



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 7MJP / pdb_00007mjp
EMDB ID : EMD-23881
Title : Vascular KATP channel: Kir6.1 SUR2B propeller-like conformation 2
Authors : Sung, M.W.; Shyng, S.L.
Deposited on : 2021-04-20
Resolution : 4.20 Å(reported)
Based on initial model : 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:

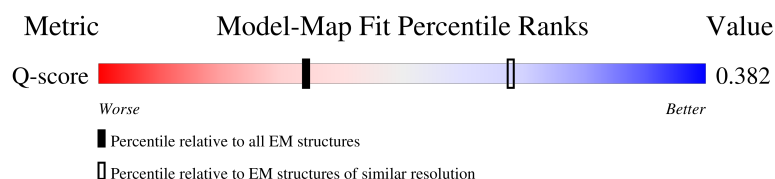
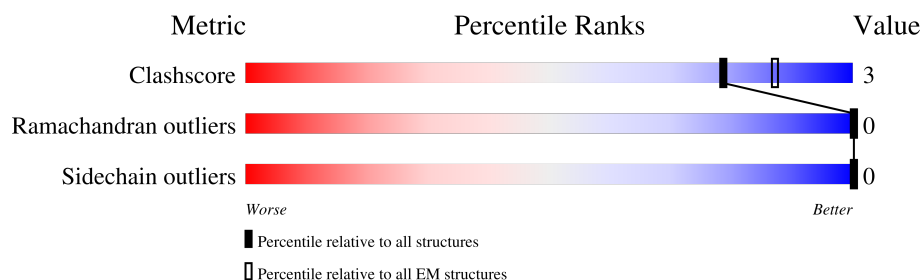
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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	5410 (3.70 - 4.70)

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	424	8% 83% 14%
1	B	424	5% 76% 20%
1	C	424	6% 78% 20%
1	D	424	5% 79% 20%

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Mol	Chain	Length	Quality of chain
2	E	1545	11% 88% 5% 7%
3	N	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14163 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 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	366	Total	C	N	O	0	0
			1812	1080	366	366		
1	B	338	Total	C	N	O	0	0
			1674	998	338	338		
1	C	339	Total	C	N	O	0	0
			1677	999	339	339		
1	D	339	Total	C	N	O	0	0
			1677	999	339	339		

- Molecule 2 is a protein called Isoform SUR2B of ATP-binding cassette sub-family C member 9.

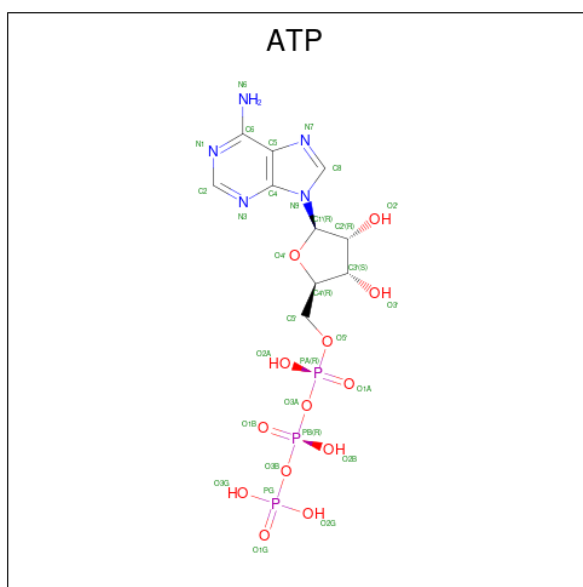
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	1436	Total	C	N	O	0	0
			7107	4233	1437	1437		

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



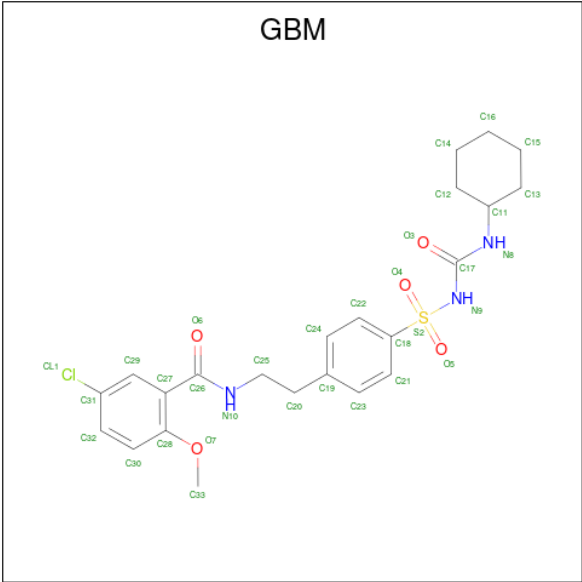
Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

- Molecule 5 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxy benzamide (CCD ID: GBM) (formula: $C_{23}H_{28}ClN_3O_5S$) (labeled as "Ligand of Interest" by depositor).

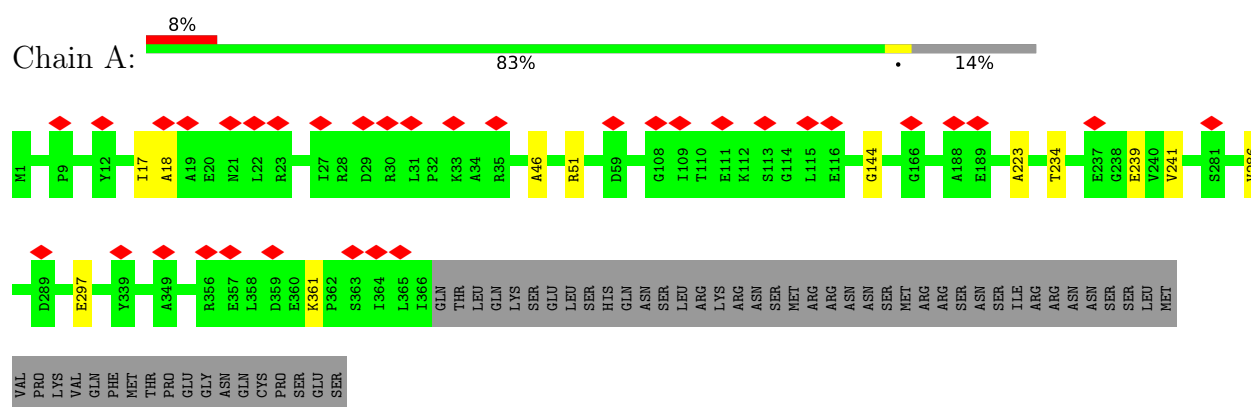


Mol	Chain	Residues	Atoms						AltConf
5	E	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	

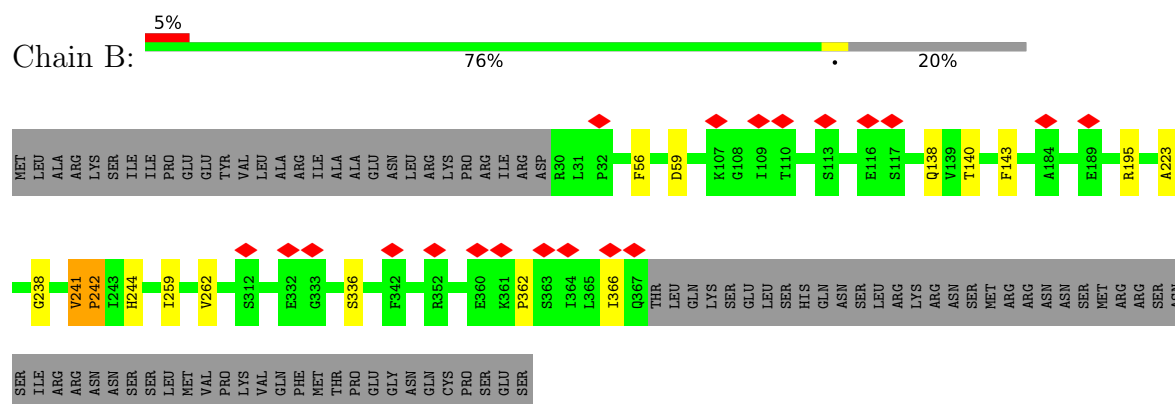
3 Residue-property plots

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

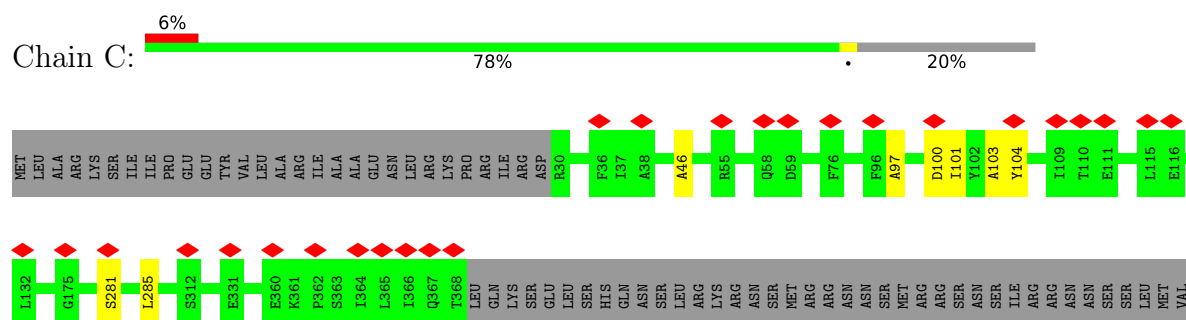
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



PRO
LYS
VAL
GLN
ARG
PHE
MET
THR
PRO
GLU
GLY
ASN
GLN
CYS
PRO
SER
GLU
SER

- Molecule 1: ATP-sensitive inward rectifier potassium channel 8

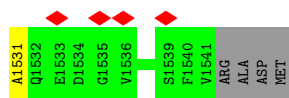
Chain D:  5% 79% 20%

MET LEU ALA ARG LYS SER ILE ILE PRO GLU GLY ASN GLN CYS PRO SER GLU SER
R195 K217 H322 S336 S363 I364 I365 I366 Q367 T368 LEU GLN LYS SER GLU LEU LYS PRO ARG ILE ASN ARG ASP R30 L31 A38 Q53 G54 R55 F61 C82 E106 K107 G108 I109 T110 S113 G114 S117 Q138 V139 T140 G166 A188
R195 K217 H322 S336 S363 I364 I365 I366 Q367 T368 LEU GLN LYS SER GLU LEU LYS PRO ARG ILE ASN ARG ASP R30 L31 A38 Q53 G54 R55 F61 C82 E106 K107 G108 I109 T110 S113 G114 S117 Q138 V139 T140 G166 A188
THR PRO GLY GLN CYS SER GLU SER

- Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

Chain E:  11% 88% 5% 7%

M1 G50 S51 Q52 S53 S54 K55 V56 Q57 I58 L139 Y140 A144 F145 G161 R166 A182 R191 E206 L216 I253 V258 A267 Y268 E269 E270 Q271 A276 D277 R281 R291 A292 F315 P328 K329 N330 N331 T332 T333 R334 T338 L339
S340 E343 F344 L345 E346 N347 Q437 G450 L496 L501 E516 H555 A558 N562 L563 P565 T580 P581 L582 L585 V588 G612 E613 D614 S615 T618 G618 GLY GLY THR LEU PRO PHE GLU SER CYS LYS HIS THR VAL GLN SER LYS
PRO ILE ASN ARG LYS PRO GLY GLY THR LEU PRO PHE GLU SER CYS LYS HIS THR VAL GLN SER LYS
E664 K664 P665 V666 R669 A672 L681 A682 S695 P692 L696 T697 M698 L699 V700 G701 C705 G706 K707 S708 S709 A713 V725 N726 N729
V730 W731 F732 SER GLU PRO SER PHE GLU ALA THR R741 S742 R743 S744 R745 Y746 T761 G805 S809 Q812 C817 F849 G850 D857 D858 V862 V863 L864 W877 L878 L879 R882 S885 E889 K893 T897 K898 D899 T903 W906 K907 H910
ASN ARG GLN ASP LYS LEU GLU MET ASP ALA ASP GLN THR THR LEU LEU GLU ARG ARG THR LYS ARG ALA LYS ALA MET TYR SER ARG GLU GLU ASP ASP ASP ASP M963 R968 L969 P974 W975 K976
V1010 T1015 S1016 E1017 S1019 I1020 N1021 D1022 P1023 G1024 K1025 Y1031 G1034 A1041 M1067 R1078 F1079 T1082 T1083 M1090 I1133 N1240 L1243 E1285 Q1297 V1298 V1302 P1303 Q1304 E1307 H1311 D1312 L1313 C1314 V1315 R1316 Y1317 N1318 N1319 N1320 P1323
K1326 H1327 V1328 K1337 I1340 G1342 R1343 T1344 G1345 S1346 G1347 S1352 F1356 F1362 K1375 L1376 P1377 T1380 R1384 L1385 S1386 Q1390 L1394 G1397 S1398 C1409 T1410 D1411 D1412 R1413 L1414 W1415 E1416 A1417 A1421 K1424 N1425 W1426 V1427 K1428 S1429 E1527 S1528
D1435 A1436 H1437 T1437 G1441 S1446 Q1449 Q1450 Q1451 L1452 F1453 C1454 L1455 A1458 F1459 V1460 L1466 D1469 E1470 A1473 M1477 N1481 V1486 V1487 M1488 T1489 A1490 F1491 A1492 D1493 T1499 A1500 H1501 T1505 A1509 D1510 L1511 V1512 V1513 V1514 I1520 T1525 P1526 E1527 S1528



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

Chain N:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70830	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	16.729	Depositor
Minimum map value	-13.303	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	134.32779, 180.77759, 164.4574	wwPDB
Map dimensions	107, 144, 131	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2554, 1.2554, 1.2554	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: NAG, ATP, GBM

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	0.35	0/1811	0.76	3/2523 (0.1%)
1	B	0.44	1/1674 (0.1%)	0.74	5/2332 (0.2%)
1	C	0.39	1/1676 (0.1%)	0.67	2/2334 (0.1%)
1	D	0.39	0/1676	0.62	1/2334 (0.0%)
2	E	0.41	0/7104	0.73	30/9891 (0.3%)
All	All	0.40	2/13941 (0.0%)	0.71	41/19414 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	ILE	CA-C	-6.36	1.44	1.52
1	B	262	VAL	C-N	-5.26	1.23	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	VAL	N-CA-C	-11.67	96.94	107.56
1	C	101	ILE	N-CA-C	-11.37	99.03	110.62
1	B	241	VAL	CA-C-N	11.36	134.03	119.84
1	B	241	VAL	C-N-CA	11.36	134.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	582	LEU	N-CA-C	9.50	121.23	111.07
2	E	338	THR	N-CA-C	9.06	120.76	111.07
1	D	217	LYS	N-CA-C	8.75	120.90	111.36
2	E	1525	THR	CA-C-N	8.63	128.25	118.85
2	E	1525	THR	C-N-CA	8.63	128.25	118.85
2	E	330	ASN	N-CA-C	8.53	120.36	111.14
2	E	555	HIS	N-CA-C	8.48	120.30	111.14
2	E	347	ASN	N-CA-C	-8.47	96.95	109.15
2	E	331	ASN	N-CA-C	8.29	120.70	108.60
2	E	968	ARG	N-CA-C	7.58	122.42	112.72
2	E	332	THR	N-CA-C	7.33	121.63	111.74
2	E	1531	ALA	N-CA-C	7.16	120.48	111.24
2	E	706	GLY	N-CA-C	7.08	129.96	113.18
2	E	1527	GLU	N-CA-C	6.78	121.41	112.13
1	A	286	VAL	N-CA-C	-6.77	107.28	113.71
1	C	97	ALA	N-CA-C	6.51	118.38	111.28
2	E	580	THR	CA-C-N	-6.25	112.41	119.28
2	E	580	THR	C-N-CA	-6.25	112.41	119.28
1	B	244	HIS	N-CA-C	5.90	118.62	110.35
2	E	588	VAL	CB-CA-C	-5.85	104.25	112.14
1	B	238	GLY	N-CA-C	5.73	123.25	115.00
2	E	969	LEU	N-CA-C	5.64	117.51	111.36
2	E	258	VAL	N-CA-C	5.63	116.36	110.62
2	E	253	ILE	N-CA-C	5.61	117.01	110.62
1	B	242	PRO	N-CA-C	5.49	123.77	112.47
2	E	1397	GLY	N-CA-C	5.38	118.07	111.45
2	E	1390	GLN	CB-CA-C	-5.35	110.39	116.54
2	E	558	ALA	N-CA-C	5.31	119.74	112.68
2	E	253	ILE	CB-CA-C	-5.30	105.09	112.04
2	E	564	LYS	CA-C-N	5.18	124.80	119.05
2	E	564	LYS	C-N-CA	5.18	124.80	119.05
2	E	705	CYS	O-C-N	5.15	129.73	123.14
2	E	580	THR	O-C-N	5.12	125.04	120.48
2	E	705	CYS	CA-C-N	5.07	131.34	121.41
2	E	705	CYS	C-N-CA	5.07	131.34	121.41
2	E	345	LEU	N-CA-C	5.02	117.49	111.71
1	A	361	LYS	N-CA-C	-5.02	98.62	109.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	104	TYR	Mainchain
2	E	581	PRO	Mainchain

5.2 Too-close contacts ⓘ

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	1812	0	827	6	0
1	B	1674	0	764	8	0
1	C	1677	0	760	4	0
1	D	1677	0	760	4	0
2	E	7107	0	3231	37	0
3	N	28	0	25	0	0
4	A	31	0	12	0	0
4	B	62	0	24	2	0
4	D	31	0	12	0	0
4	E	31	0	12	1	0
5	E	33	0	28	1	0
All	All	14163	0	6455	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (57) 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:565:PRO:HA	2:E:1015:THR:CB	1.98	0.94
2:E:565:PRO:HB3	2:E:1015:THR:C	1.93	0.93
2:E:1486:VAL:HA	2:E:1490:ALA:HB3	1.53	0.87
2:E:562:ASN:HA	2:E:1025:LYS:CB	2.09	0.82
2:E:1386:SER:O	2:E:1466:LEU:CB	2.29	0.80
2:E:1397:GLY:O	2:E:1437:THR:O	1.99	0.80
1:B:195:ARG:N	4:B:501:ATP:O2A	2.23	0.70
1:C:100:ASP:O	1:C:103:ALA:N	2.27	0.68
2:E:565:PRO:HB3	2:E:1015:THR:O	1.95	0.66
1:A:46:ALA:HB3	1:B:336:SER:HA	1.77	0.65
1:D:106:GLU:O	1:D:110:THR:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:709:SER:N	4:E:1601:ATP:O1A	2.31	0.62
1:B:362:PRO:O	1:B:366:ILE:N	2.33	0.61
2:E:1341:CYS:CB	2:E:1513:ILE:O	2.49	0.60
1:C:281:SER:O	1:C:285:LEU:N	2.35	0.59
2:E:563:LEU:CB	2:E:1018:TYR:CB	2.82	0.58
2:E:696:LEU:HA	2:E:862:VAL:O	2.05	0.56
1:C:100:ASP:O	1:C:103:ALA:HB3	2.06	0.55
2:E:562:ASN:CA	2:E:1025:LYS:CB	2.84	0.54
2:E:562:ASN:CB	2:E:1025:LYS:CB	2.86	0.53
1:D:138:GLN:C	1:D:140:THR:H	2.16	0.52
2:E:1386:SER:CB	2:E:1458:ALA:HB2	2.41	0.51
1:A:223:ALA:HA	1:A:297:GLU:O	2.11	0.50
1:A:144:GLY:HA3	1:B:143:PHE:O	2.12	0.50
2:E:744:SER:O	2:E:746:TYR:N	2.44	0.50
1:A:51:ARG:N	4:B:501:ATP:N1	2.60	0.50
2:E:565:PRO:HB3	2:E:1016:SER:N	2.27	0.50
1:B:223:ALA:HB3	1:B:259:ILE:O	2.13	0.49
2:E:1398:SER:HA	2:E:1437:THR:H	1.78	0.49
2:E:1328:VAL:CB	2:E:1520:ILE:CB	2.90	0.49
1:B:241:VAL:HA	1:B:242:PRO:HD2	1.61	0.47
2:E:565:PRO:CA	2:E:1015:THR:CB	2.84	0.46
2:E:1446:SER:HA	2:E:1449:GLN:CB	2.46	0.45
2:E:1425:ASN:C	2:E:1427:VAL:H	2.25	0.45
5:E:1602:GBM:O7	5:E:1602:GBM:N10	2.49	0.45
2:E:612:GLY:C	2:E:614:ASP:H	2.24	0.45
2:E:878:ILE:O	2:E:889:GLU:HA	2.17	0.45
1:B:56:PHE:O	1:B:59:ASP:N	2.36	0.44
2:E:666:VAL:HA	2:E:692:PRO:HA	1.99	0.44
2:E:340:SER:O	2:E:343:GLU:N	2.51	0.44
2:E:1486:VAL:O	2:E:1491:PHE:N	2.51	0.44
2:E:565:PRO:CB	2:E:1015:THR:O	2.65	0.43
2:E:698:MET:HA	2:E:864:LEU:O	2.17	0.43
2:E:269:GLU:C	2:E:271:GLN:N	2.75	0.43
2:E:267:ALA:CB	2:E:292:ALA:HB2	2.49	0.43
2:E:1398:SER:HA	2:E:1437:THR:N	2.34	0.43
1:A:234:THR:HA	1:A:239:GLU:O	2.20	0.42
1:C:46:ALA:HB3	1:D:336:SER:HA	2.01	0.42
2:E:139:LEU:O	2:E:140:TYR:C	2.62	0.42
2:E:974:PRO:C	2:E:976:LYS:H	2.28	0.42
1:B:138:GLN:C	1:B:140:THR:H	2.27	0.41
1:D:138:GLN:C	1:D:140:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:ALA:O	2:E:145:PHE:C	2.62	0.41
2:E:565:PRO:HB3	2:E:1016:SER:HA	2.02	0.41
2:E:697:THR:HA	2:E:877:TRP:O	2.20	0.41
2:E:699:ILE:HA	2:E:879:ILE:O	2.21	0.40
1:A:17:ILE:O	1:A:18:ALA:C	2.63	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	364/424 (86%)	314 (86%)	50 (14%)	0	100	100
1	B	336/424 (79%)	306 (91%)	30 (9%)	0	100	100
1	C	337/424 (80%)	311 (92%)	26 (8%)	0	100	100
1	D	337/424 (80%)	306 (91%)	31 (9%)	0	100	100
2	E	1426/1545 (92%)	1308 (92%)	118 (8%)	0	100	100
All	All	2800/3241 (86%)	2545 (91%)	255 (9%)	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	B	1/376 (0%)	1 (100%)	0	100	100
2	E	3/1348 (0%)	3 (100%)	0	100	100
All	All	4/1724 (0%)	4 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	N	1	3	14,14,15	2.92	8 (57%)	17,19,21	2.00	6 (35%)
3	NAG	N	2	3	14,14,15	2.78	9 (64%)	17,19,21	1.25	2 (11%)

