	65I	C3-C4-C5-O1
8	E	1610	65I	C3-C4-C5-O
4	B	401	ATP	PA-O3A-PB-O1B
4	C	401	ATP	PA-O3A-PB-O1B
7	B	403	P5S	C30-C31-C32-C33
8	E	1605	65I	C12-C11-O6-C7
6	B	402	POV	C21-C22-C23-C24
7	E	1607	P5S	C49-C50-C51-C52
8	E	1606	65I	O7-C11-C12-C13
9	E	1602	BJX	N1-C16-C17-C18
8	E	1604	65I	C17-C18-C19-C20
8	E	1610	65I	C14-C15-C16-C17
7	D	402	P5S	C2-C3-O16-P12
4	D	401	ATP	C5'-O5'-PA-O1A
7	A	405	P5S	C3-O16-P12-O13
8	E	1604	65I	N-C10-C9-O5
8	E	1605	65I	C3-C4-C5-O
8	E	1606	65I	C3-C4-C5-O
6	D	403	POV	C12-C11-O12-P
8	E	1605	65I	C6-C7-O6-C11
8	E	1610	65I	C10-C9-O5-P
7	A	405	P5S	O37-C38-C39-C40
6	C	402	POV	C2-C1-O11-P
7	A	405	P5S	C20-C21-C22-C23
7	C	403	P5S	O19-C17-C20-C21
6	D	403	POV	C32-C33-C34-C35
7	C	403	P5S	O18-C17-C20-C21
8	E	1601	65I	C3-C4-C5-O

There are no ring outliers.

15 monomers are involved in 41 short contacts:

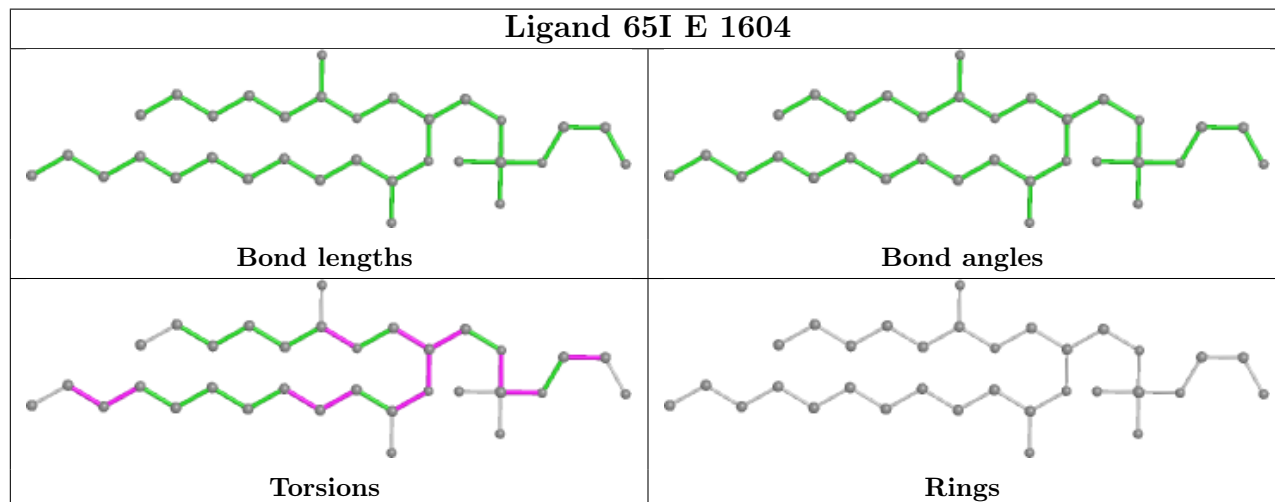
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	ATP	4	0
4	B	401	ATP	3	0
6	E	1608	POV	1	0

