



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 12:04 PM EDT

PDB ID : 7M1T
Title : Crystal structure of an archaeal CNM, MtCorB, with C-terminal deletion in complex with Mg²⁺-ATP
Authors : Chen, Y.S.; Kozlov, G.; Gehring, K.
Deposited on : 2021-03-15
Resolution : 3.26 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

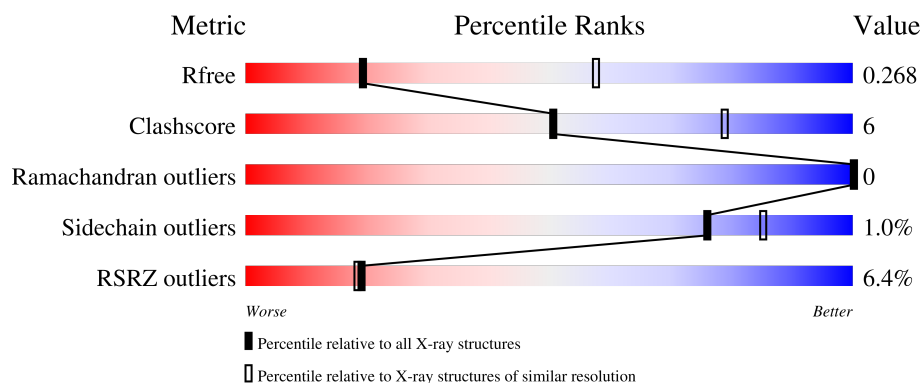
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	 2% 85% 13% •
1	B	326	 10% 84% 13% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10065 atoms, of which 4980 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemolysin, contains CBS domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	H	N	O	S	0	0	0
			4790	1557	2378	386	462	7			
1	B	316	Total	C	H	N	O	S	0	0	0
			4727	1534	2353	379	454	7			

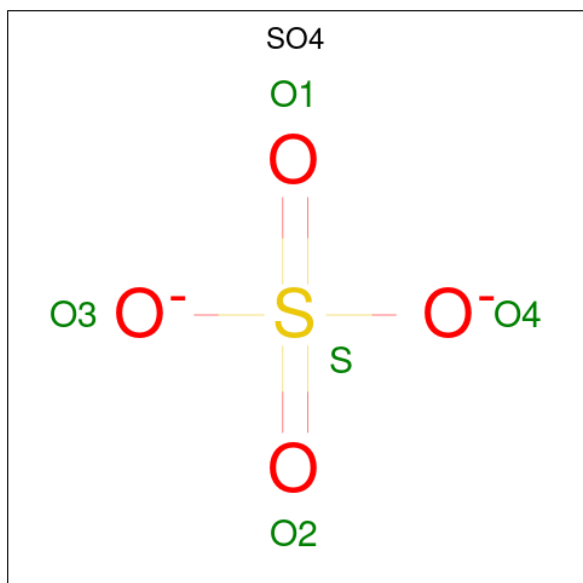
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP A0A1G8XA46
A	?	-	PHE	deletion	UNP A0A1G8XA46
A	?	-	ARG	deletion	UNP A0A1G8XA46
A	?	-	GLN	deletion	UNP A0A1G8XA46
A	323	LEU	-	expression tag	UNP A0A1G8XA46
A	324	GLU	-	expression tag	UNP A0A1G8XA46
A	325	HIS	-	expression tag	UNP A0A1G8XA46
A	326	HIS	-	expression tag	UNP A0A1G8XA46
A	327	HIS	-	expression tag	UNP A0A1G8XA46
A	328	HIS	-	expression tag	UNP A0A1G8XA46
A	329	HIS	-	expression tag	UNP A0A1G8XA46
A	330	HIS	-	expression tag	UNP A0A1G8XA46
B	?	-	VAL	deletion	UNP A0A1G8XA46
B	?	-	PHE	deletion	UNP A0A1G8XA46
B	?	-	ARG	deletion	UNP A0A1G8XA46
B	?	-	GLN	deletion	UNP A0A1G8XA46
B	323	LEU	-	expression tag	UNP A0A1G8XA46
B	324	GLU	-	expression tag	UNP A0A1G8XA46
B	325	HIS	-	expression tag	UNP A0A1G8XA46
B	326	HIS	-	expression tag	UNP A0A1G8XA46
B	327	HIS	-	expression tag	UNP A0A1G8XA46
B	328	HIS	-	expression tag	UNP A0A1G8XA46
B	329	HIS	-	expression tag	UNP A0A1G8XA46
B	330	HIS	-	expression tag	UNP A0A1G8XA46

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

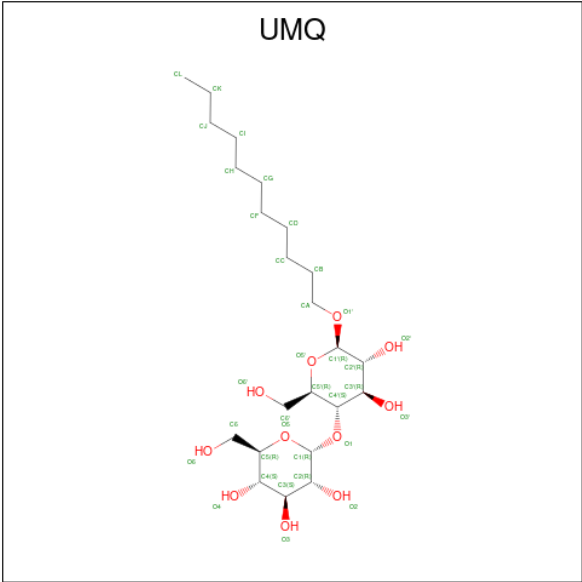
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



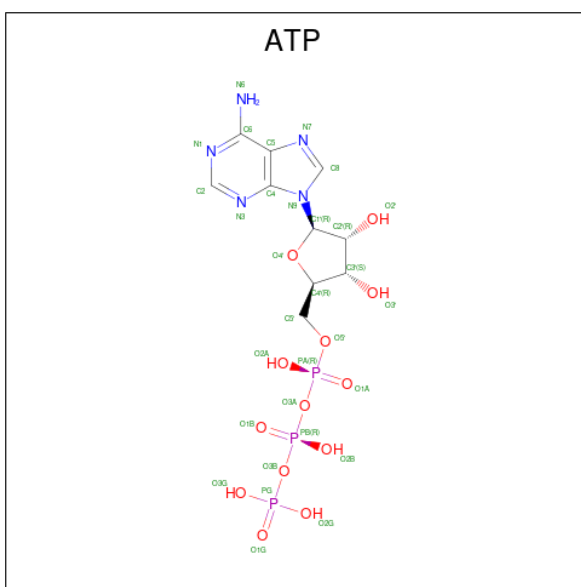
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