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	N	1	3	-	5/6/23/26	0/1/1/1

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O5-C5	5.88	1.54	1.43
3	N	2	NAG	O5-C5	5.44	1.54	1.43
3	N	1	NAG	C2-N2	4.62	1.53	1.46
3	N	2	NAG	C2-N2	4.03	1.52	1.46
3	N	1	NAG	C7-N2	3.88	1.46	1.34
3	N	2	NAG	C7-N2	3.78	1.46	1.34
3	N	2	NAG	C6-C5	-3.24	1.40	1.51
3	N	2	NAG	C3-C2	-3.11	1.46	1.52
3	N	1	NAG	C3-C2	-3.07	1.46	1.52
3	N	1	NAG	C6-C5	-3.05	1.41	1.51
3	N	1	NAG	O5-C1	2.75	1.48	1.43
3	N	2	NAG	O5-C1	2.67	1.48	1.43
3	N	1	NAG	C8-C7	2.22	1.55	1.50
3	N	2	NAG	C8-C7	2.13	1.55	1.50
3	N	2	NAG	C1-C2	-2.02	1.49	1.52
3	N	1	NAG	C4-C5	2.01	1.57	1.53
3	N	2	NAG	O3-C3	2.01	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C8-C7-N2	4.89	124.22	116.12
3	N	1	NAG	C2-N2-C7	3.58	127.70	122.90
3	N	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	N	2	NAG	C2-N2-C7	-2.52	119.53	122.90
3	N	1	NAG	O7-C7-N2	-2.50	117.56	121.98
3	N	2	NAG	C8-C7-N2	2.41	120.12	116.12
3	N	1	NAG	O5-C5-C6	2.32	112.19	107.66
3	N	1	NAG	O7-C7-C8	-2.16	118.22	122.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2

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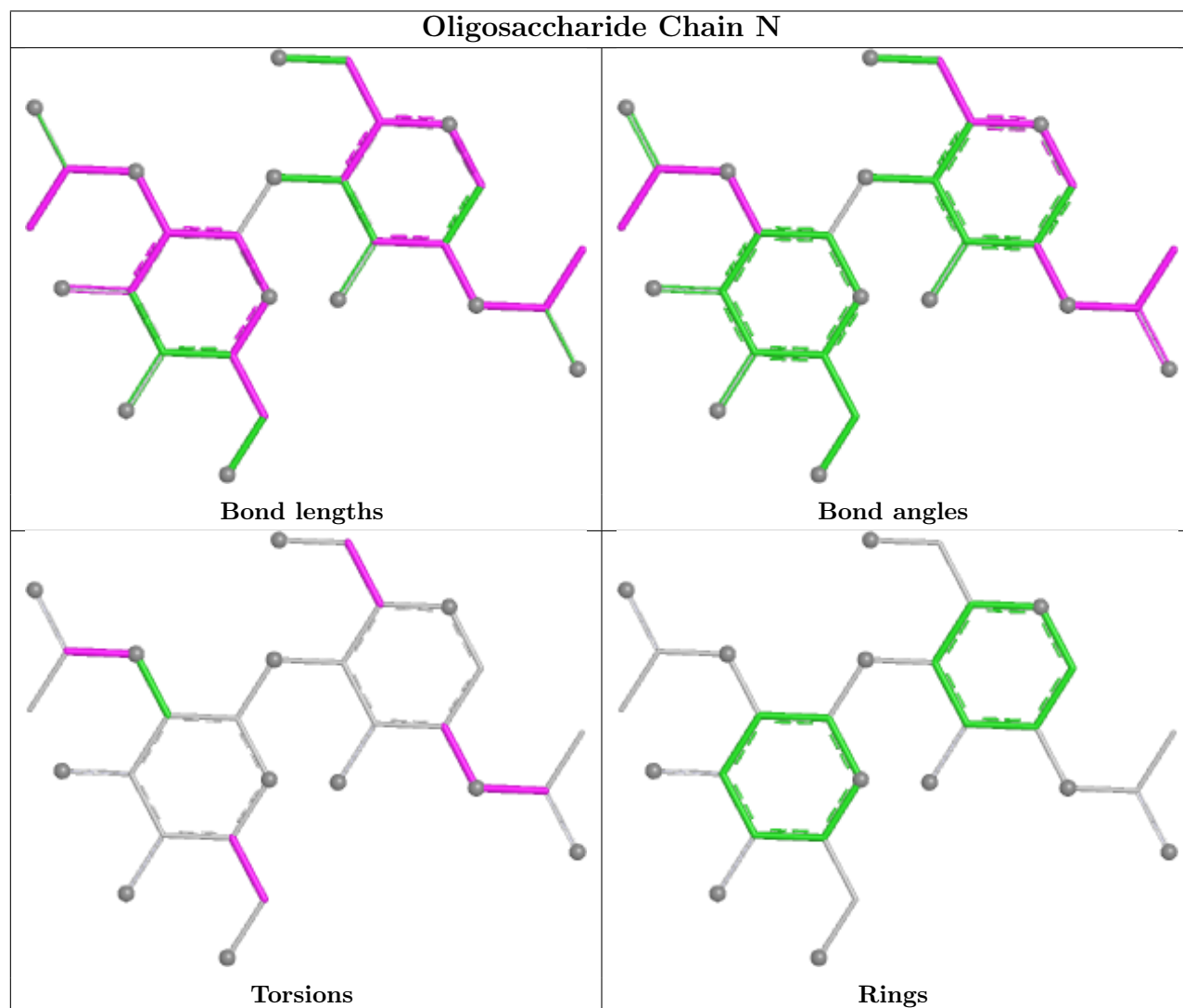
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Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	N	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C1-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7