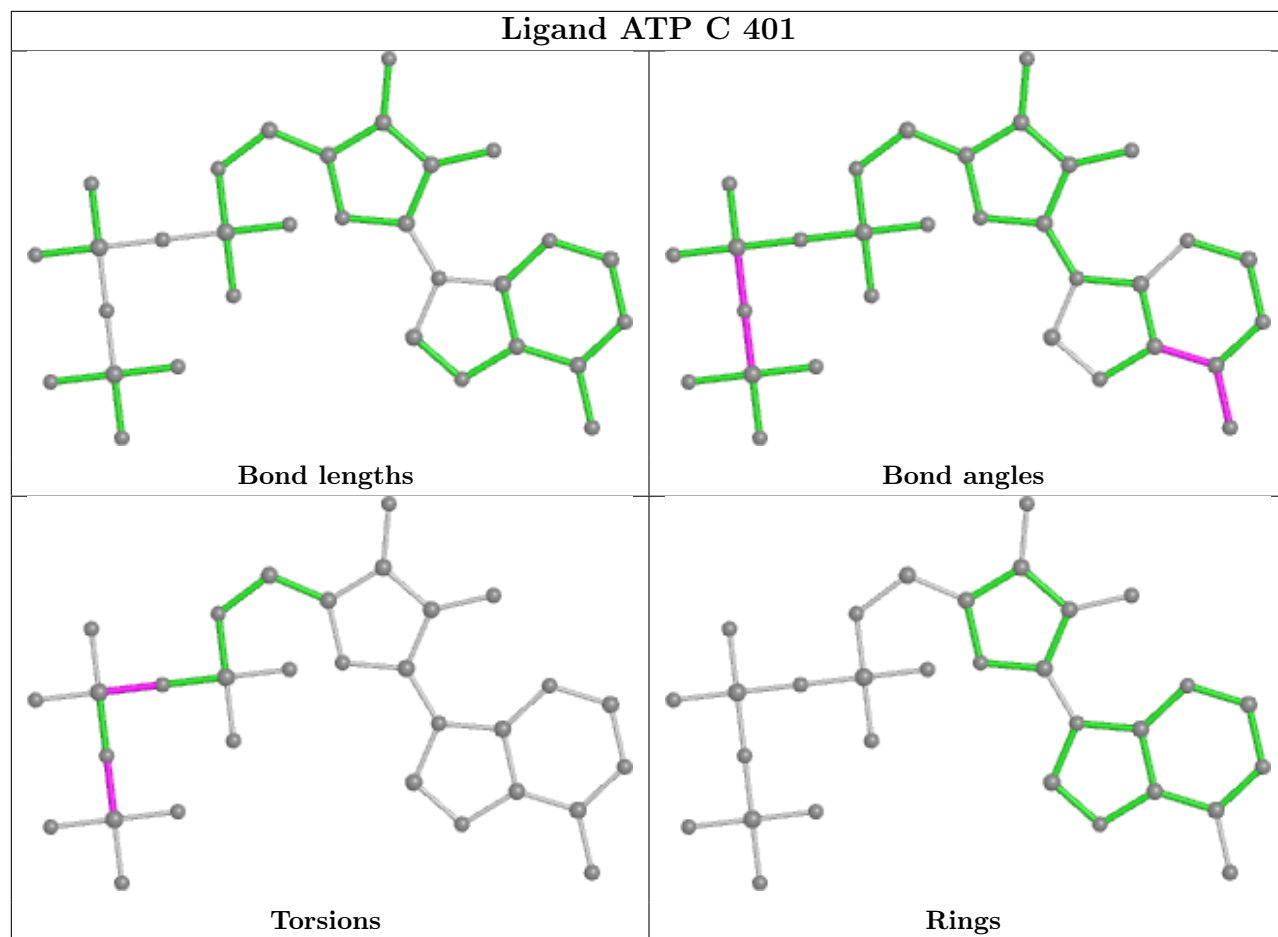
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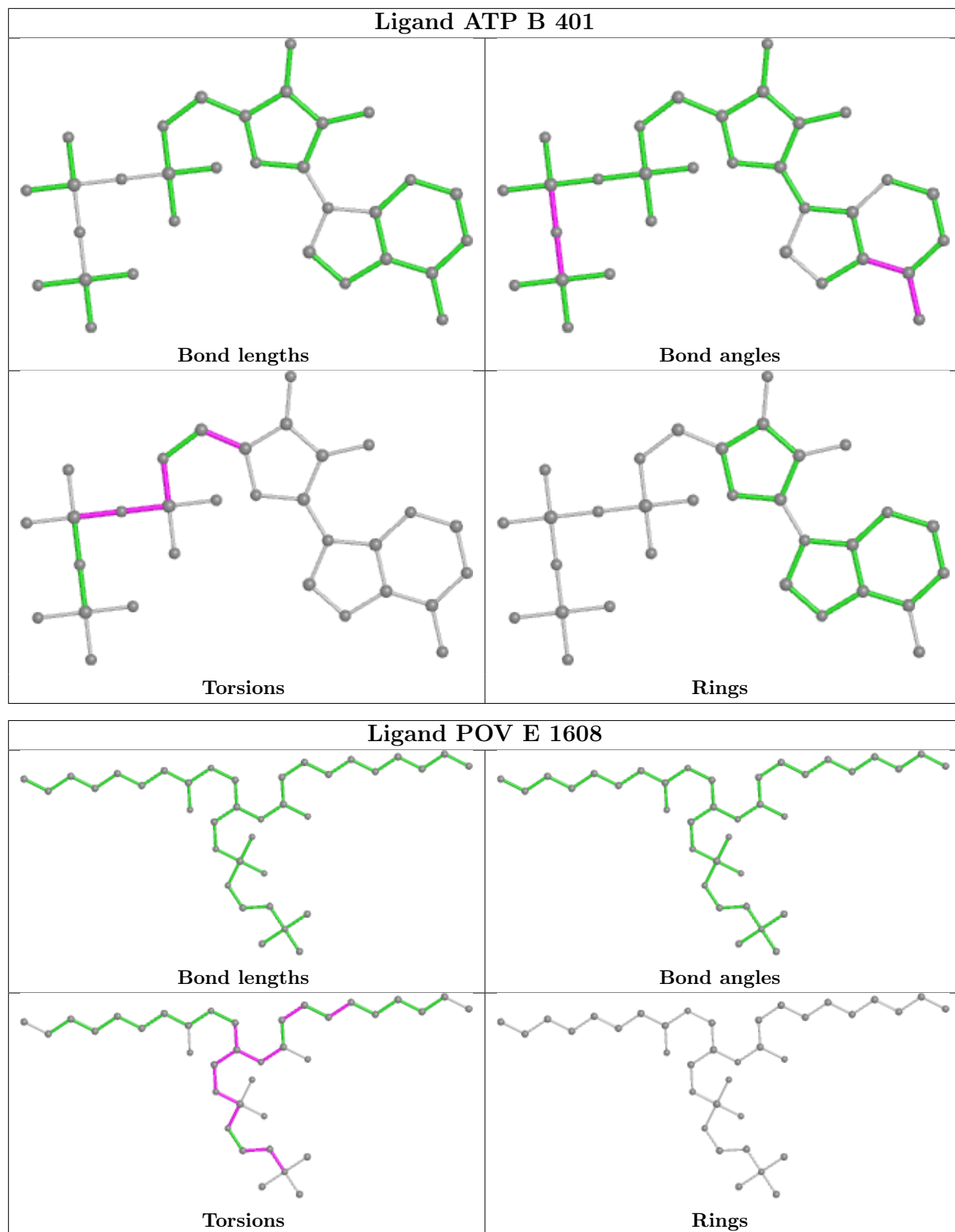
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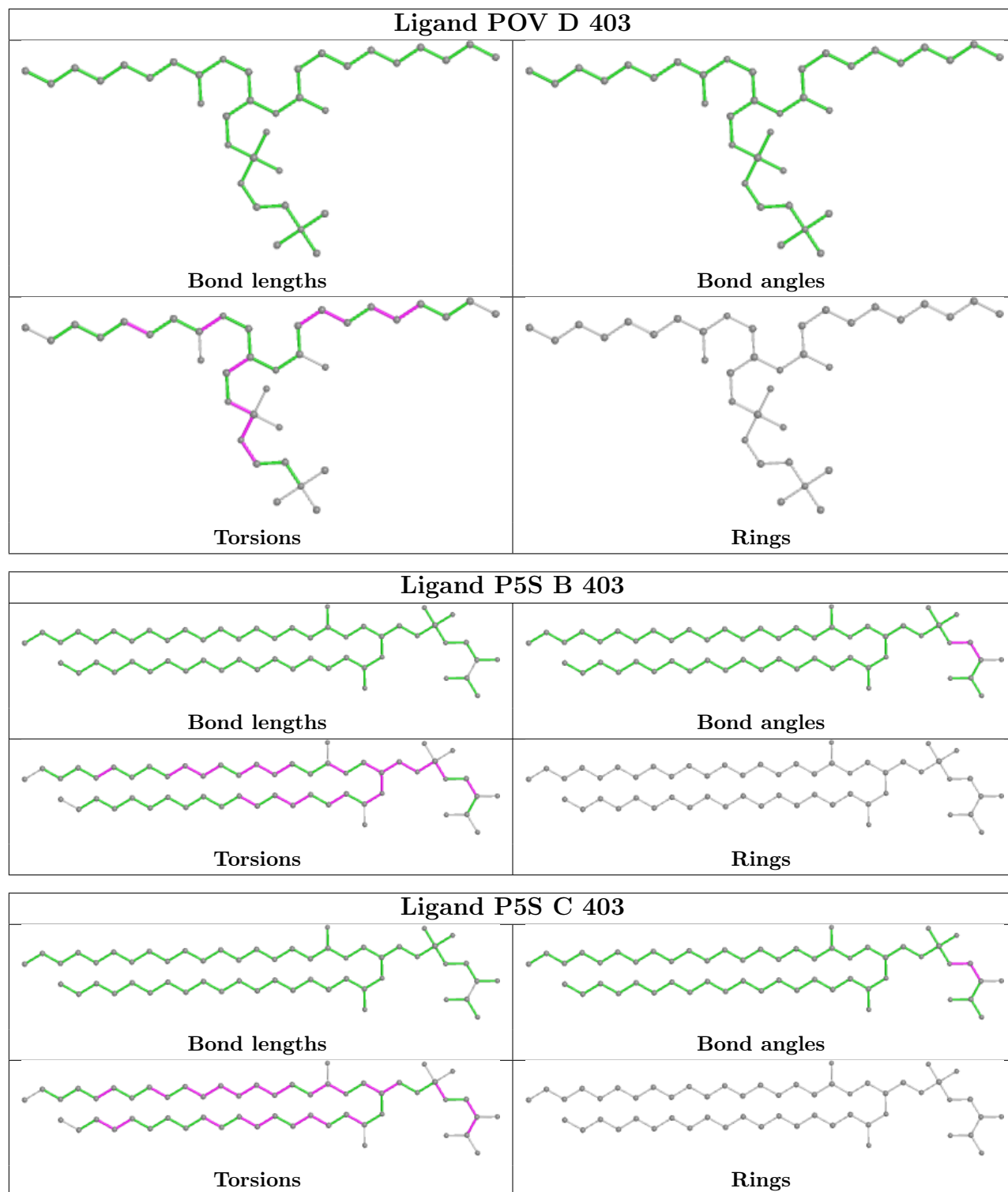
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	403	POV	1	0
7	B	403	P5S	4	0
7	C	403	P5S	6	0
6	A	404	POV	1	0
7	E	1607	P5S	5	0
6	C	402	POV	1	0
7	A	406	P5S	3	0
9	E	1602	BJX	1	0
4	A	401	ATP	3	0
7	D	402	P5S	5	0
7	A	405	P5S	4	0
4	E	1603	ATP	1	0