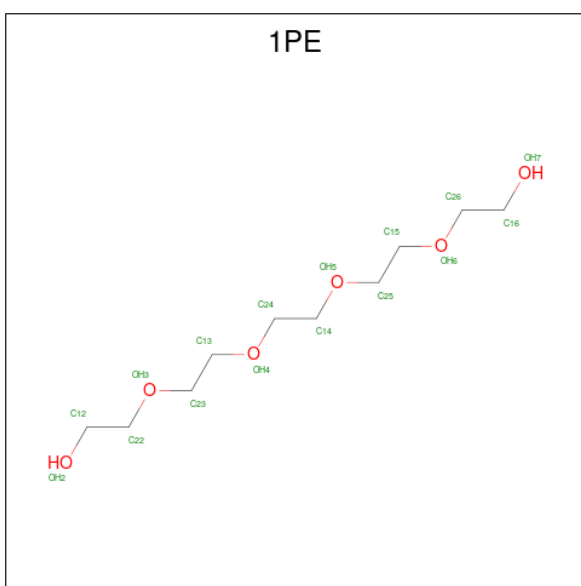
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C			0	0
			11	11				
4	A	1	Total	C			0	0
			7	7				
4	A	1	Total	C	H	O	0	0
			70	21	38	11		
4	A	1	Total	C	H	O	0	0
			77	23	43	11		
4	A	1	Total	C	H	O	0	0
			67	20	36	11		
4	B	1	Total	C	H	O	0	0
			14	12	1	1		
4	B	1	Total	C	H	O	0	0
			77	23	43	11		
4	B	1	Total	C	H	O	0	0
			77	23	43	11		
4	B	1	Total	C			0	0
			7	7				
4	B	1	Total	C			0	0
			5	5				

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
5	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).

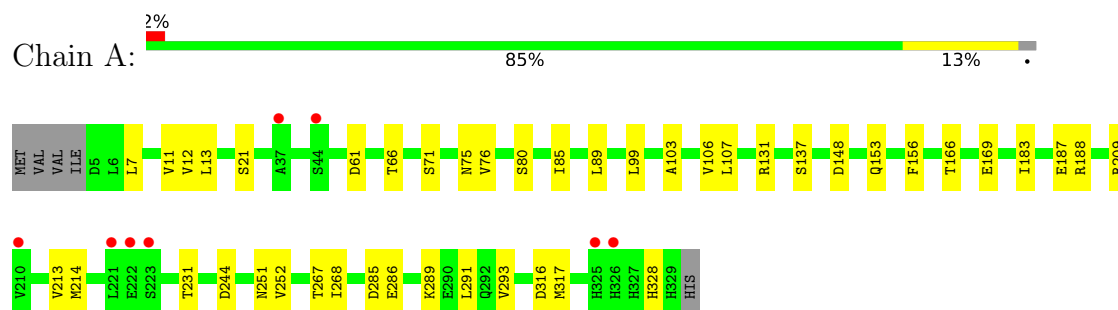


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			38	10	22	6		

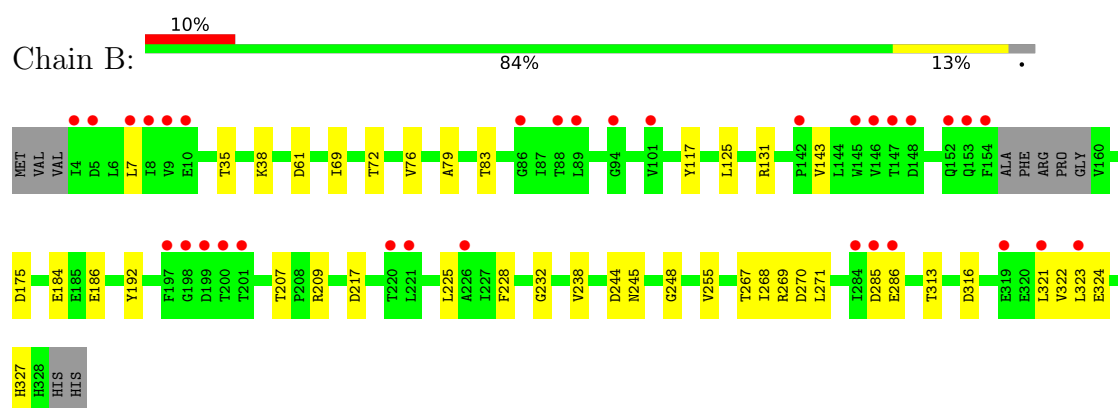
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Hemolysin, contains CBS domains



- Molecule 1: Hemolysin, contains CBS domains



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.05Å 118.68Å 177.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.26 49.31 – 3.26	Depositor EDS
% Data completeness (in resolution range)	71.2 (49.31-3.26) 68.1 (49.31-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.267 0.227 , 0.268	Depositor DCC
R_{free} test set	743 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	10065	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ATP, MG, UMQ, 1PE, SO4

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	0.24	0/2451	0.44	0/3340
1	B	0.24	0/2411	0.44	0/3286
All	All	0.24	0/4862	0.44	0/6626

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	2412	2378	2378	30	0
1	B	2374	2353	2353	34	1
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	3	1
4	A	115	117	146	0	0
4	B	93	87	133	2	0
5	A	31	11	11	0	0
5	B	31	12	11	3	0
6	A	16	22	22	1	0
All	All	5085	4980	5054	58	1

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 6.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:THR:OG1	5:B:409:ATP:O2'	1.94	0.84
1:B:131:ARG:NH1	3:B:403:SO4:O4	2.13	0.81
1:B:316:ASP:OD1	5:B:409:ATP:O3'	1.98	0.80
1:A:153:GLN:NE2	1:A:156:PHE:O	2.16	0.78
1:A:80:SER:HB2	1:B:83:THR:HG21	1.72	0.71
1:A:166:THR:HG22	1:A:169:GLU:OE1	1.92	0.70
1:B:285:ASP:OD1	1:B:286:GLU:N	2.28	0.66
1:B:131:ARG:NH1	3:B:403:SO4:O1	2.29	0.65
1:B:131:ARG:NH1	3:B:403:SO4:S	2.70	0.64
1:B:186:GLU:N	1:B:186:GLU:OE1	2.32	0.63
1:A:131:ARG:NH1	3:A:402:SO4:S	2.77	0.58
1:B:143:VAL:HG21	4:B:408:UMQ:HK2	1.86	0.57
1:A:107:LEU:HD21	1:B:69:ILE:HG12	1.87	0.57
1:A:76:VAL:HG13	1:B:79:ALA:HB2	1.85	0.57
1:A:76:VAL:HG13	1:B:79:ALA:CB	2.35	0.56
1:B:313:THR:HG21	5:B:409:ATP:O2A	2.05	0.56
1:B:125:LEU:HD23	1:B:125:LEU:O	2.09	0.52
1:B:35:THR:O	1:B:38:LYS:N	2.41	0.52
1:A:75:ASN:OD1	1:A:106:VAL:HG13	2.11	0.51
1:A:71:SER:O	1:A:75:ASN:ND2	2.43	0.51
1:A:7:LEU:HD12	1:A:89:LEU:HD11	1.93	0.51
1:B:209:ARG:NH2	1:B:244:ASP:OD1	2.38	0.50
1:A:285:ASP:OD1	1:A:286:GLU:N	2.44	0.50
1:B:117:TYR:CD2	4:B:404:UMQ:HG2	2.47	0.49
1:A:7:LEU:CD1	1:A:89:LEU:HD11	2.43	0.48
1:A:213:VAL:HG11	1:A:231:THR:HG21	1.95	0.48
1:B:321:LEU:HD12	1:B:322:VAL:N	2.28	0.48
1:A:267:THR:HG22	1:A:268:ILE:H	1.78	0.47
1:A:21:SER:OG	1:A:75:ASN:OD1	2.14	0.46
1:B:7:LEU:C	1:B:7:LEU:HD23	2.36	0.46
1:A:61:ASP:OD1	6:A:409:1PE:OH7	2.33	0.46
1:B:61:ASP:OD1	1:B:61:ASP:N	2.47	0.46
1:A:291:LEU:HD12	1:A:317:MET:HE1	1.97	0.46
1:B:267:THR:O	1:B:271:LEU:HD12	2.16	0.45
1:A:267:THR:HG22	1:A:268:ILE:N	2.31	0.45
1:B:217:ASP:OD2	1:B:269:ARG:NH1	2.48	0.45
1:A:80:SER:CB	1:B:83:THR:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:N	1:A:85:ILE:HD11	2.32	0.45
1:B:72:THR:O	1:B:76:VAL:HG23	2.16	0.45
1:A:188:ARG:NH2	1:A:328:HIS:O	2.45	0.44
1:A:289:LYS:O	1:A:293:VAL:HG23	2.18	0.44
1:B:267:THR:HG22	1:B:270:ASP:OD2	2.17	0.44
1:B:228:PHE:O	1:B:232:GLY:N	2.50	0.44
1:B:323:LEU:HD13	1:B:324:GLU:N	2.32	0.44
1:B:238:VAL:N	1:B:248:GLY:O	2.51	0.43
1:A:99:LEU:HD23	1:A:99:LEU:C	2.39	0.43
1:A:183:ILE:HG23	1:A:187:GLU:HG3	2.01	0.43
1:B:175:ASP:OD1	1:B:192:TYR:OH	2.36	0.42
1:A:12:VAL:HG13	1:A:13:LEU:N	2.33	0.42
1:B:267:THR:OG1	1:B:268:ILE:N	2.53	0.42
1:B:323:LEU:HD13	1:B:324:GLU:O	2.20	0.42
1:A:103:ALA:HA	1:B:76:VAL:HG21	2.00	0.41
1:A:251:ASN:OD1	1:A:252:VAL:N	2.52	0.41
1:A:209:ARG:NH1	1:A:244:ASP:OD1	2.53	0.41
1:A:7:LEU:C	1:A:7:LEU:HD23	2.41	0.41
1:A:66:THR:HG21	1:A:137:SER:HA	2.03	0.41
1:B:184:GLU:OE1	1:B:184:GLU:N	2.52	0.40
1:B:225:LEU:HD11	1:B:255:VAL:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HE	3:B:403:SO4:O3[4_566]	1.60	0.00