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

6 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
4	ATP	D	501	-	32,33,33	1.31	5 (15%)	48,52,52	1.72	9 (18%)
4	ATP	B	501	-	32,33,33	1.42	5 (15%)	48,52,52	1.71	9 (18%)
4	ATP	B	502	-	32,33,33	1.36	4 (12%)	48,52,52	1.77	8 (16%)
5	GBM	E	1602	-	35,35,35	4.69	9 (25%)	48,48,48	1.93	7 (14%)
4	ATP	E	1601	-	32,33,33	1.34	5 (15%)	48,52,52	1.71	8 (16%)
4	ATP	A	501	-	32,33,33	1.46	7 (21%)	48,52,52	1.76	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	501	-	-	3/22/38/38	0/3/3/3
4	ATP	B	501	-	-	5/22/38/38	0/3/3/3
4	ATP	B	502	-	-	0/22/38/38	0/3/3/3
5	GBM	E	1602	-	-	9/27/35/35	0/3/3/3
4	ATP	E	1601	-	-	5/22/38/38	0/3/3/3
4	ATP	A	501	-	-	2/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1602	GBM	O4-S2	18.52	1.65	1.43
5	E	1602	GBM	O5-S2	18.32	1.64	1.43
5	E	1602	GBM	C26-N10	5.46	1.45	1.33
4	A	501	ATP	C5-C4	4.57	1.47	1.39
4	B	501	ATP	C5-C4	4.53	1.47	1.39
4	E	1601	ATP	C5-C4	4.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	ATP	C5-C4	4.30	1.46	1.39
4	B	502	ATP	C5-C4	4.28	1.46	1.39
5	E	1602	GBM	C18-S2	3.47	1.81	1.76
5	E	1602	GBM	C17-N8	3.15	1.44	1.35
4	B	502	ATP	C5-N7	-2.83	1.33	1.39
5	E	1602	GBM	S2-N9	2.82	1.71	1.64
4	D	501	ATP	C5-N7	-2.73	1.34	1.39
4	A	501	ATP	C5-C6	2.64	1.48	1.41
4	D	501	ATP	C4-N9	-2.61	1.32	1.37
4	B	501	ATP	C5-N7	-2.60	1.34	1.39
4	B	501	ATP	C5-C6	2.55	1.48	1.41
5	E	1602	GBM	O3-C17	-2.52	1.18	1.23
4	E	1601	ATP	C5-C6	2.52	1.48	1.41
4	E	1601	ATP	C5-N7	-2.48	1.34	1.39
5	E	1602	GBM	C17-N9	2.43	1.44	1.39
4	A	501	ATP	PB-O3A	2.42	1.62	1.59
4	A	501	ATP	C5-N7	-2.38	1.34	1.39
4	B	501	ATP	C4-N9	-2.38	1.32	1.37
4	A	501	ATP	C8-N7	2.31	1.36	1.31
4	B	502	ATP	C4-N9	-2.27	1.33	1.37
4	B	501	ATP	C8-N7	2.26	1.36	1.31
4	A	501	ATP	PB-O3B	2.25	1.61	1.59
4	A	501	ATP	PA-O3A	2.21	1.61	1.59
4	D	501	ATP	C5-C6	2.19	1.47	1.41
4	E	1601	ATP	C8-N7	2.16	1.35	1.31
4	B	502	ATP	C5-C6	2.10	1.46	1.41
4	E	1601	ATP	C4-N9	-2.09	1.33	1.37
4	D	501	ATP	C8-N7	2.03	1.35	1.31
5	E	1602	GBM	O6-C26	-2.03	1.18	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1602	GBM	O5-S2-O4	-9.36	108.15	119.52
4	A	501	ATP	C5-C4-N3	-6.07	118.36	126.72
4	B	501	ATP	C5-C4-N3	-5.63	118.96	126.72
4	E	1601	ATP	C5-C4-N3	-5.56	119.06	126.72
4	B	502	ATP	C5-C4-N3	-5.52	119.12	126.72
4	D	501	ATP	C5-C4-N3	-5.35	119.34	126.72
4	B	502	ATP	N3-C4-N9	4.94	135.56	127.17
4	A	501	ATP	N3-C4-N9	4.58	134.96	127.17
4	E	1601	ATP	N3-C4-N9	4.41	134.67	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	ATP	N3-C4-N9	4.38	134.62	127.17
4	B	501	ATP	N3-C4-N9	4.27	134.43	127.17
5	E	1602	GBM	C33-O7-C28	-3.92	111.76	117.51
5	E	1602	GBM	C28-C27-C26	-3.81	119.36	126.24
4	A	501	ATP	C4-C5-N7	-3.75	106.30	110.58
4	A	501	ATP	C2-N3-C4	3.71	120.88	111.83
4	B	501	ATP	C2-N3-C4	3.55	120.49	111.83
4	E	1601	ATP	C2-N3-C4	3.54	120.49	111.83
4	B	502	ATP	C2-N3-C4	3.46	120.29	111.83
4	B	501	ATP	C4-C5-N7	-3.35	106.75	110.58
4	D	501	ATP	C2-N3-C4	3.31	119.91	111.83
4	B	502	ATP	N3-C2-N1	-3.25	123.66	128.58
4	E	1601	ATP	C4-C5-N7	-3.24	106.88	110.58
5	E	1602	GBM	C11-N8-C17	-3.23	115.97	122.92
4	E	1601	ATP	N3-C2-N1	-3.22	123.71	128.58
4	A	501	ATP	N3-C2-N1	-3.12	123.86	128.58
4	B	502	ATP	C4-N9-C8	3.11	109.00	105.74
4	B	501	ATP	N3-C2-N1	-2.95	124.11	128.58
4	D	501	ATP	C4-C5-N7	-2.95	107.21	110.58
4	D	501	ATP	N3-C2-N1	-2.93	124.15	128.58
4	D	501	ATP	C2'-C1'-N9	-2.86	106.20	113.30
4	D	501	ATP	C4-N9-C8	2.81	108.69	105.74
4	A	501	ATP	C5-N7-C8	2.64	107.60	103.45
4	E	1601	ATP	C4-N9-C8	2.53	108.40	105.74
4	B	501	ATP	C3'-C2'-C1'	2.46	106.12	101.46
5	E	1602	GBM	O7-C28-C30	-2.44	120.18	124.30
4	B	502	ATP	C4-C5-N7	-2.44	107.79	110.58
4	A	501	ATP	C4-N9-C8	2.36	108.22	105.74
4	D	501	ATP	C3'-C2'-C1'	2.33	105.86	101.46
4	E	1601	ATP	C5-N7-C8	2.32	107.10	103.45
4	B	501	ATP	C4-N9-C8	2.30	108.15	105.74
4	B	502	ATP	C3'-C2'-C1'	2.20	105.62	101.46
4	B	501	ATP	C5-N7-C8	2.17	106.86	103.45
4	A	501	ATP	C6-C5-N7	2.13	136.21	132.09
4	E	1601	ATP	C3'-C2'-C1'	2.13	105.49	101.46
4	B	502	ATP	C2'-C1'-N9	-2.11	108.06	113.30
5	E	1602	GBM	N9-C17-N8	2.10	121.94	115.06
4	D	501	ATP	C5-N7-C8	2.05	106.67	103.45
5	E	1602	GBM	C17-N9-S2	-2.04	117.91	123.55
4	B	501	ATP	C6-C5-N7	2.03	135.99	132.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	ATP	C5'-O5'-PA-O2A
4	D	501	ATP	C5'-O5'-PA-O1A
4	D	501	ATP	C5'-O5'-PA-O3A
4	E	1601	ATP	C5'-O5'-PA-O1A
4	E	1601	ATP	C5'-O5'-PA-O2A
4	E	1601	ATP	C5'-O5'-PA-O3A
5	E	1602	GBM	C30-C28-O7-C33
5	E	1602	GBM	C27-C28-O7-C33
5	E	1602	GBM	C22-C18-S2-O5
5	E	1602	GBM	C21-C18-S2-O5
5	E	1602	GBM	C17-N9-S2-O4
5	E	1602	GBM	C21-C18-S2-N9
5	E	1602	GBM	C22-C18-S2-N9
4	B	501	ATP	PB-O3A-PA-O1A
4	B	501	ATP	PA-O3A-PB-O2B
5	E	1602	GBM	C17-N9-S2-C18
5	E	1602	GBM	C17-N9-S2-O5
4	D	501	ATP	PA-O3A-PB-O1B
4	A	501	ATP	C3'-C4'-C5'-O5'
4	B	501	ATP	PA-O3A-PB-O1B
4	B	501	ATP	PB-O3A-PA-O2A
4	E	1601	ATP	PG-O3B-PB-O2B
4	A	501	ATP	O4'-C4'-C5'-O5'
4	E	1601	ATP	PG-O3B-PB-O1B

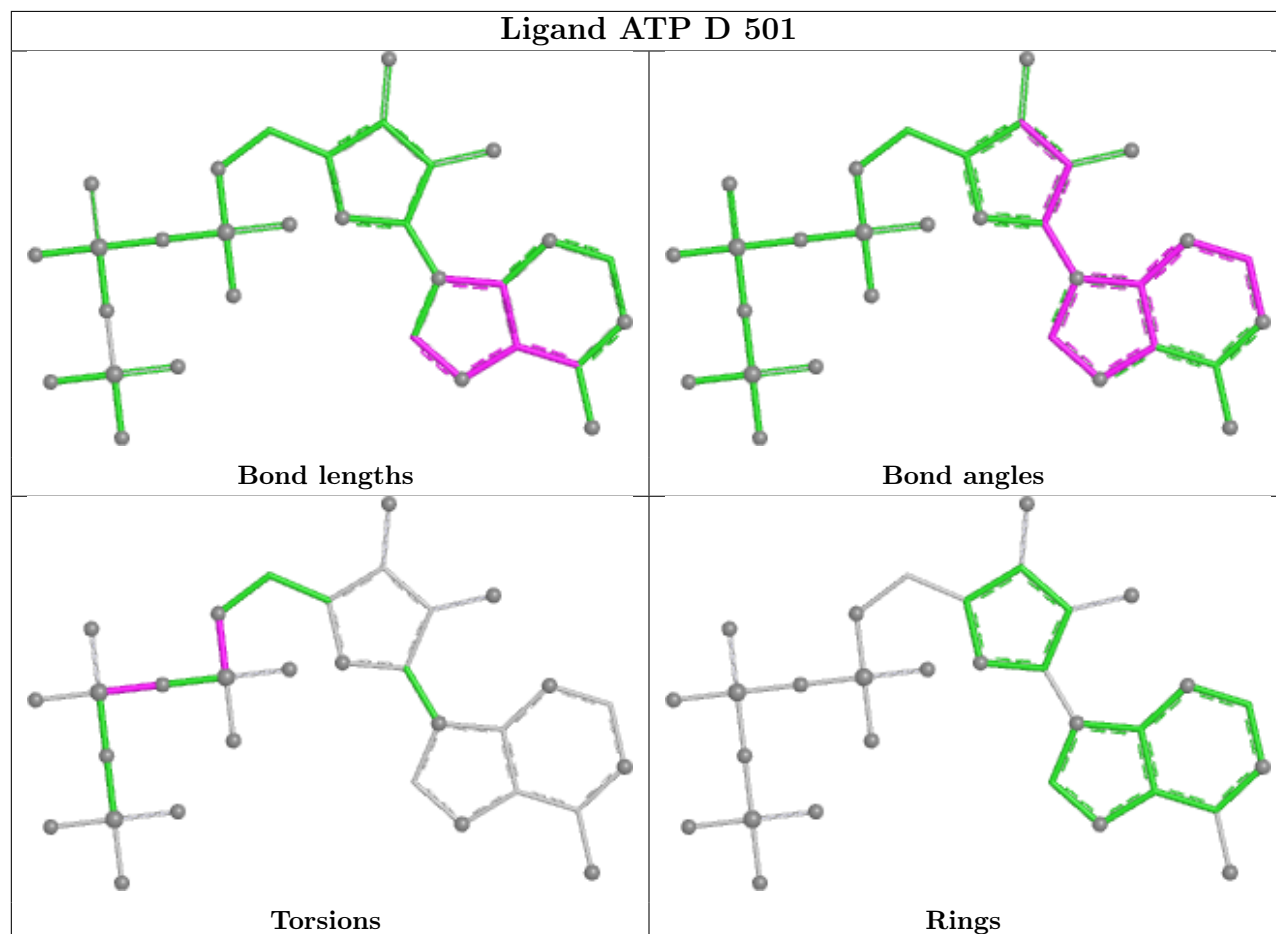
There are no ring outliers.