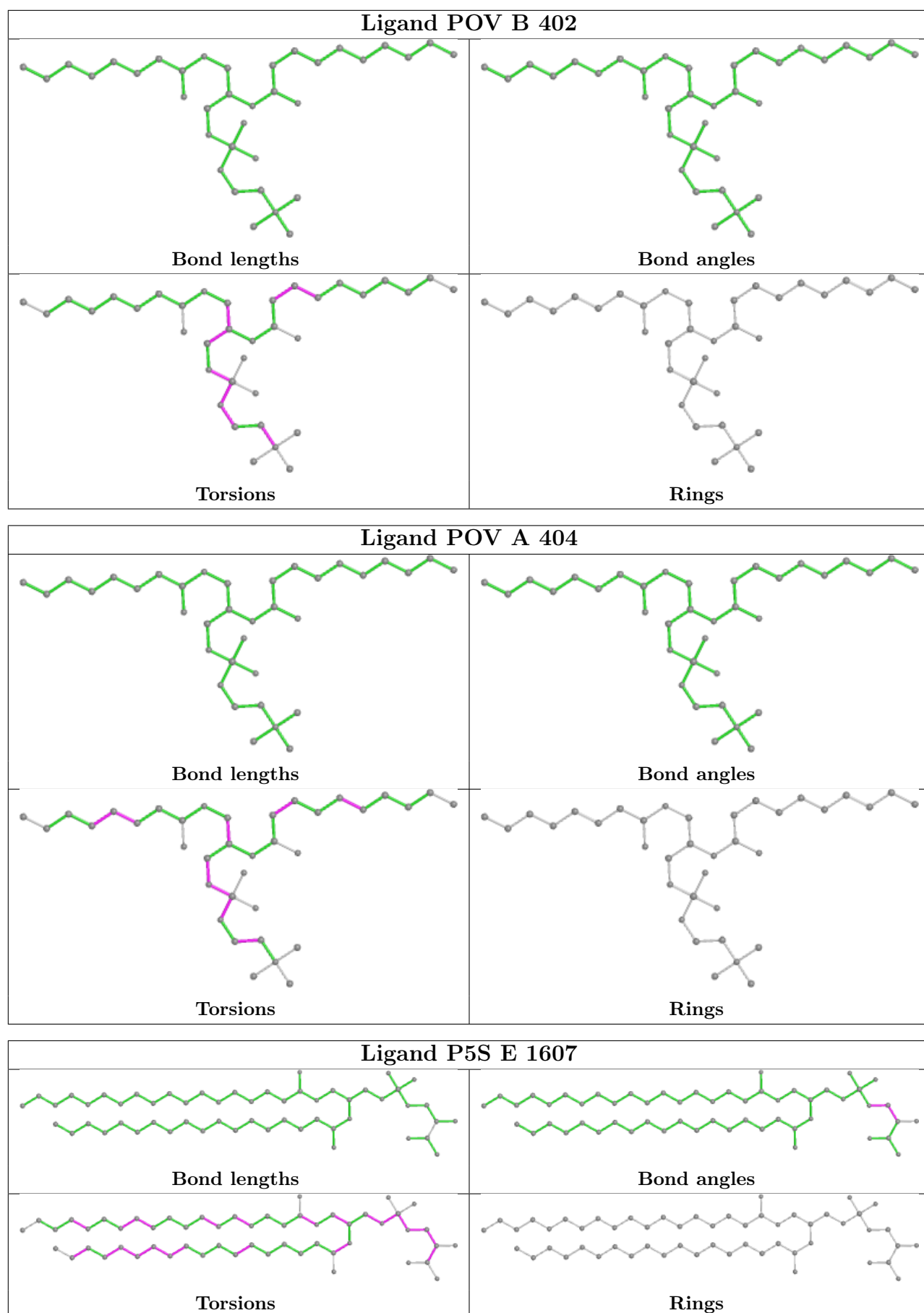
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