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 X-ray entries followed by that with respect to entries of similar resolution.

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	319/326 (98%)	307 (96%)	12 (4%)	0	100	100
1	B	312/326 (96%)	303 (97%)	9 (3%)	0	100	100
All	All	631/652 (97%)	610 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	249/281 (89%)	246 (99%)	3 (1%)	71	83
1	B	248/281 (88%)	246 (99%)	2 (1%)	81	89
All	All	497/562 (88%)	492 (99%)	5 (1%)	76	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	214	MET
1	A	316	ASP
1	B	245	ASN
1	B	327	HIS

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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
6	1PE	A	409	-	15,15,15	0.52	0	14,14,14	0.27	0
4	UMQ	A	403	-	10,10,35	0.72	0	9,9,46	0.78	0
4	UMQ	B	405	-	35,35,35	1.48	7 (20%)	46,46,46	0.92	1 (2%)
4	UMQ	A	407	-	32,32,35	1.59	7 (21%)	43,43,46	1.24	4 (9%)
5	ATP	B	409	2	26,33,33	4.59	7 (26%)	31,52,52	2.34	7 (22%)
4	UMQ	B	404	-	12,12,35	0.81	0	11,11,46	0.76	0
4	UMQ	A	404	-	6,6,35	0.58	0	5,5,46	0.69	0
4	UMQ	B	408	-	4,4,35	0.46	0	3,3,46	0.56	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
5	ATP	A	408	2	26,33,33	4.57	8 (30%)	31,52,52	2.19	5 (16%)
4	UMQ	B	407	-	6,6,35	0.58	0	5,5,46	0.68	0
4	UMQ	A	406	-	35,35,35	1.51	7 (20%)	46,46,46	1.02	1 (2%)
4	UMQ	B	406	-	35,35,35	1.50	8 (22%)	46,46,46	1.05	3 (6%)
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.06	0
4	UMQ	A	405	-	32,32,35	1.47	7 (21%)	41,42,46	1.32	4 (9%)