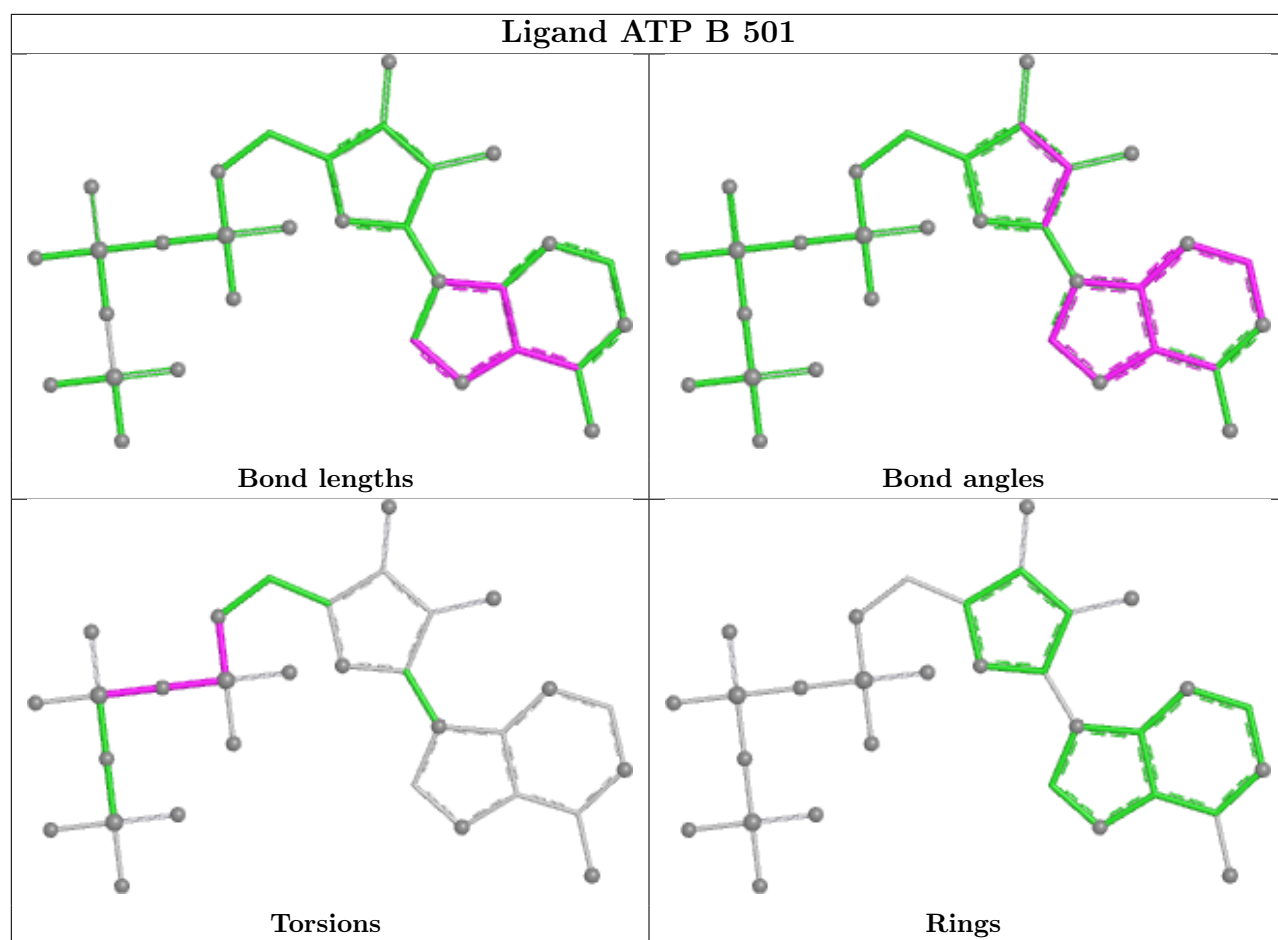
3 monomers are involved in 4 short contacts:

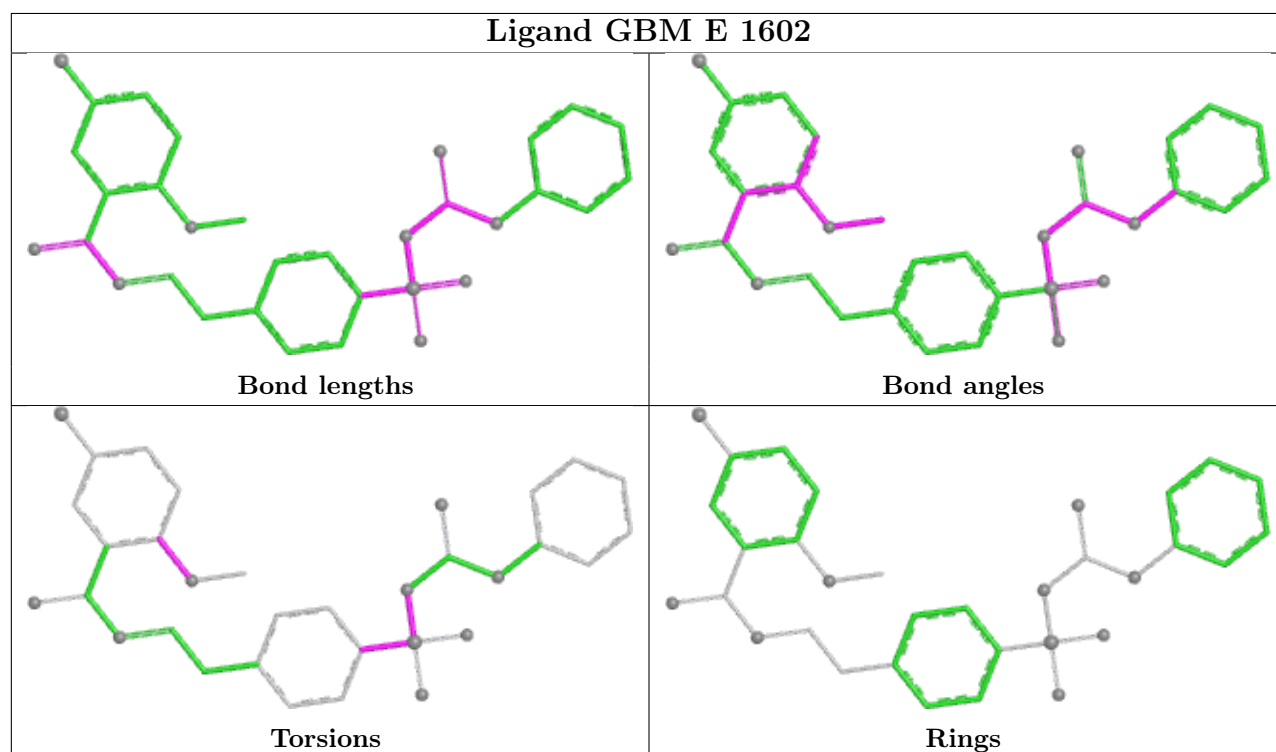
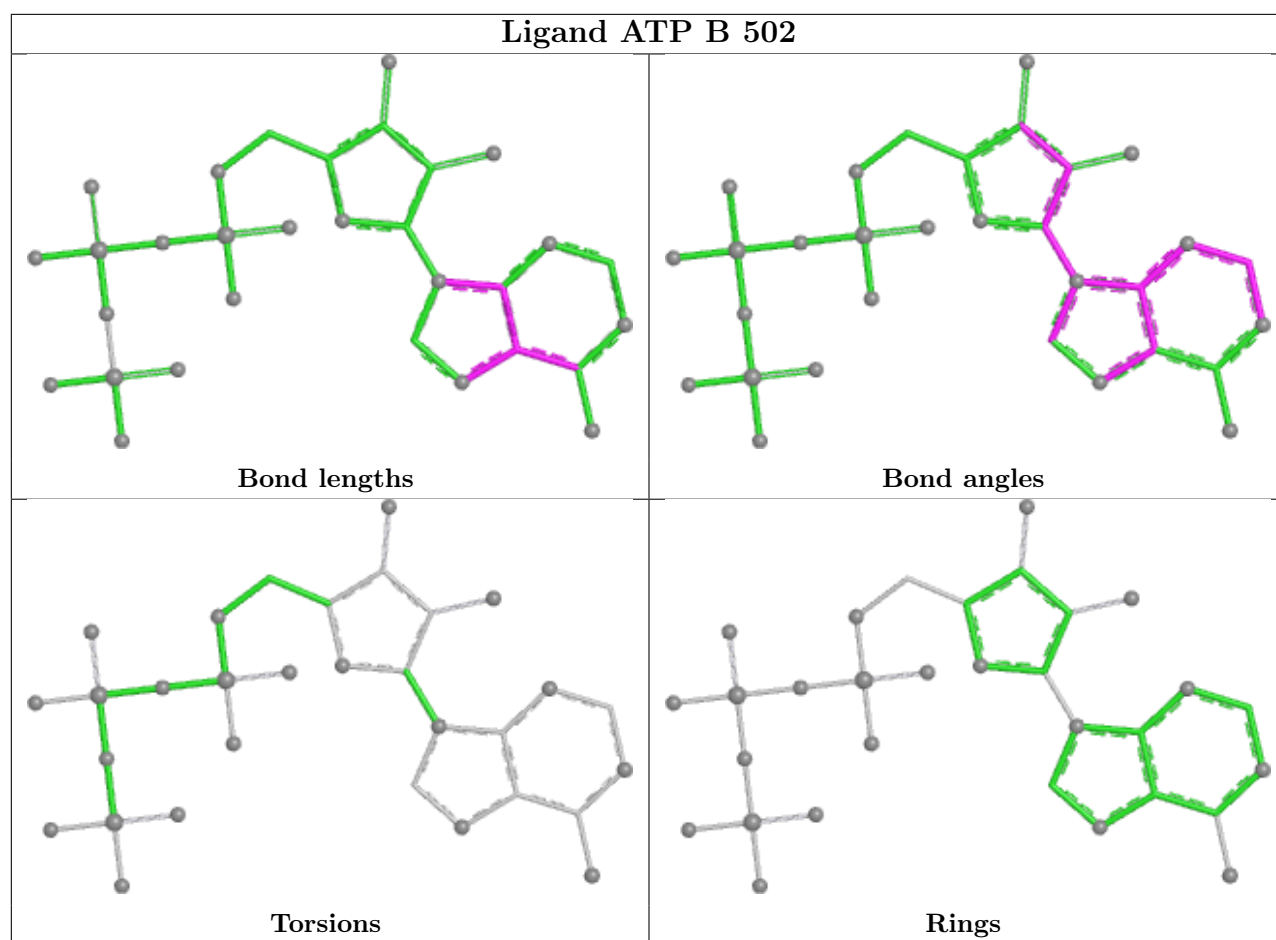
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	ATP	2	0
5	E	1602	GBM	1	0
4	E	1601	ATP	1	0