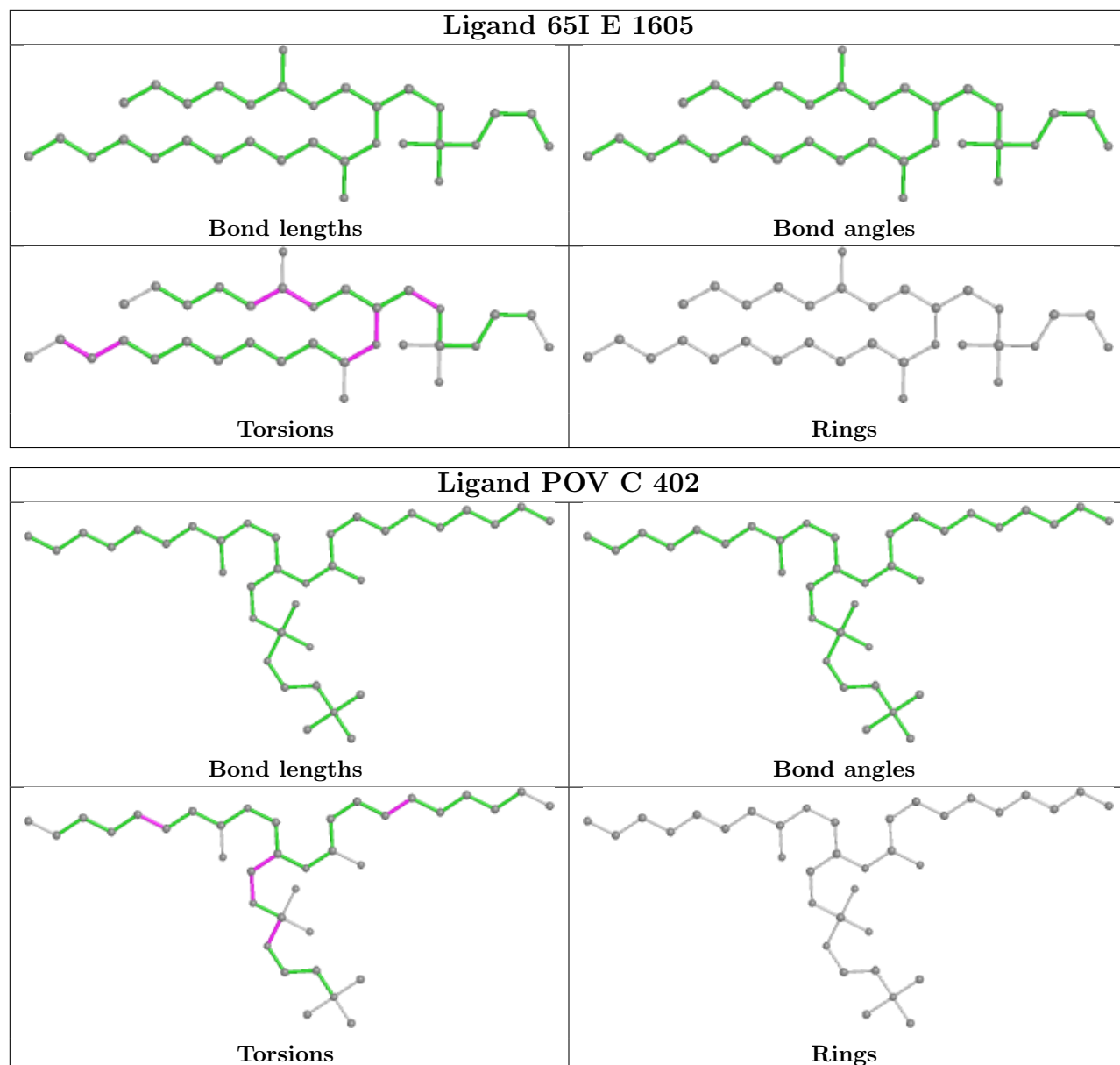


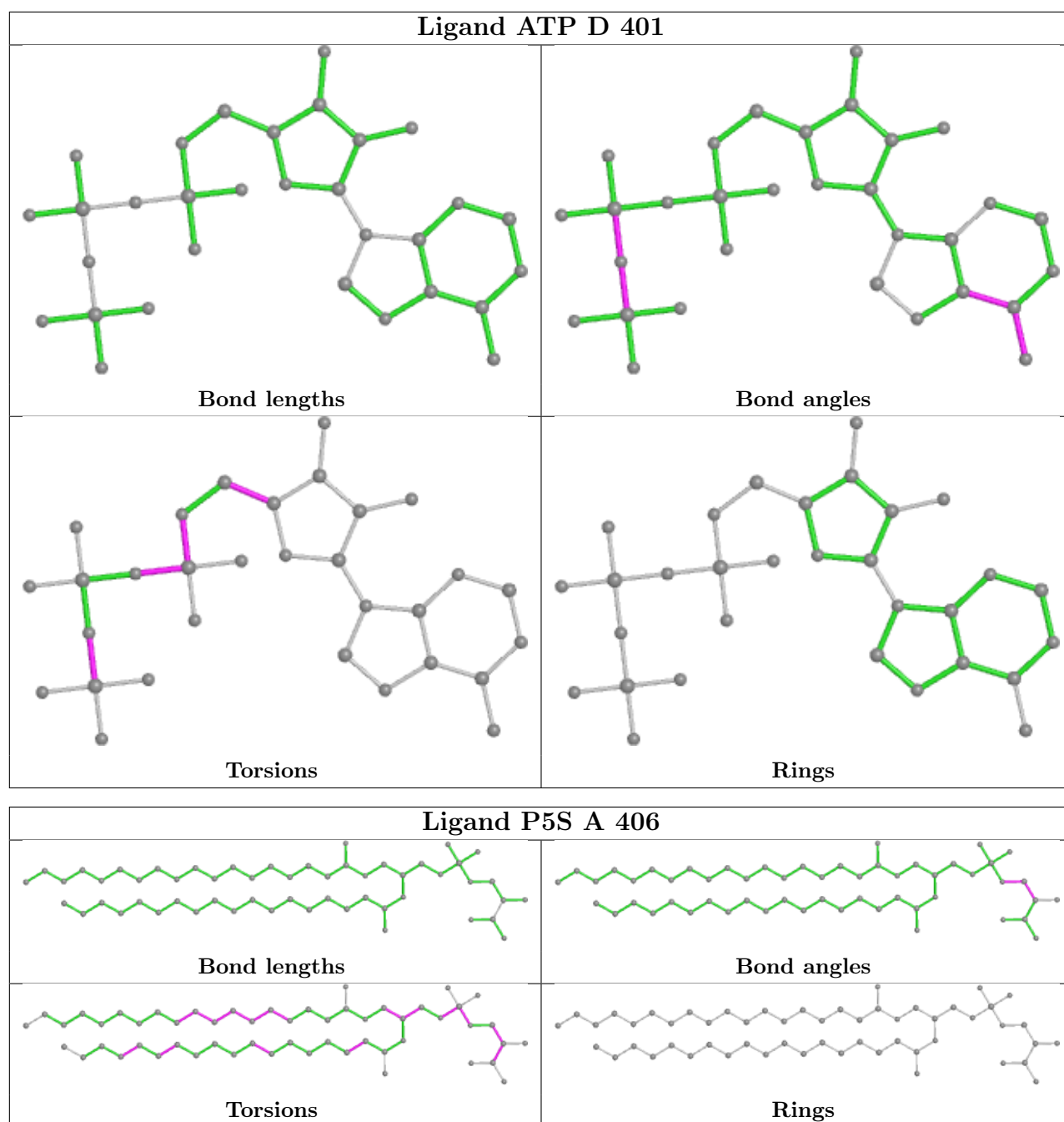


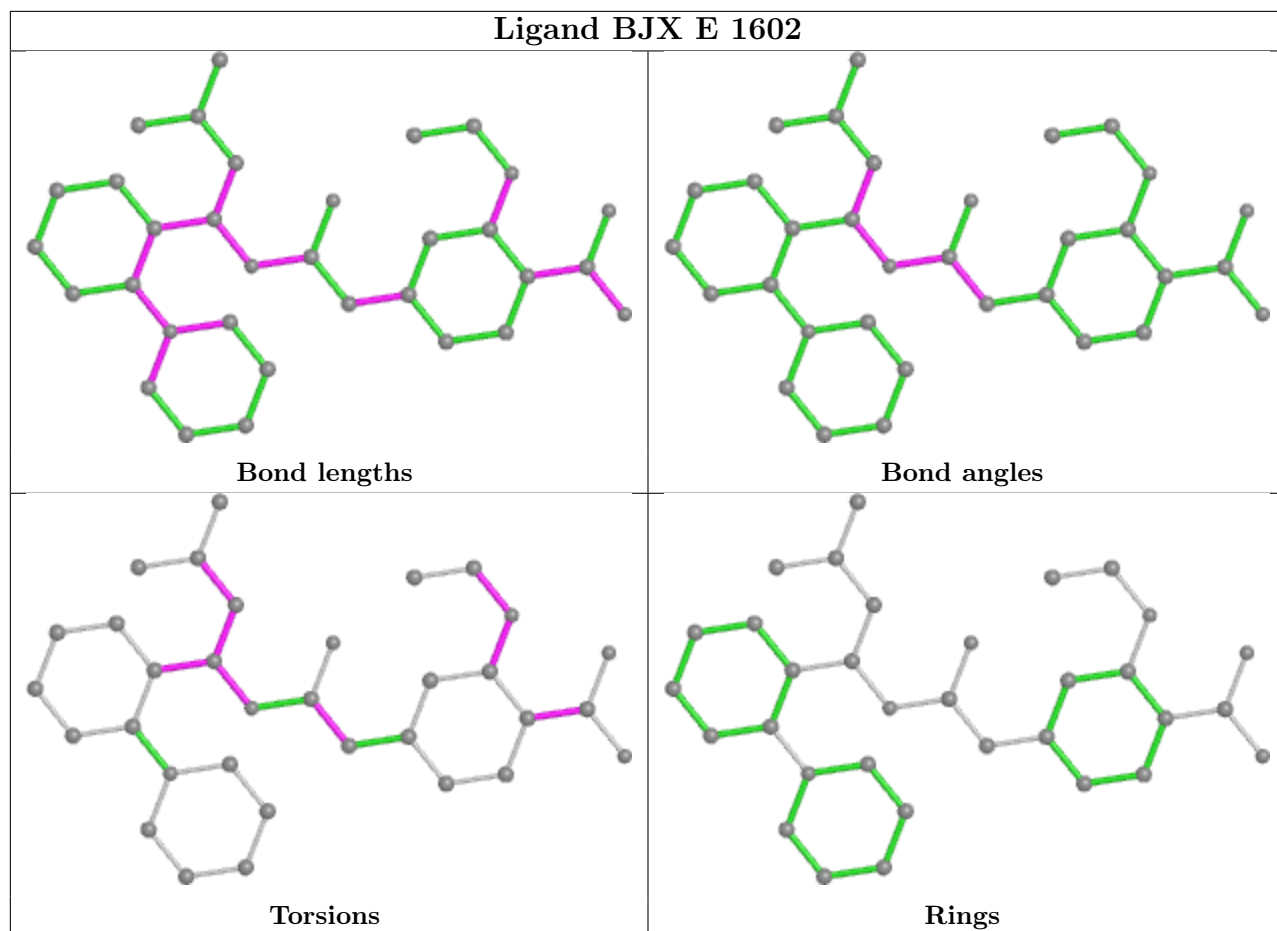