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
6	1PE	A	409	-	-	6/13/13/13	-
4	UMQ	A	403	-	-	0/8/8/60	-
4	UMQ	B	405	-	-	8/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UMQ	A	407	-	-	11/17/57/60	0/2/2/2
5	ATP	B	409	2	-	3/18/38/38	0/3/3/3
4	UMQ	B	404	-	-	2/10/10/60	-
4	UMQ	A	404	-	-	0/4/4/60	-
4	UMQ	B	408	-	-	0/2/2/60	-
5	ATP	A	408	2	-	0/18/38/38	0/3/3/3
4	UMQ	B	407	-	-	1/4/4/60	-
4	UMQ	A	406	-	-	5/20/60/60	0/2/2/2
4	UMQ	B	406	-	-	8/20/60/60	0/2/2/2
4	UMQ	A	405	-	-	7/15/55/60	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	409	ATP	O4'-C1'	15.10	1.62	1.41
5	B	409	ATP	C2'-C1'	-15.02	1.31	1.53
5	A	408	ATP	O4'-C1'	15.02	1.62	1.41
5	A	408	ATP	C2'-C1'	-14.92	1.31	1.53
5	B	409	ATP	O4'-C4'	-6.44	1.30	1.45
5	A	408	ATP	O4'-C4'	-6.30	1.30	1.45
4	A	407	UMQ	O5-C5	4.23	1.54	1.44
4	B	406	UMQ	O5-C5	4.08	1.54	1.44
4	A	406	UMQ	O5-C5	4.00	1.54	1.44
4	B	405	UMQ	O5-C5	3.95	1.53	1.44
4	A	405	UMQ	O5-C5	3.80	1.53	1.44
4	A	406	UMQ	O5'-C1'	3.73	1.51	1.41
4	A	407	UMQ	O5'-C1'	3.48	1.50	1.41
4	A	405	UMQ	O5'-C1'	3.39	1.50	1.41
4	B	406	UMQ	O5'-C1'	3.36	1.50	1.41
4	B	405	UMQ	O5'-C1'	3.35	1.50	1.41
5	A	408	ATP	C6-N6	3.18	1.45	1.34
5	B	409	ATP	C6-N6	3.11	1.45	1.34
4	A	407	UMQ	O5-C1	3.04	1.49	1.41
5	B	409	ATP	O3'-C3'	-3.00	1.35	1.43
5	A	408	ATP	O3'-C3'	-2.93	1.36	1.43
5	A	408	ATP	O2'-C2'	2.93	1.49	1.43
4	B	405	UMQ	C6-C5	-2.82	1.42	1.51
5	B	409	ATP	O2'-C2'	2.81	1.49	1.43
4	A	407	UMQ	C6-C5	-2.78	1.42	1.51
4	B	406	UMQ	C6-C5	-2.77	1.42	1.51
4	A	406	UMQ	C6-C5	-2.77	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	407	UMQ	C3-C2	-2.76	1.45	1.52
4	A	405	UMQ	C6-C5	-2.69	1.42	1.51
5	A	408	ATP	C5-C4	-2.67	1.33	1.40
5	B	409	ATP	C5-C4	-2.67	1.33	1.40
4	B	406	UMQ	C3-C2	-2.65	1.45	1.52
4	A	406	UMQ	C3-C2	-2.61	1.45	1.52
4	B	405	UMQ	C3-C2	-2.60	1.45	1.52
4	B	406	UMQ	O5-C1	2.57	1.48	1.41
4	A	406	UMQ	O5-C1	2.56	1.48	1.41
4	B	405	UMQ	O5-C1	2.56	1.48	1.41
4	A	405	UMQ	C3-C2	-2.32	1.46	1.52
4	A	405	UMQ	O5-C1	2.30	1.47	1.41
4	A	405	UMQ	O2-C2	2.22	1.48	1.43
4	A	407	UMQ	O2-C2	2.20	1.48	1.43
4	A	406	UMQ	O2-C2	2.17	1.48	1.43
4	B	405	UMQ	O2-C2	2.17	1.48	1.43
4	B	406	UMQ	O2-C2	2.16	1.48	1.43
4	A	405	UMQ	O3-C3	2.15	1.48	1.43
4	B	405	UMQ	O3-C3	2.15	1.48	1.43
4	B	406	UMQ	O5'-C5'	2.14	1.49	1.44
4	B	406	UMQ	O3-C3	2.12	1.48	1.43
4	A	406	UMQ	O3-C3	2.12	1.48	1.43
5	A	408	ATP	C2-N3	2.10	1.35	1.32
4	A	407	UMQ	O3-C3	2.10	1.47	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	409	ATP	C5-C6-N6	7.34	131.51	120.35
5	A	408	ATP	C5-C6-N6	7.26	131.38	120.35
5	A	408	ATP	N3-C2-N1	-5.46	120.14	128.68
5	B	409	ATP	N3-C2-N1	-5.39	120.26	128.68
5	B	409	ATP	N6-C6-N1	-4.86	108.49	118.57
5	A	408	ATP	N6-C6-N1	-4.75	108.72	118.57
5	B	409	ATP	PA-O3A-PB	-4.36	117.86	132.83
4	A	405	UMQ	C4-C3-C2	4.11	117.99	110.82
5	B	409	ATP	C3'-C2'-C1'	3.99	106.99	100.98
4	A	405	UMQ	C3-C4-C5	3.86	117.13	110.24
4	A	407	UMQ	O5-C1-C2	3.64	118.06	110.35
5	A	408	ATP	PB-O3B-PG	-3.56	120.62	132.83
5	A	408	ATP	PA-O3A-PB	-3.44	121.02	132.83
4	A	407	UMQ	C1-O5-C5	3.12	119.81	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	407	UMQ	C1-O1-C4'	-2.85	110.90	117.96
4	A	407	UMQ	C1-C2-C3	2.82	115.86	110.00
4	A	405	UMQ	C1-O1-C4'	-2.75	111.16	117.96
4	B	406	UMQ	CA-O1'-C1'	2.72	118.36	113.84
5	B	409	ATP	PB-O3B-PG	-2.64	123.78	132.83
4	A	406	UMQ	O5'-C1'-C2'	2.59	115.84	110.35
4	B	406	UMQ	O5'-C5'-C4'	2.57	115.16	109.75
4	A	405	UMQ	C1-C2-C3	2.45	115.10	110.00
4	B	405	UMQ	C1-O1-C4'	-2.40	112.02	117.96
4	B	406	UMQ	C1-O1-C4'	-2.25	112.40	117.96
5	B	409	ATP	C1'-N9-C4	-2.20	122.77	126.64

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	406	UMQ	C2'-C1'-O1'-CA
4	B	406	UMQ	O5'-C1'-O1'-CA
4	B	406	UMQ	CB-CA-O1'-C1'
5	B	409	ATP	C5'-O5'-PA-O1A
4	A	405	UMQ	O5-C5-C6-O6
4	A	406	UMQ	C3'-C4'-O1-C1
4	A	407	UMQ	O5-C5-C6-O6
4	A	405	UMQ	C4-C5-C6-O6
4	B	405	UMQ	O5-C5-C6-O6
6	A	409	1PE	OH4-C13-C23-OH3
6	A	409	1PE	OH6-C15-C25-OH5
4	B	406	UMQ	O5'-C5'-C6'-O6'
6	A	409	1PE	OH5-C14-C24-OH4
4	B	405	UMQ	C4-C5-C6-O6
4	A	405	UMQ	O5'-C5'-C6'-O6'
4	B	406	UMQ	O1'-CA-CB-CC
4	B	406	UMQ	C4'-C5'-C6'-O6'
4	A	407	UMQ	O5'-C1'-O1'-CA
4	A	407	UMQ	O1'-CA-CB-CC
4	A	407	UMQ	C2'-C1'-O1'-CA
4	B	405	UMQ	C2'-C1'-O1'-CA
4	A	407	UMQ	C4-C5-C6-O6
4	B	406	UMQ	CG-CH-CI-CJ
4	B	405	UMQ	CB-CC-CD-CF
4	B	405	UMQ	O5'-C1'-O1'-CA
4	A	405	UMQ	CF-CG-CH-CI

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Mol	Chain	Res	Type	Atoms
4	A	407	UMQ	CC-CD-CF-CG
4	B	404	UMQ	CF-CG-CH-CI
4	A	405	UMQ	O1'-CA-CB-CC
4	B	404	UMQ	CG-CH-CI-CJ
4	A	406	UMQ	C5'-C4'-O1-C1
6	A	409	1PE	OH2-C12-C22-OH3
4	A	405	UMQ	C4'-C5'-C6'-O6'
6	A	409	1PE	C23-C13-OH4-C24
5	B	409	ATP	C5'-O5'-PA-O3A
4	B	405	UMQ	C2-C1-O1-C4'
6	A	409	1PE	C24-C14-OH5-C25
4	A	407	UMQ	O5'-C5'-C6'-O6'
4	A	405	UMQ	CH-CI-CJ-CK
5	B	409	ATP	C5'-O5'-PA-O2A
4	B	405	UMQ	O5-C1-O1-C4'
4	A	407	UMQ	CF-CG-CH-CI
4	B	407	UMQ	CH-CI-CJ-CK
4	B	405	UMQ	CA-CB-CC-CD
4	A	406	UMQ	CA-CB-CC-CD
4	B	406	UMQ	CB-CC-CD-CF
4	A	407	UMQ	C3'-C4'-O1-C1
4	A	407	UMQ	C5'-C4'-O1-C1
4	A	406	UMQ	CF-CG-CH-CI
4	A	406	UMQ	CB-CA-O1'-C1'
4	A	407	UMQ	CB-CA-O1'-C1'