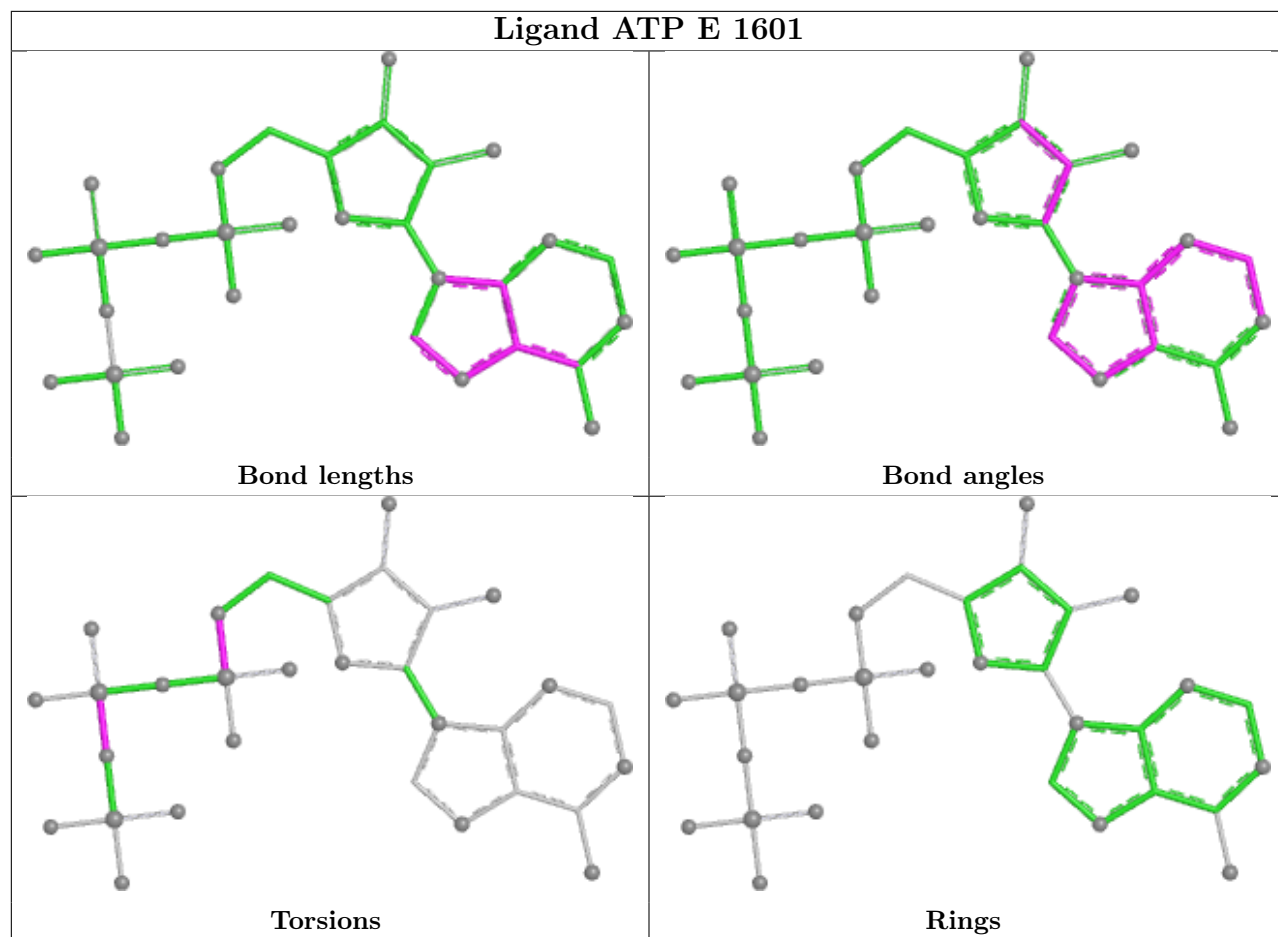
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

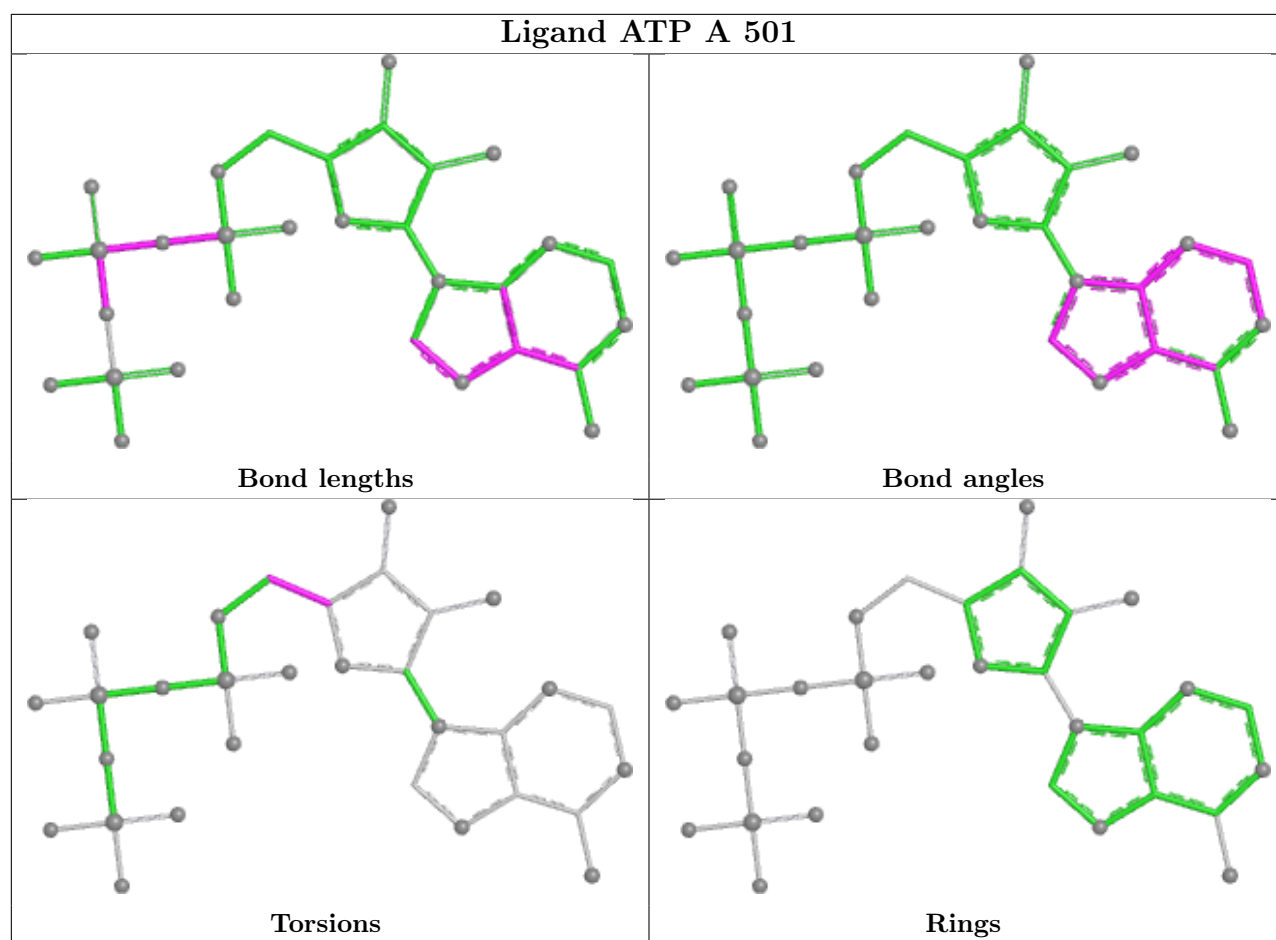
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	205:PRO	C	206:GLU	N	3.35

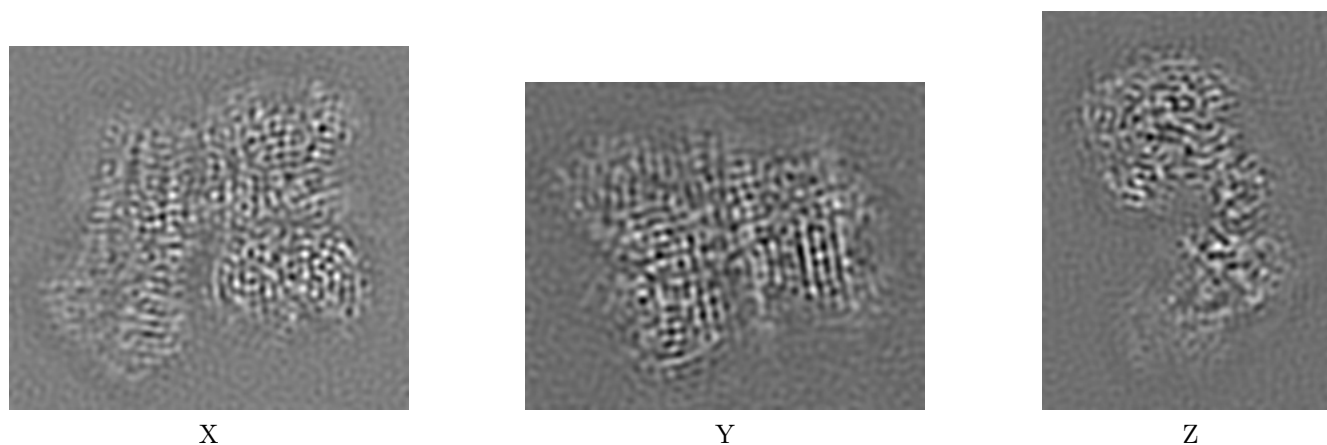
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23881. 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](#)