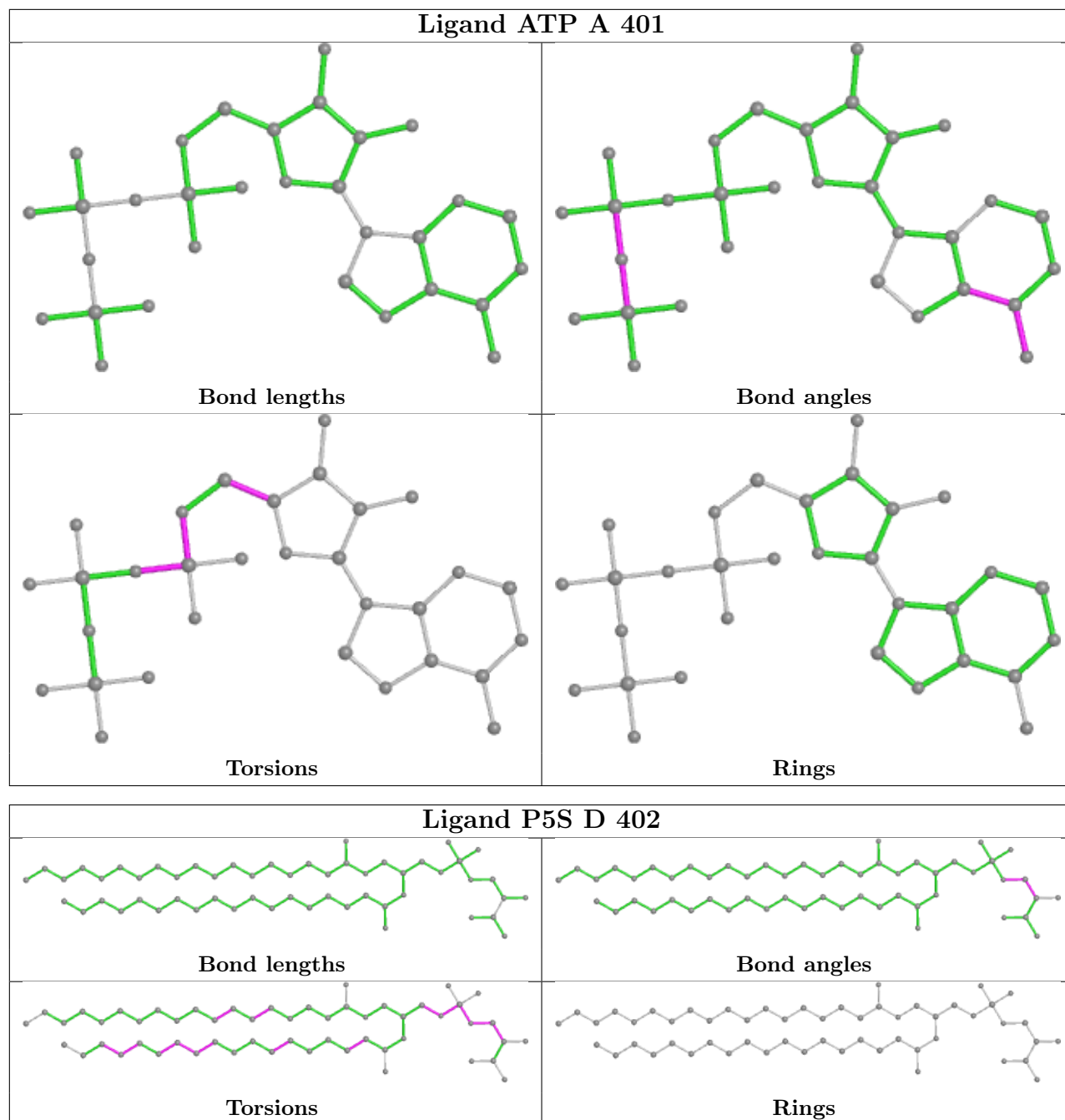


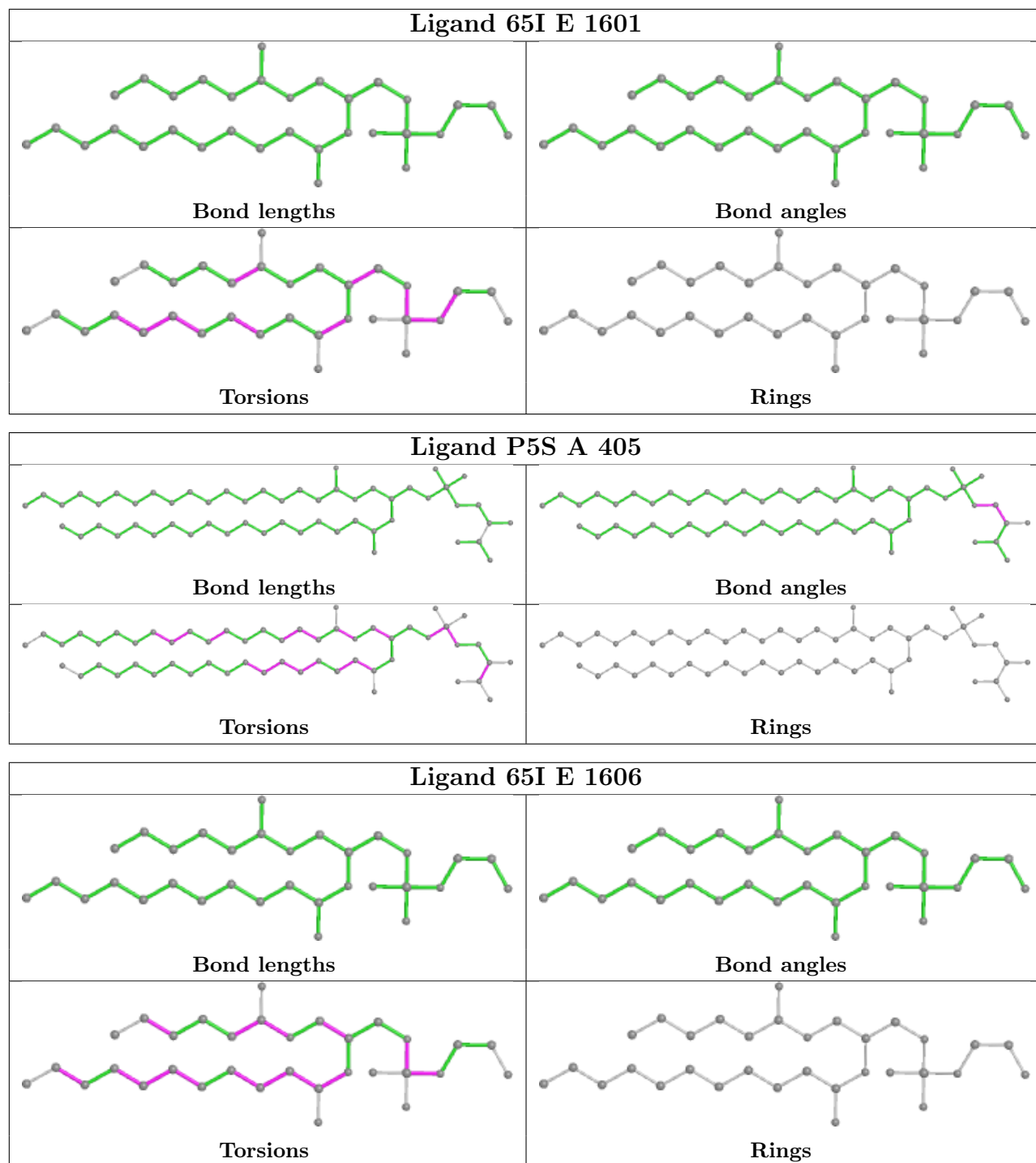


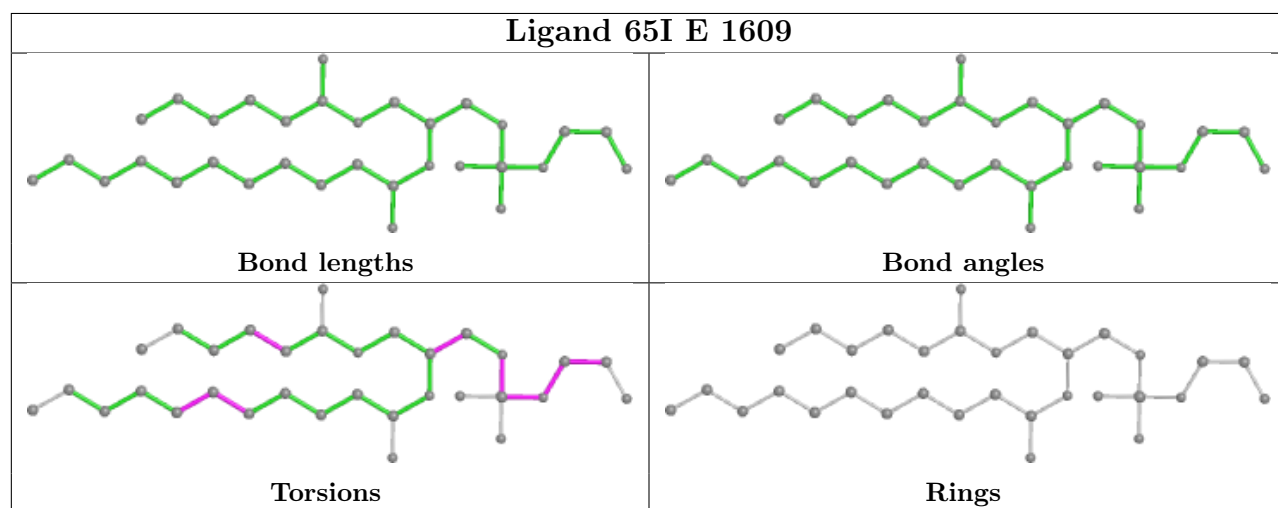
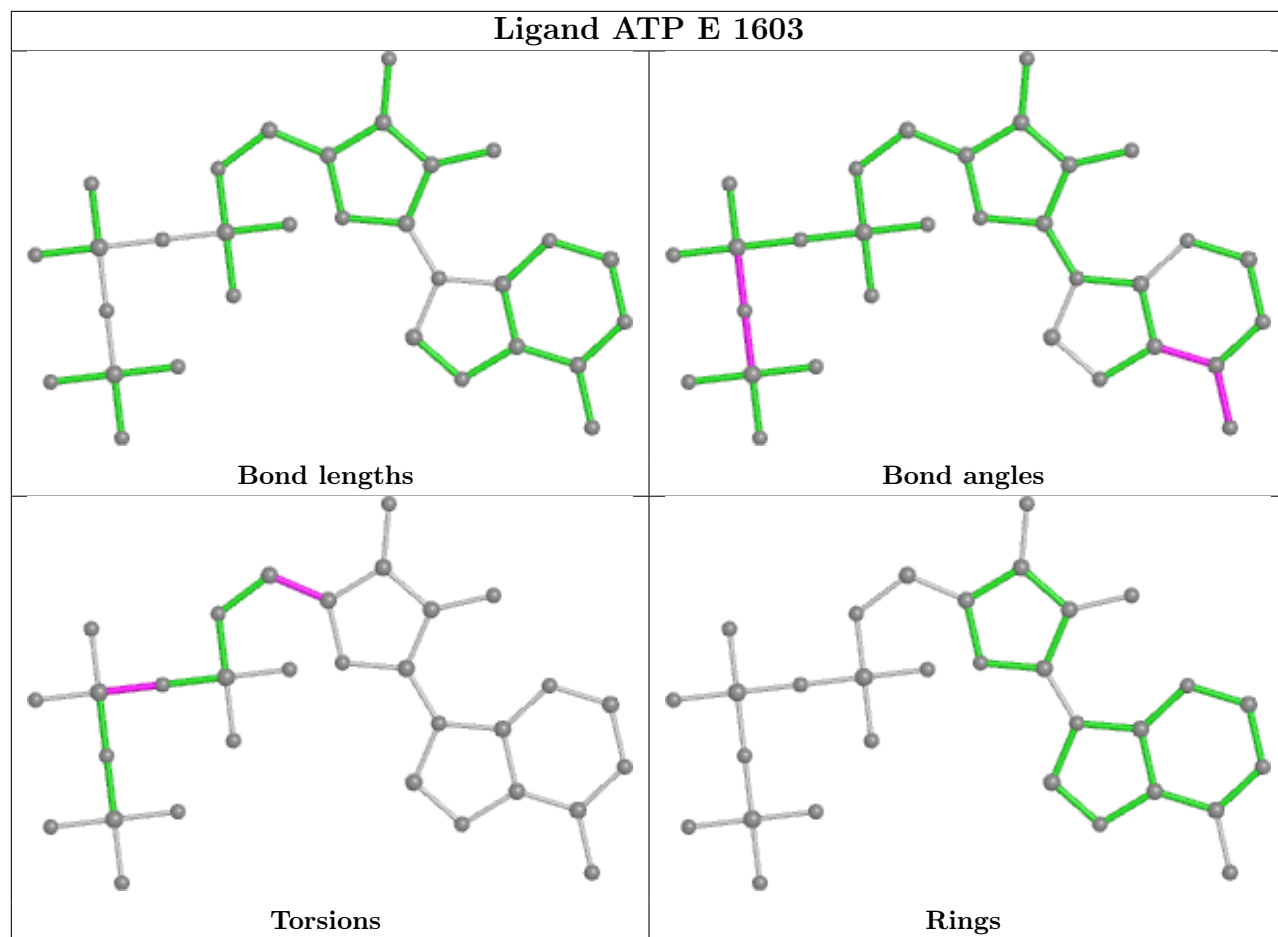