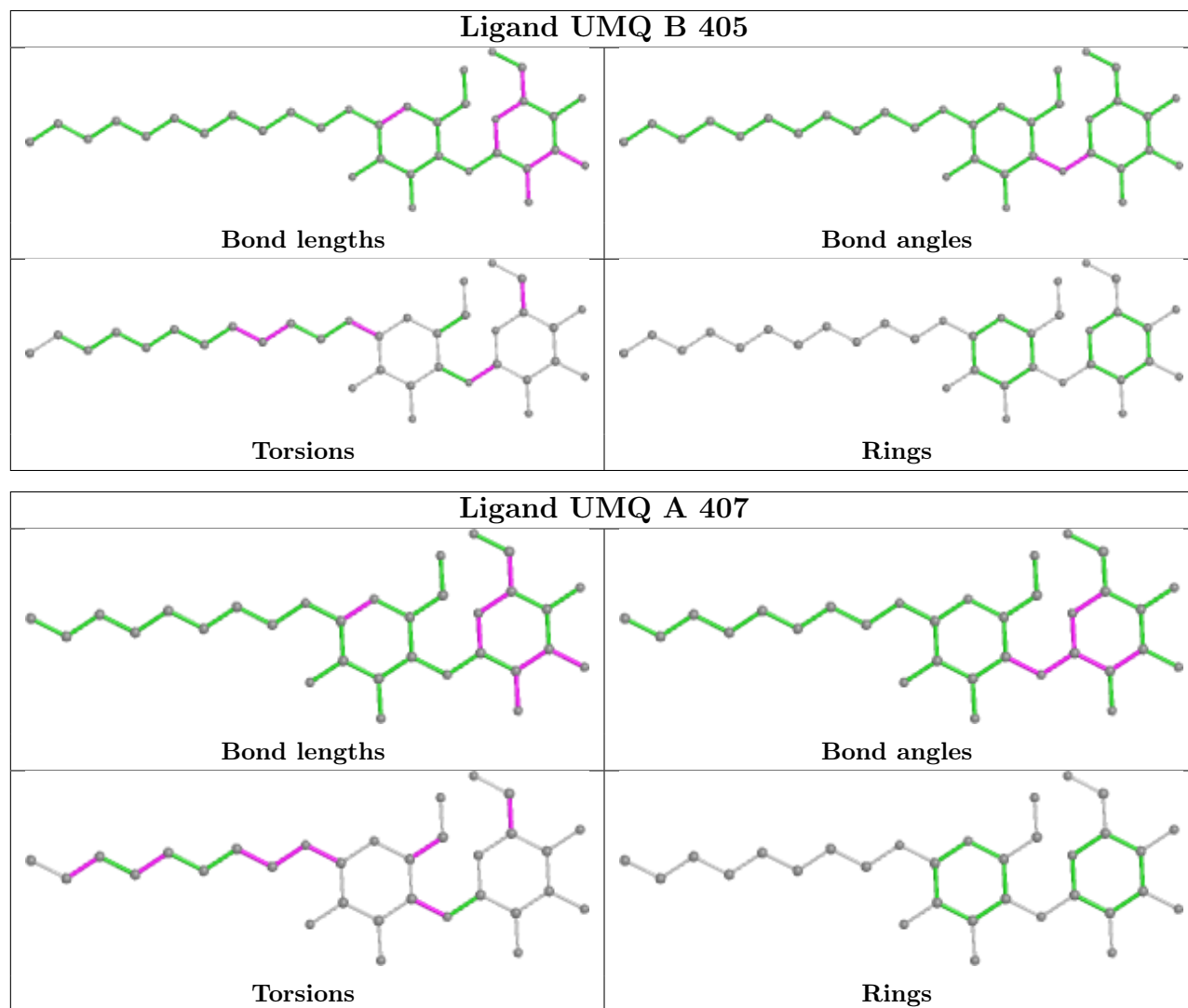
There are no ring outliers.

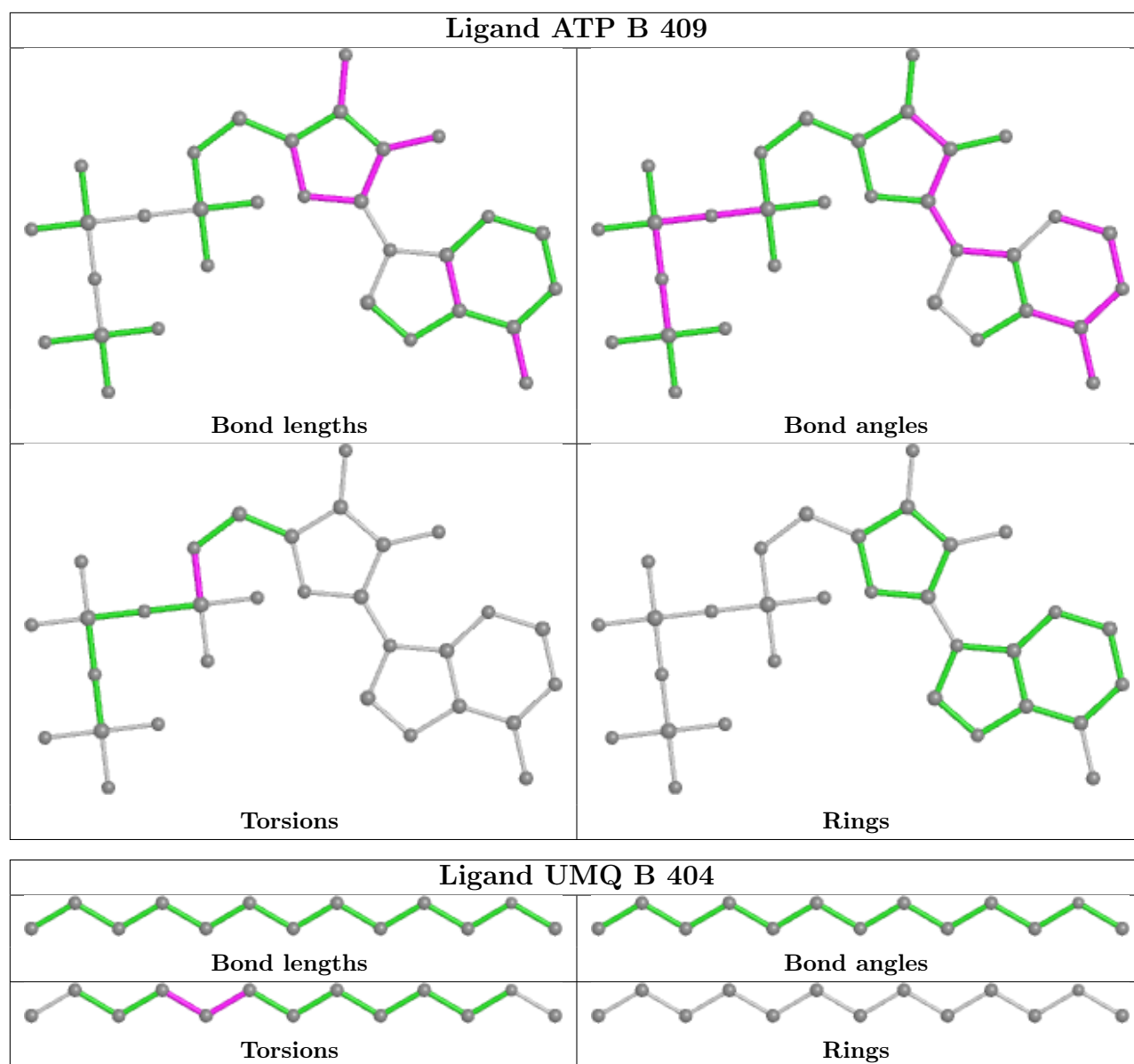
6 monomers are involved in 11 short contacts:

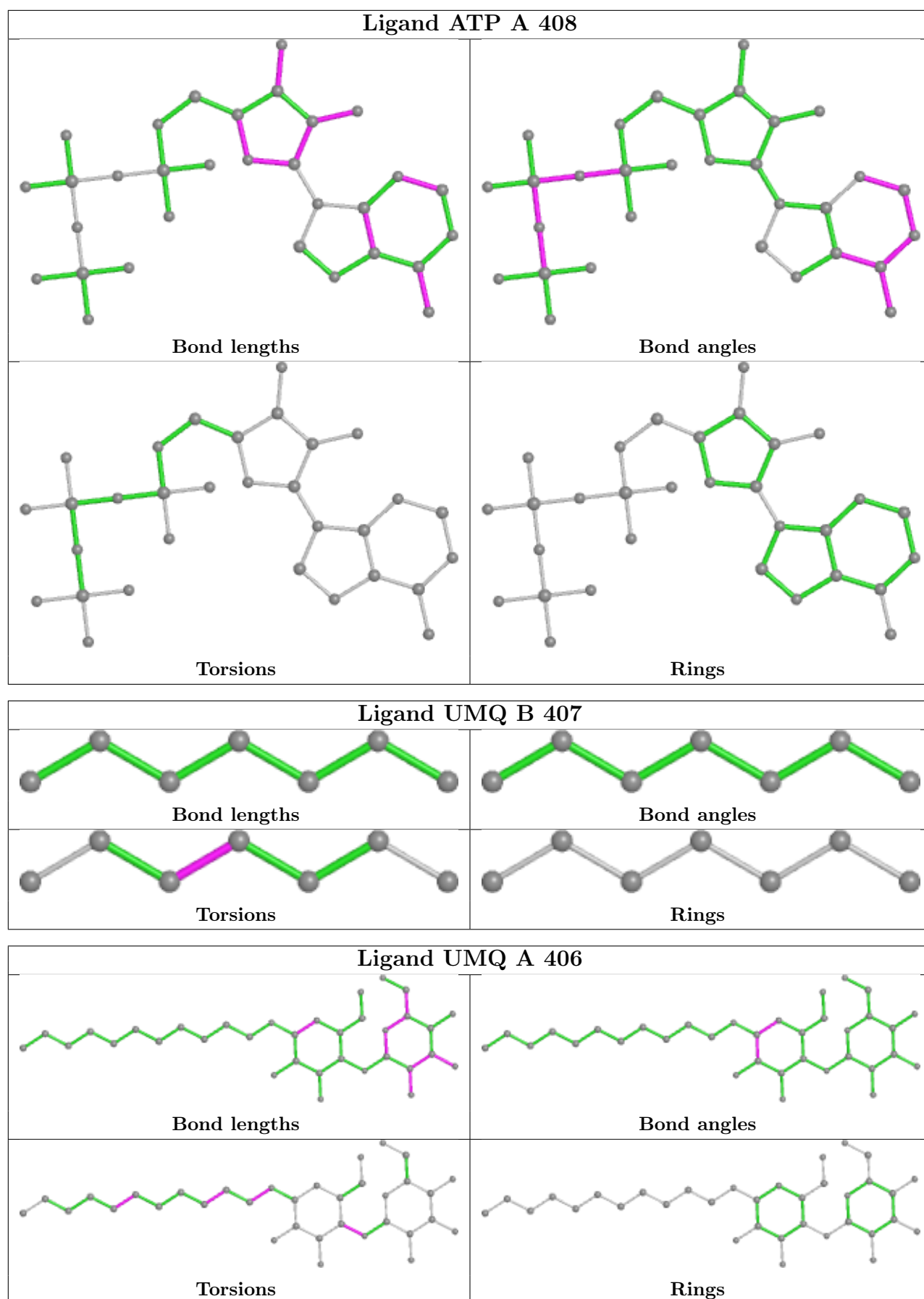
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	409	1PE	1	0
5	B	409	ATP	3	0
4	B	404	UMQ	1	0
4	B	408	UMQ	1	0
3	A	402	SO4	1	0
3	B	403	SO4	3	1

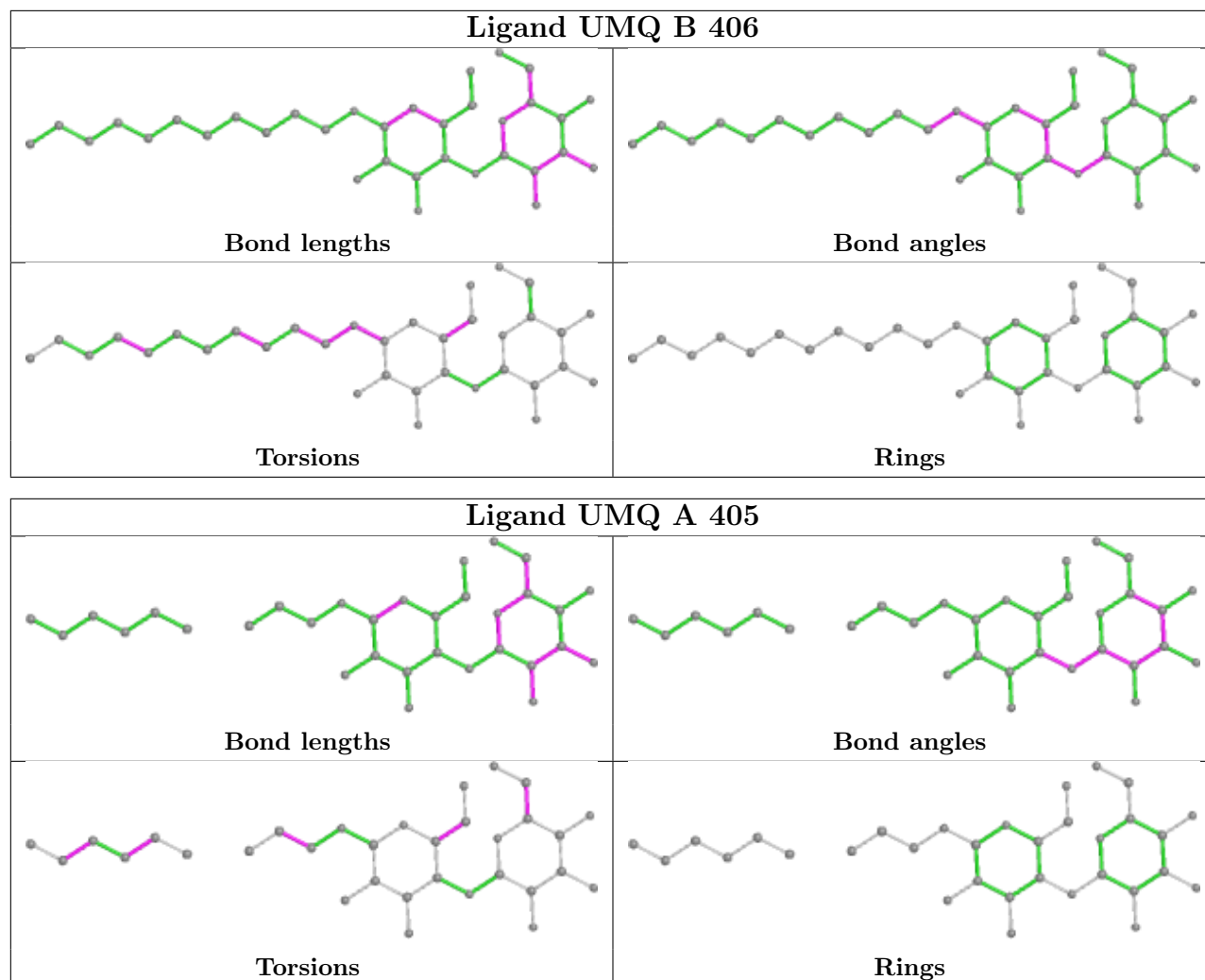
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/326 (98%)	0.12	8 (2%) 57 53	8, 24, 54, 74	0
1	B	316/326 (96%)	0.37	33 (10%) 6 6	9, 24, 60, 72	0
All	All	637/652 (97%)	0.24	41 (6%) 19 18	8, 24, 57, 74	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	HIS	7.1
1	B	197	PHE	5.2
1	B	146	VAL	4.6
1	B	145	TRP	4.4
1	B	198	GLY	4.0
1	B	147	THR	3.8
1	B	142	PRO	3.6
1	B	323	LEU	3.5
1	A	326	HIS	3.5
1	B	285	ASP	3.4
1	B	94	GLY	3.2
1	B	8	ILE	3.2
1	B	153	GLN	3.2
1	B	89	LEU	3.2
1	B	284	ILE	3.0
1	B	88	THR	3.0
1	B	199	ASP	3.0
1	B	220	THR	2.9
1	B	221	LEU	2.9
1	B	152	GLN	2.9
1	A	37	ALA	2.8
1	A	223	SER	2.7
1	B	9	VAL	2.7
1	B	321	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	319	GLU	2.6
1	B	101	VAL	2.5
1	A	44	SER	2.5
1	B	7	LEU	2.4
1	A	222	GLU	2.4
1	B	226	ALA	2.4
1	B	5	ASP	2.4
1	B	154	PHE	2.3
1	A	221	LEU	2.3
1	B	200	THR	2.3
1	B	286	GLU	2.1
1	B	10	GLU	2.1
1	B	4	ILE	2.1
1	B	148	ASP	2.1
1	A	210	VAL	2.0
1	B	201	THR	2.0
1	B	86	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