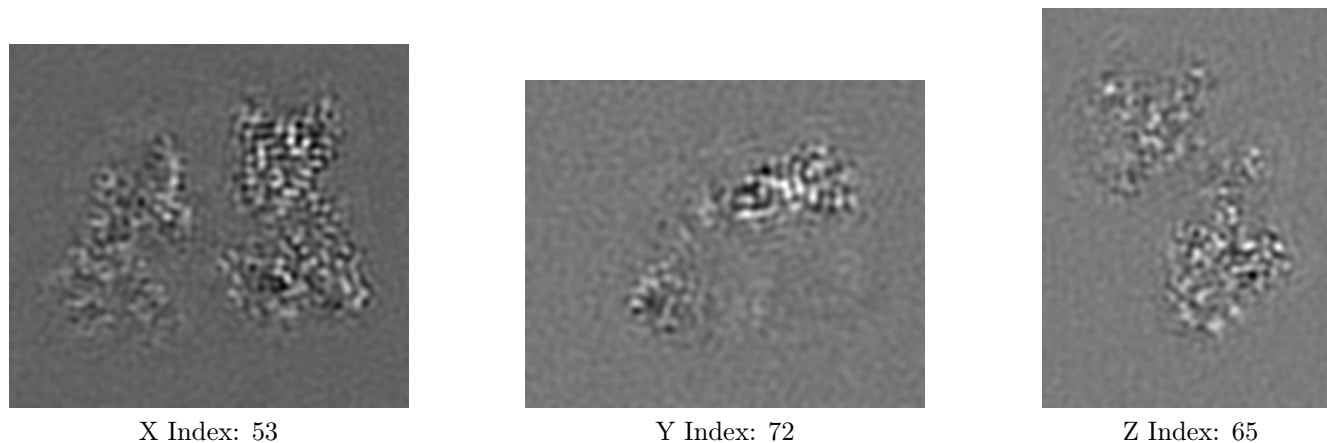
6.1.1 Primary map



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

6.2 Central slices [i](#)

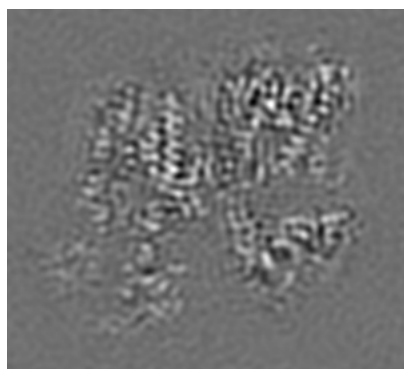
6.2.1 Primary map



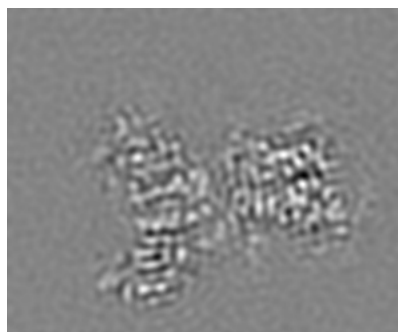
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

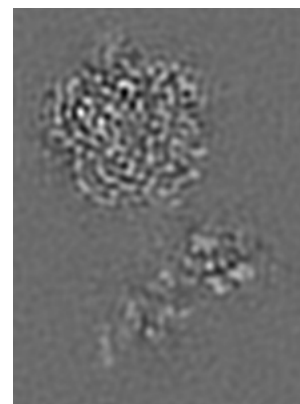
6.3.1 Primary map



X Index: 62



Y Index: 104

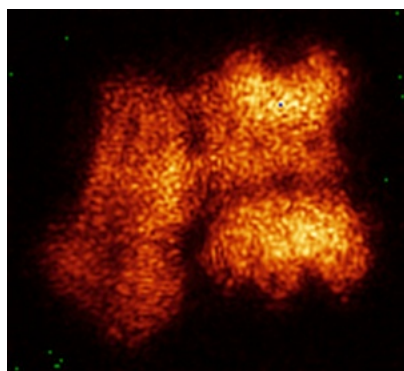


Z Index: 51

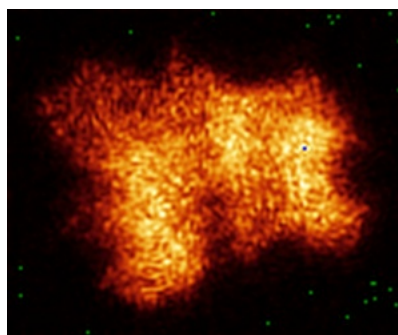
The images above show the largest variance slices of the map in three orthogonal directions.

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

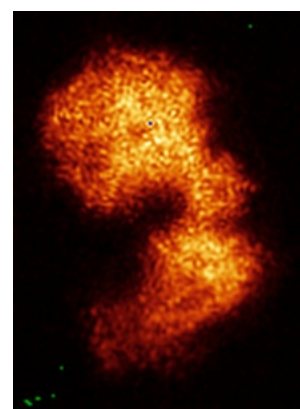
6.4.1 Primary map



X



Y

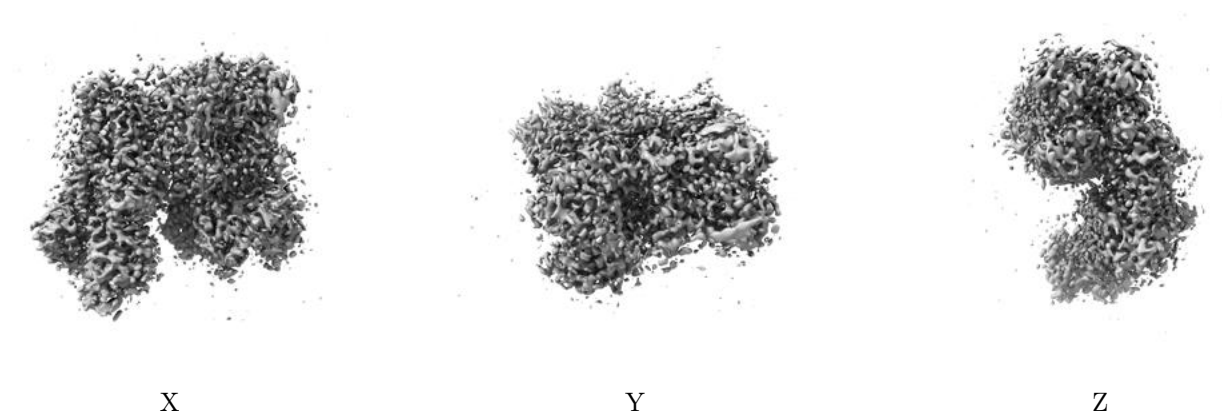


Z

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.

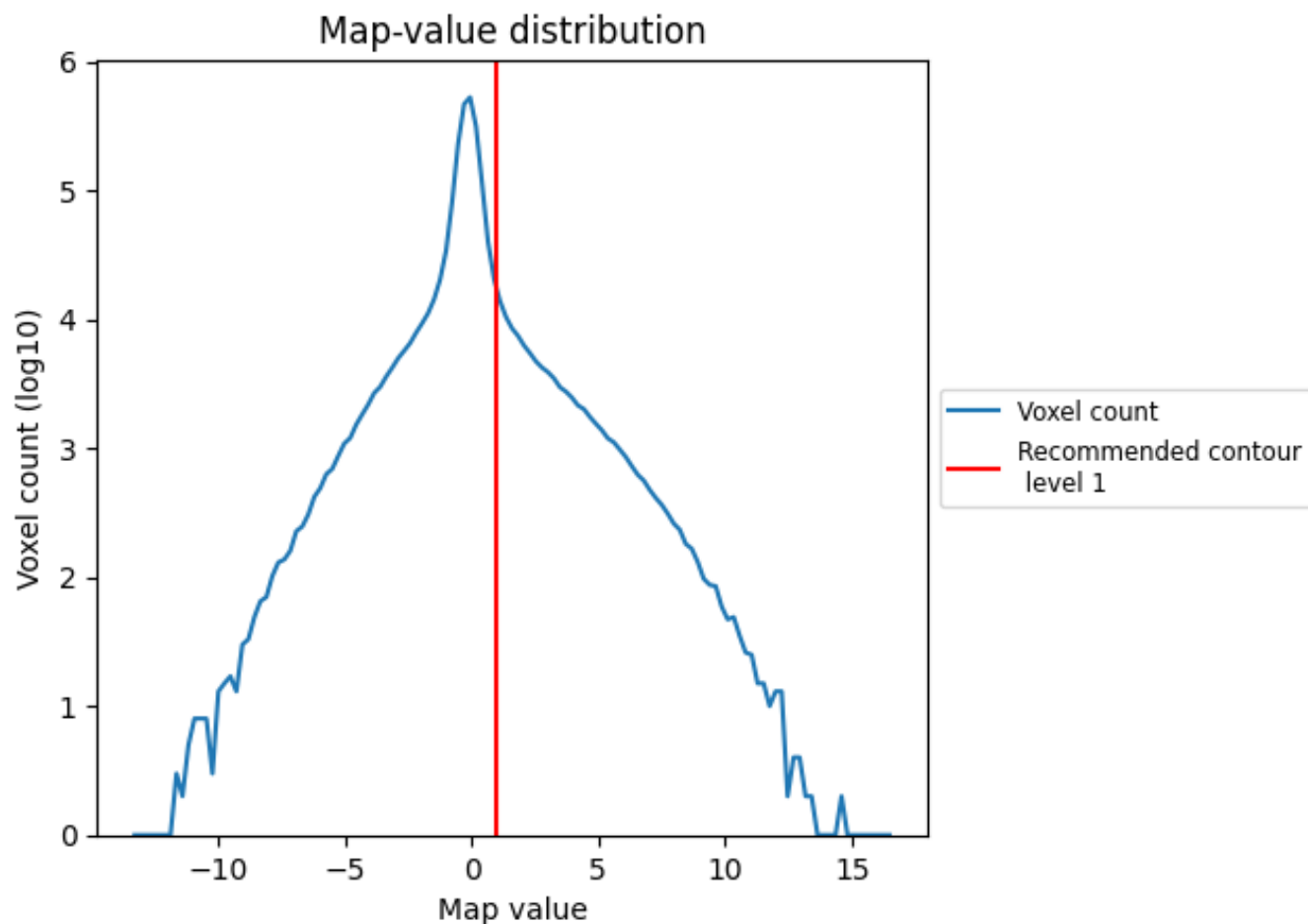
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