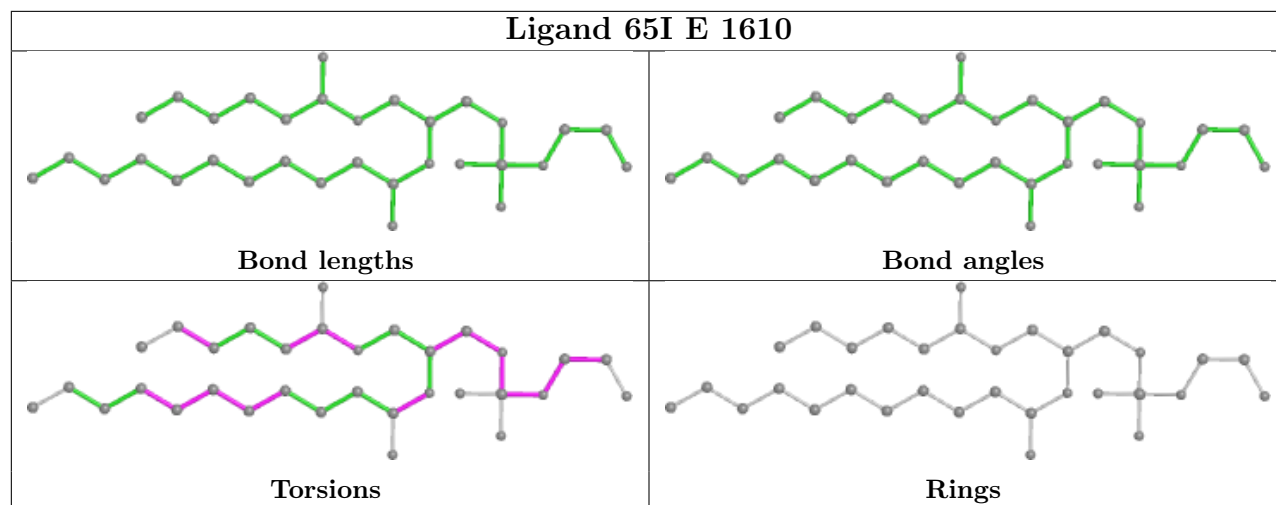












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

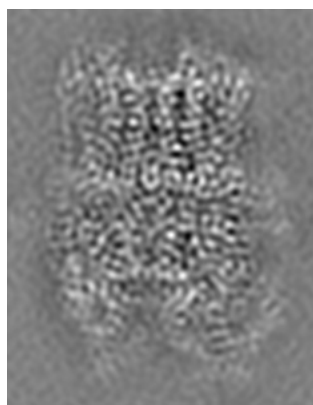
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26193. These allow visual inspection of the internal detail of the map and identification of artifacts.

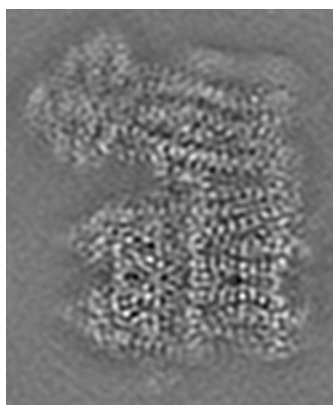
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

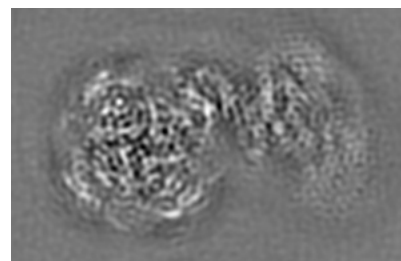
6.1.1 Primary map



X



Y

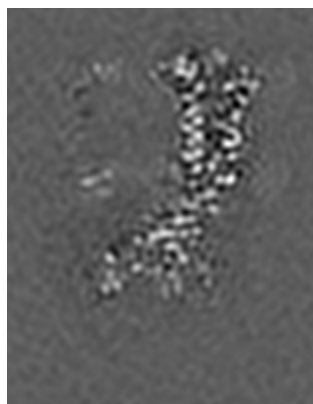


Z

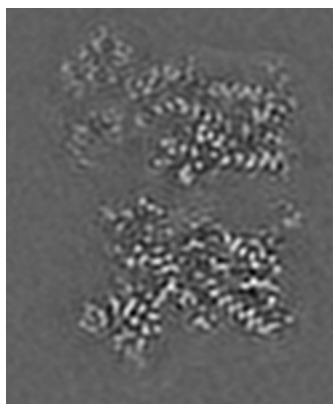
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

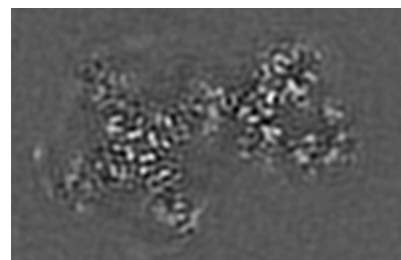
6.2.1 Primary map



X Index: 84



Y Index: 54

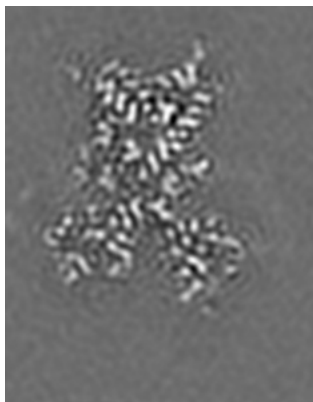


Z Index: 70

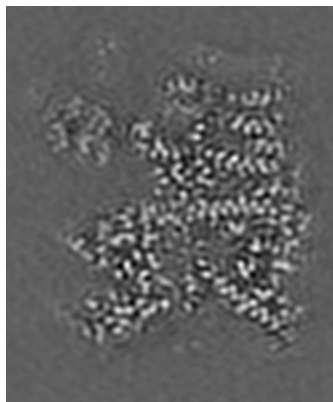
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