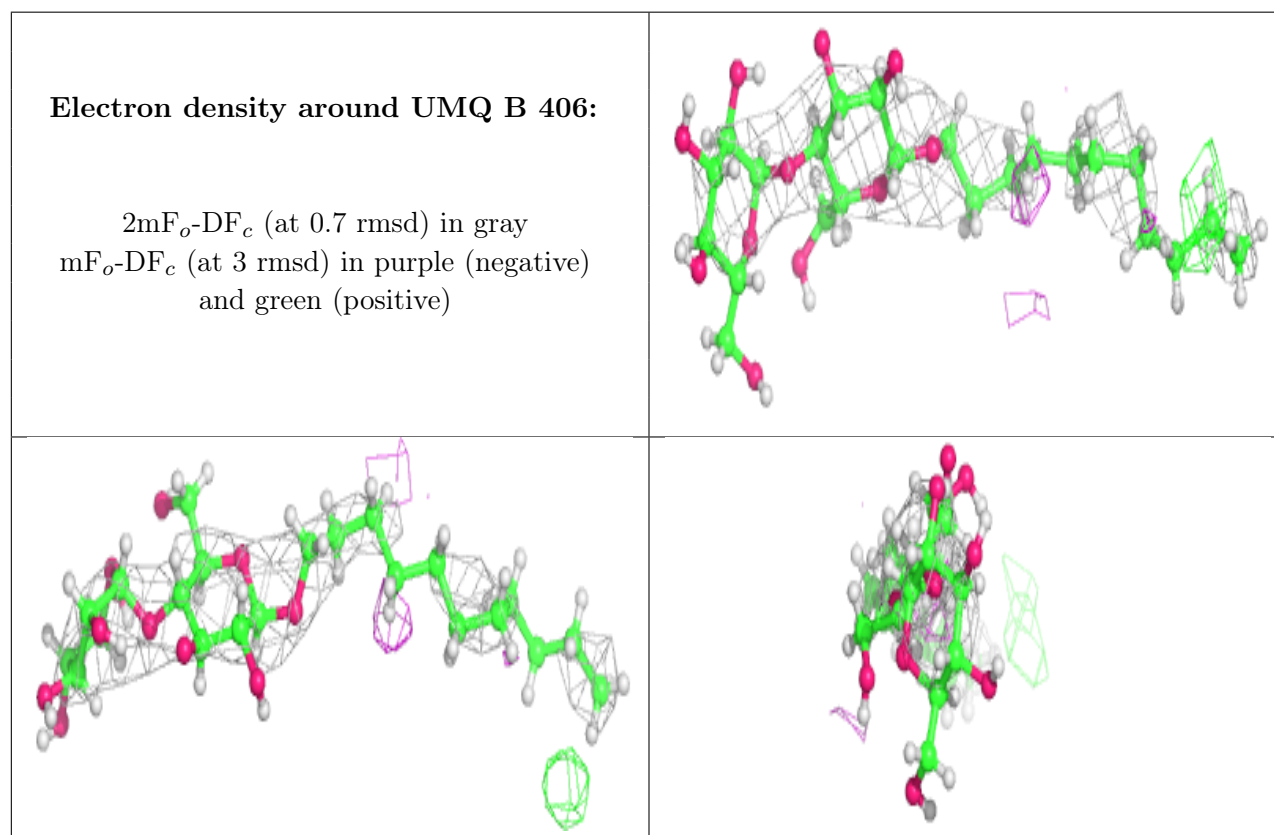
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	402	1/1	0.75	0.27	25,25,25,25	0
2	MG	B	401	1/1	0.78	0.37	16,16,16,16	0
4	UMQ	B	406	34/34	0.82	0.80	29,85,130,157	0
4	UMQ	A	405	32/34	0.85	0.48	18,76,107,113	0
4	UMQ	A	406	34/34	0.90	0.32	17,52,76,84	0
4	UMQ	A	403	11/34	0.90	0.35	20,21,22,23	0