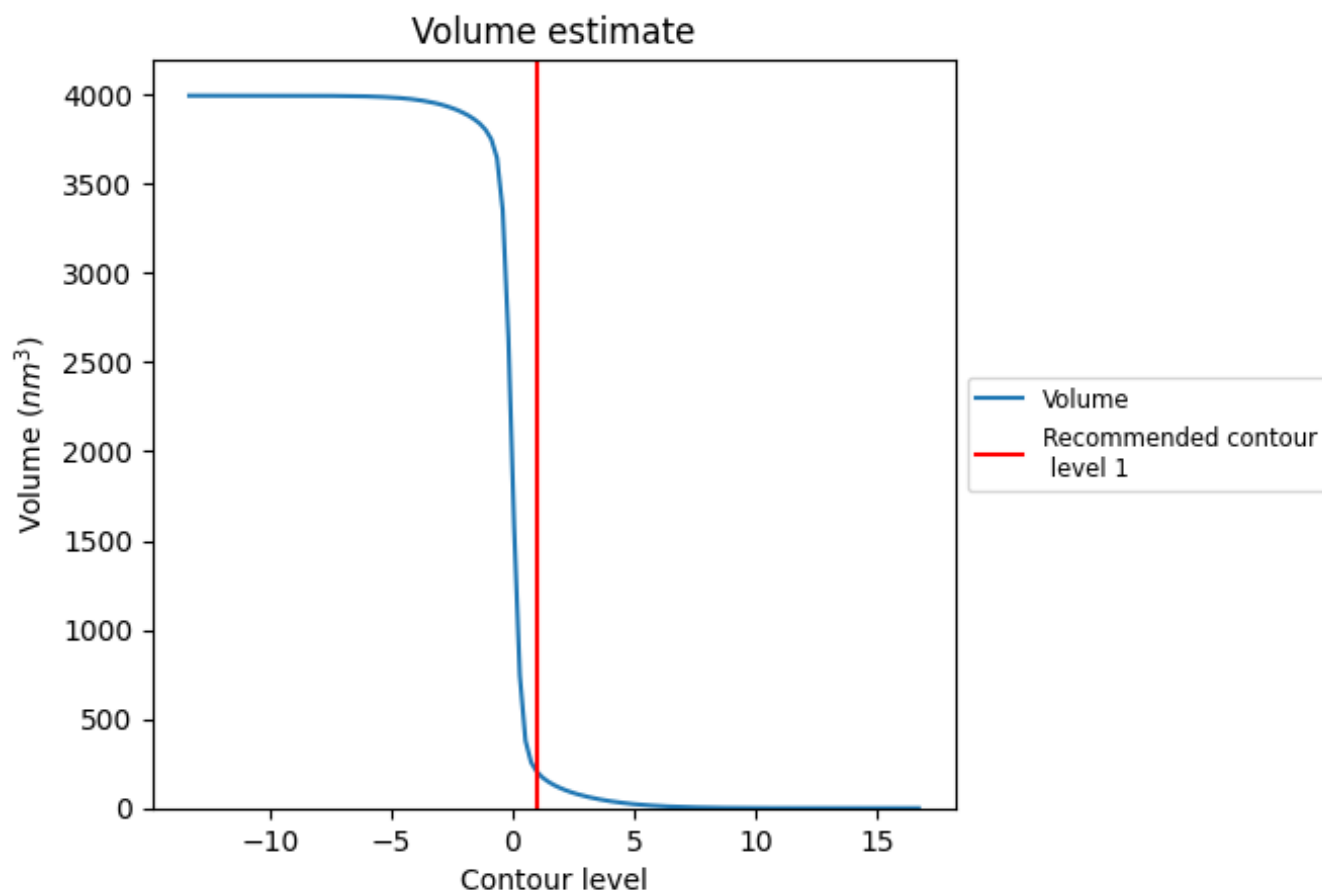
This section contains the results of statistical analysis of the map.

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 205 nm³; this corresponds to an approximate mass of 186 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.

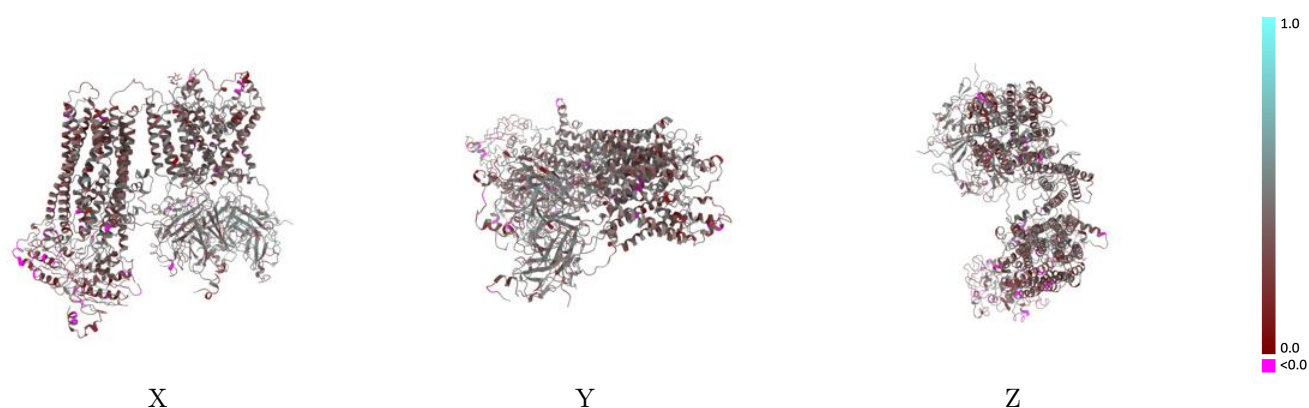
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23881 and PDB model 7MJP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

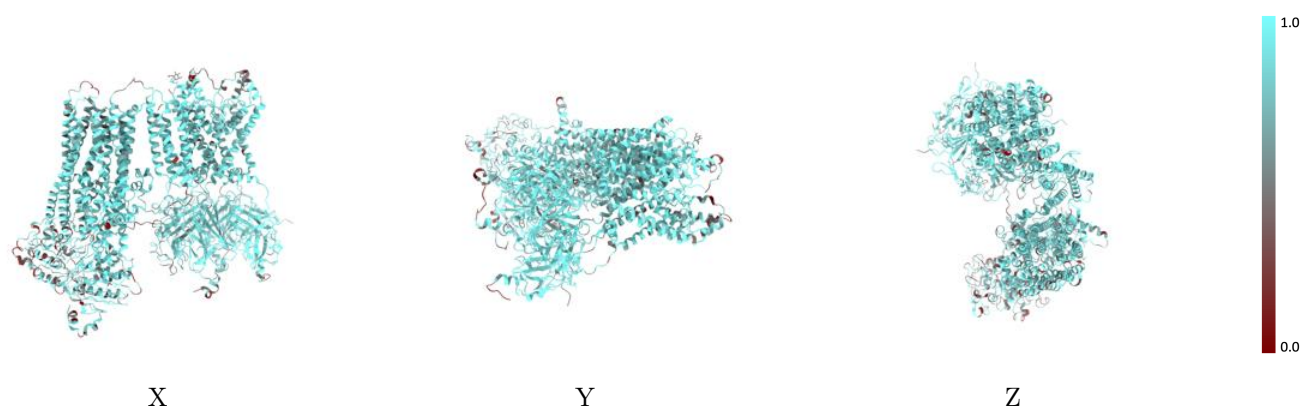
This section was not generated.

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



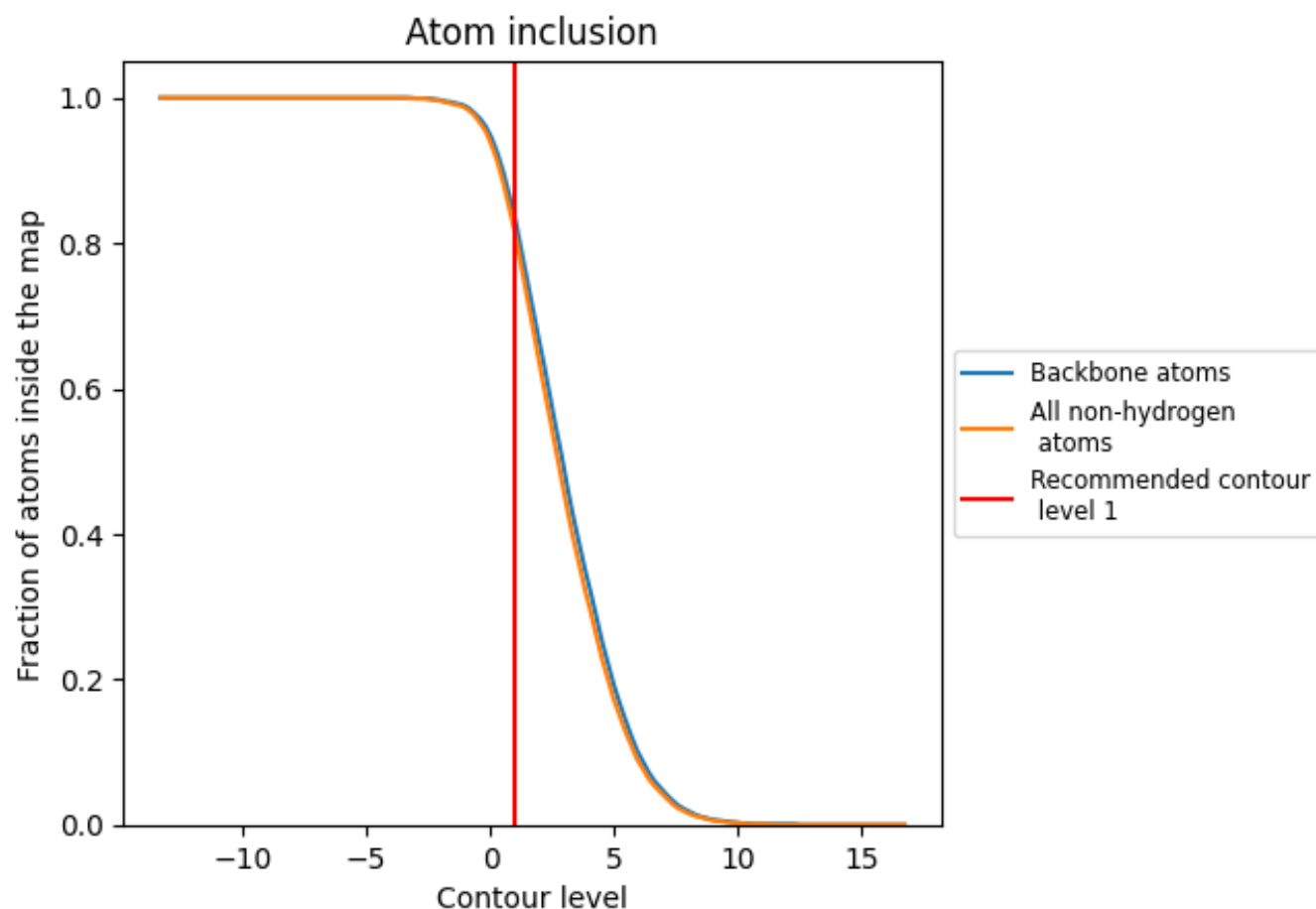
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 82% 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	0.8160	0.3820
A	0.8190	0.4100
B	0.8570	0.4080
C	0.8460	0.4120
D	0.8510	0.4080
E	0.7900	0.3560
N	0.6070	0.3210

1.0

0.0

<0.0