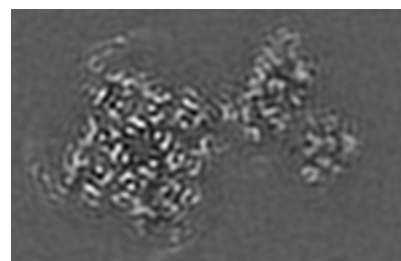
6.3.1 Primary map



X Index: 59



Y Index: 65

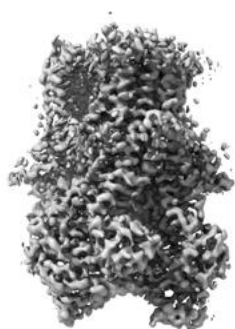


Z Index: 63

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

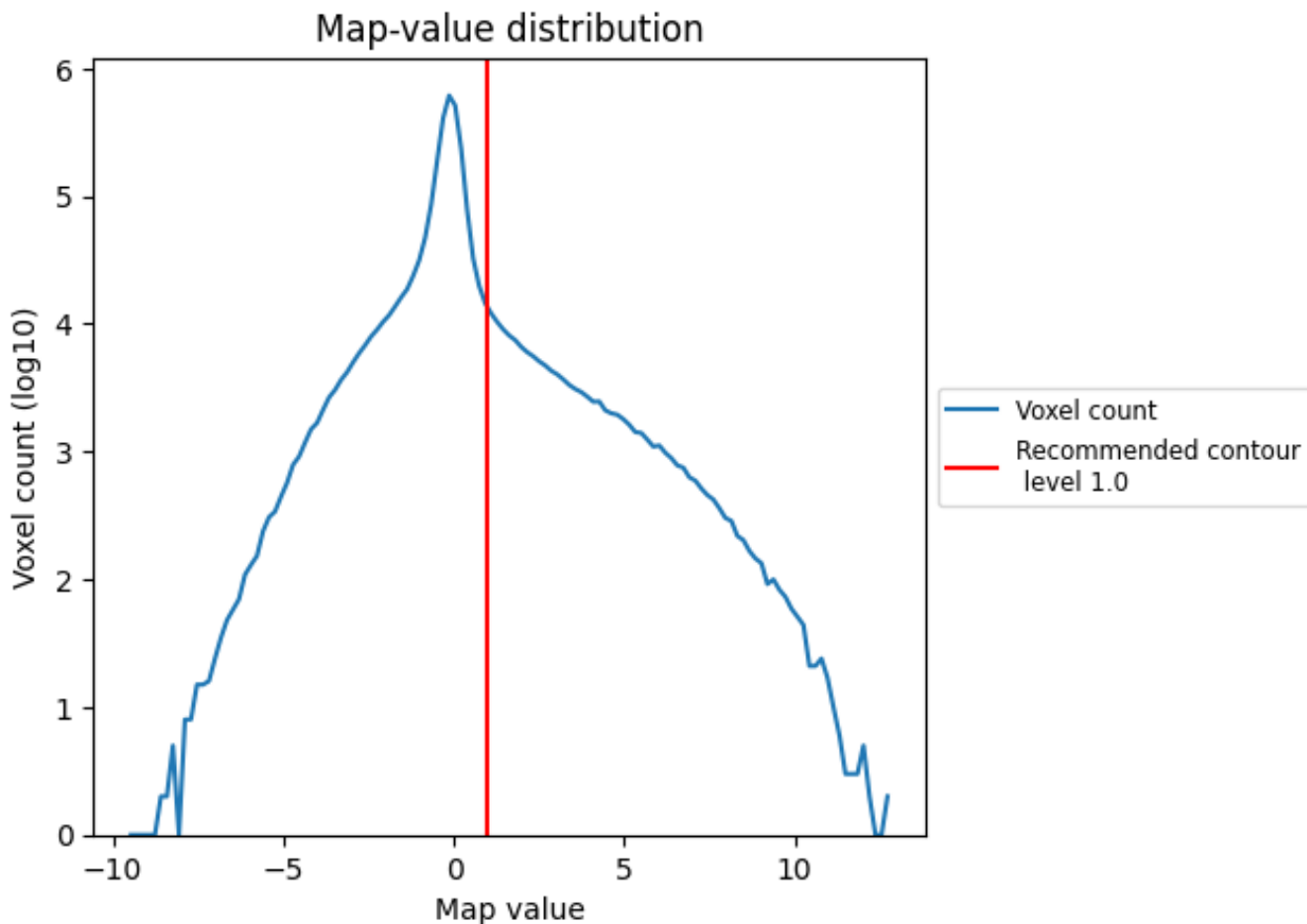
6.5 Mask visualisation

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

7 Map analysis [i](#)

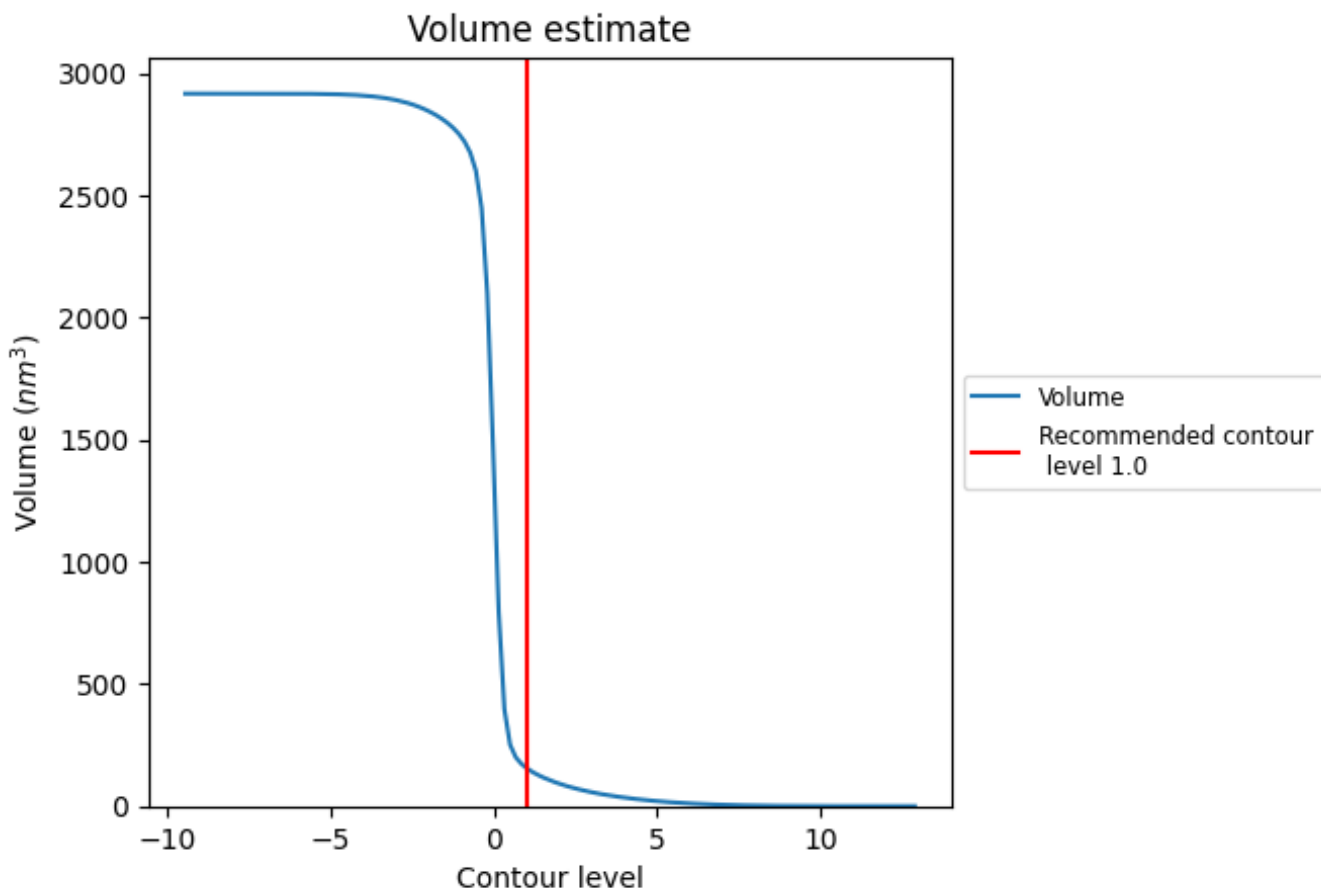
This section contains the results of statistical analysis of the map.

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 156 nm^3 ; this corresponds to an approximate mass of 141 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.

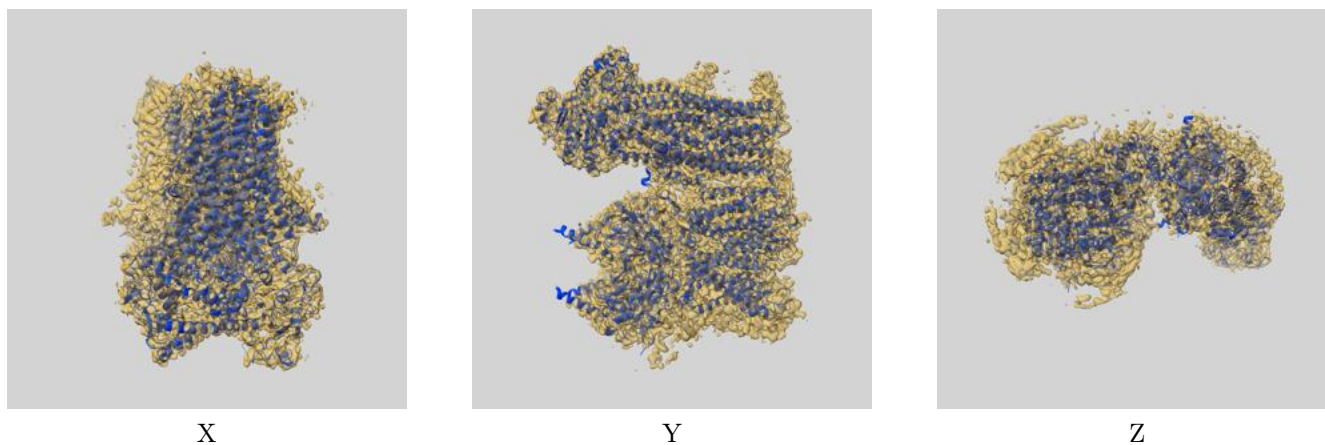
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

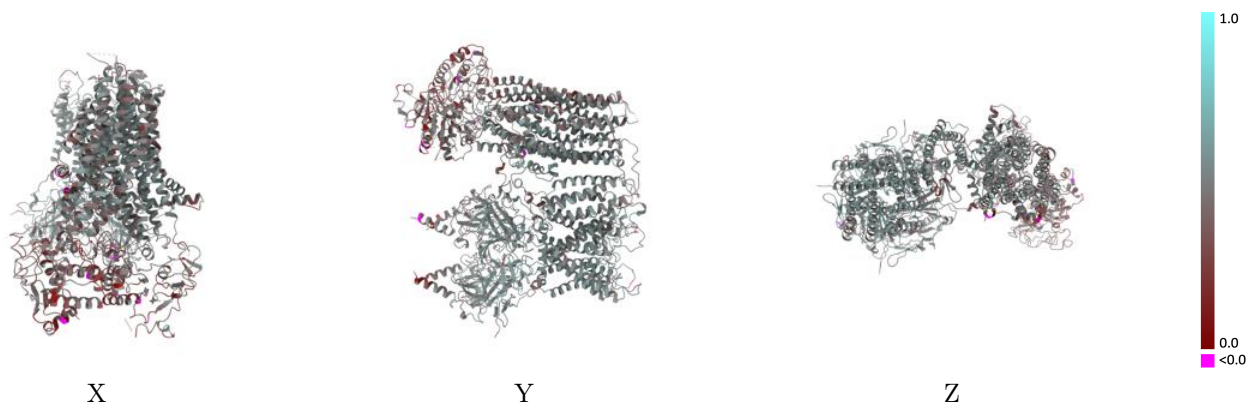
This section contains information regarding the fit between EMDB map EMD-26193 and PDB model 7TYS. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



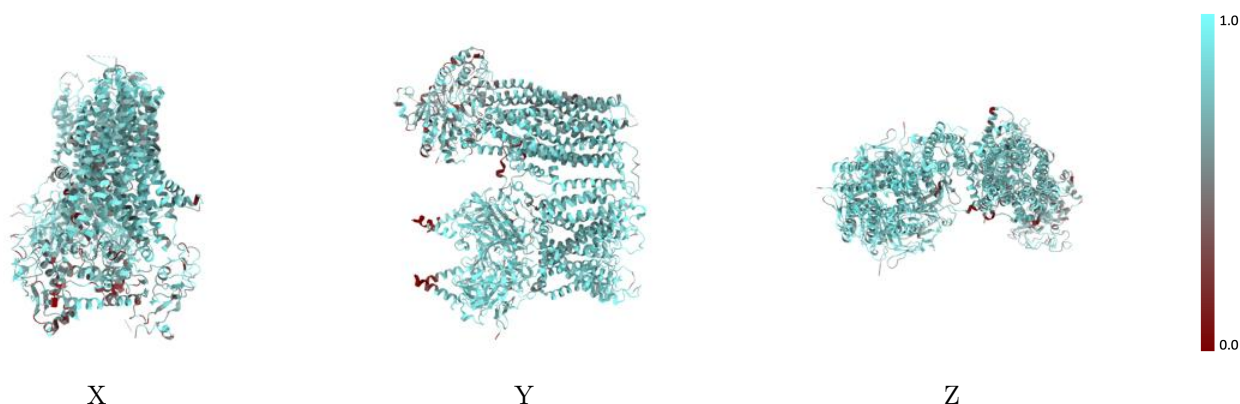
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



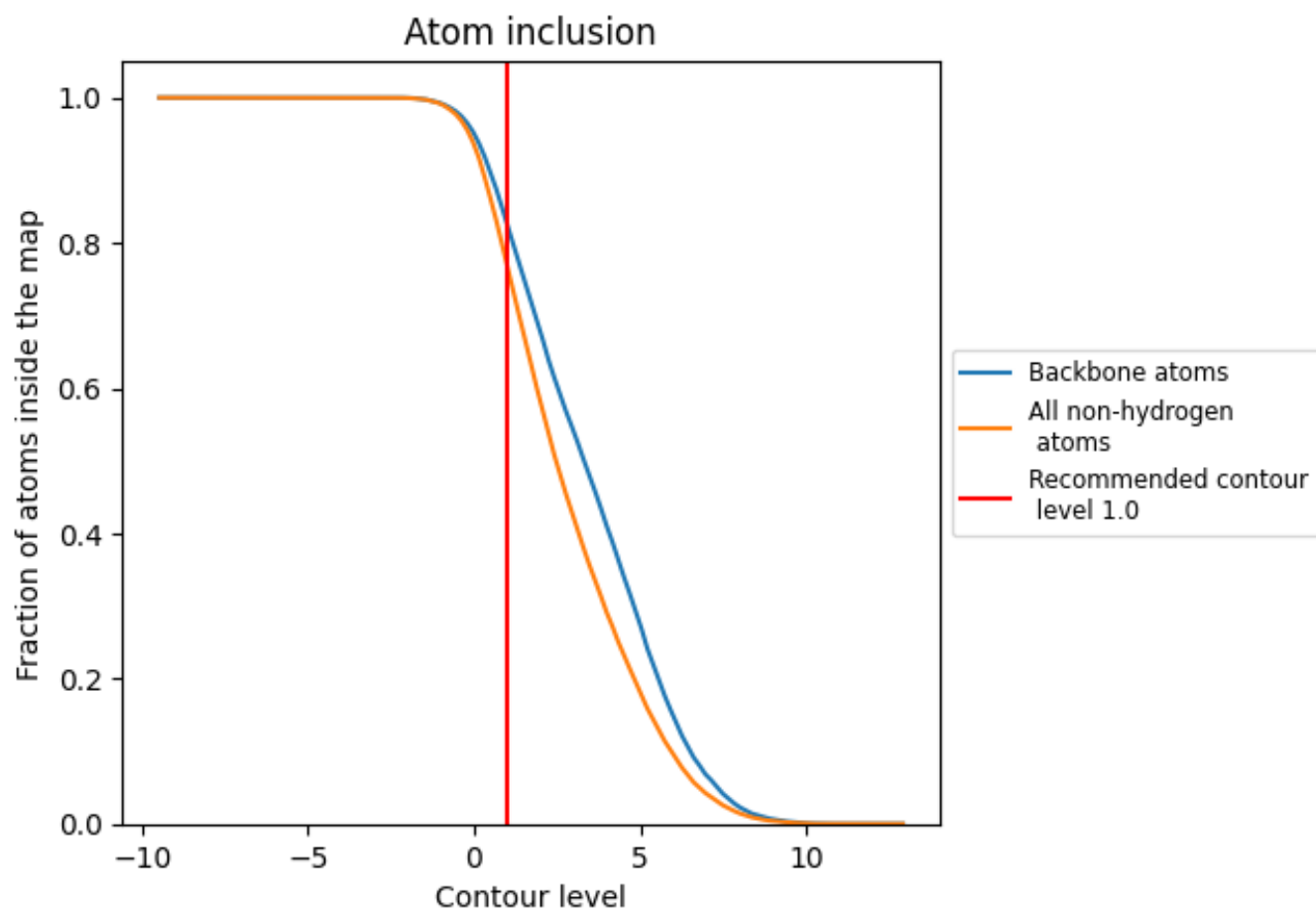
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).















9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7676	 0.4780
A	 0.7830	 0.5010
B	 0.8115	 0.5070
C	 0.8088	 0.5050
D	 0.8131	 0.5090
E	 0.7318	 0.4510
F	 0.3214	 0.2940