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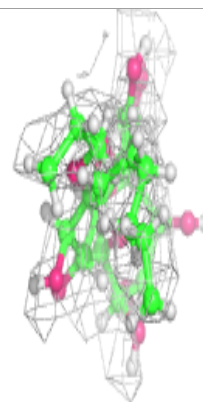
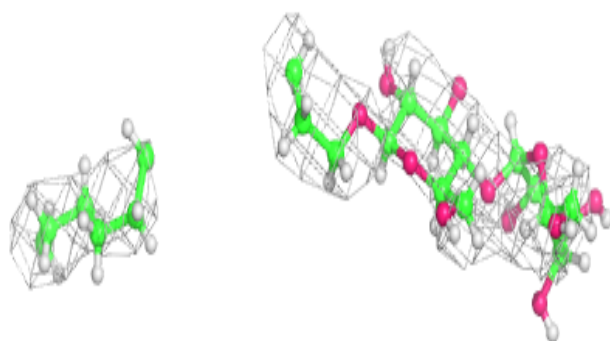
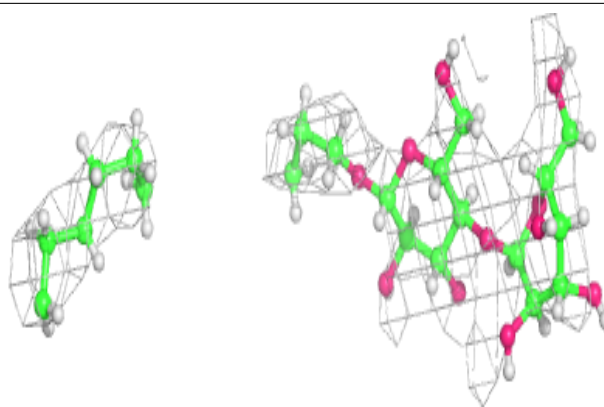
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	UMQ	B	404	13/34	0.91	0.23	14,20,36,36	0
4	UMQ	B	405	34/34	0.92	0.19	15,41,80,97	0
4	UMQ	A	407	31/34	0.92	0.20	20,46,69,95	0
6	1PE	A	409	16/16	0.92	0.33	10,52,88,93	0
4	UMQ	A	404	7/34	0.94	0.25	19,19,21,27	0
4	UMQ	B	407	7/34	0.95	0.20	18,18,18,18	0
2	MG	A	401	1/1	0.95	0.22	18,18,18,18	0
5	ATP	B	409	31/31	0.96	0.16	10,21,34,56	0
4	UMQ	B	408	5/34	0.96	0.24	19,19,20,20	0
5	ATP	A	408	31/31	0.97	0.19	12,19,40,46	0
3	SO4	B	403	5/5	0.99	0.14	11,11,15,26	0
3	SO4	A	402	5/5	0.99	0.14	17,17,21,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

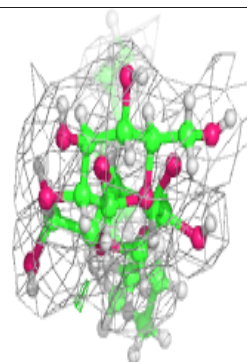
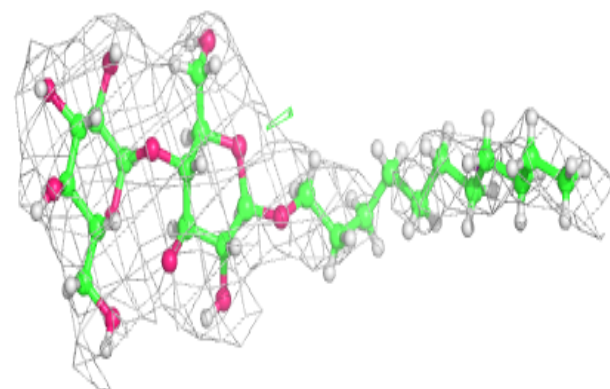
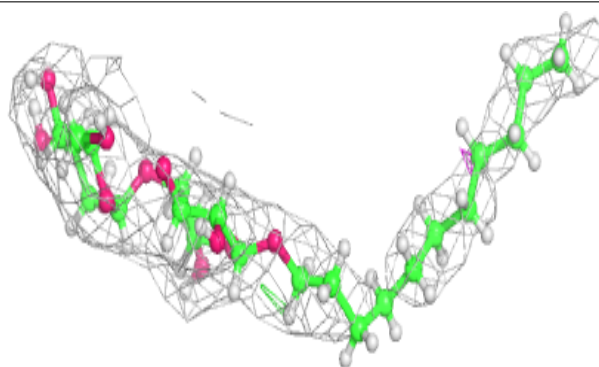


Electron density around UMQ A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

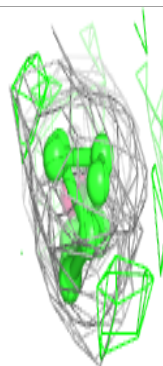
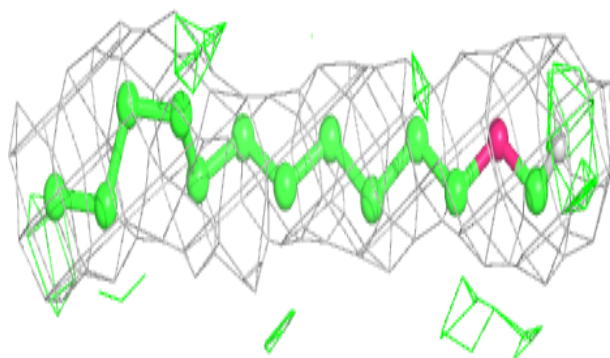
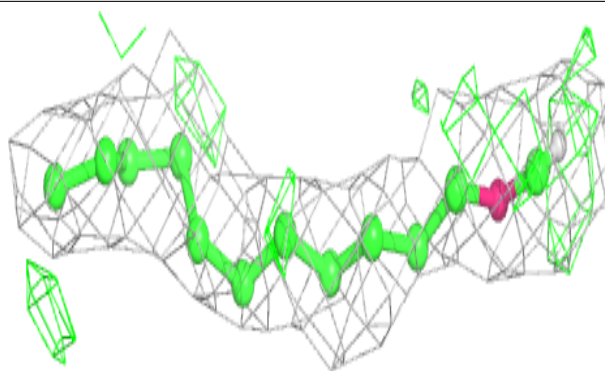
**Electron density around UMQ A 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

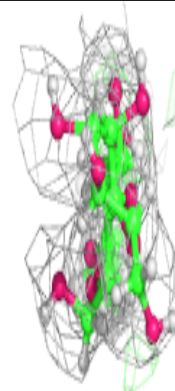
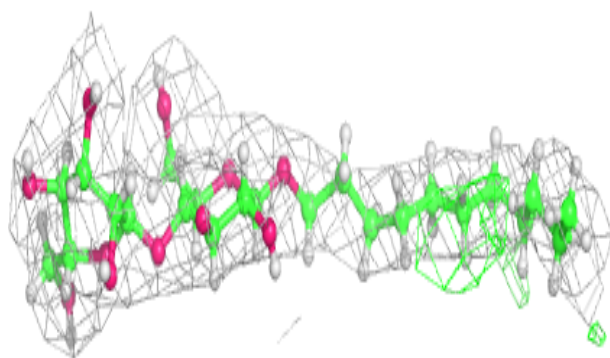
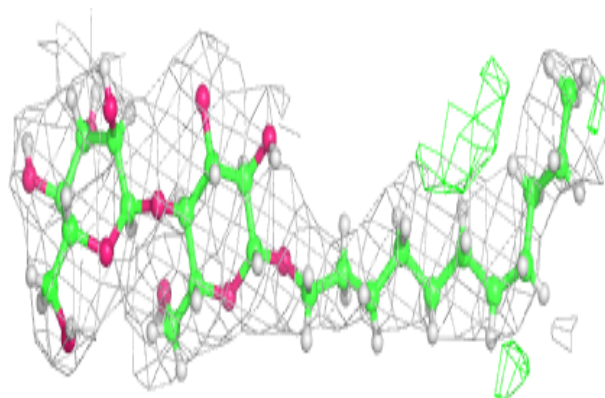


Electron density around UMQ B 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

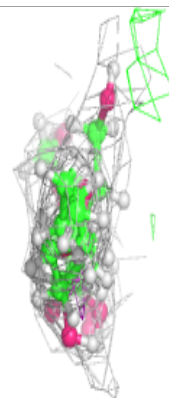
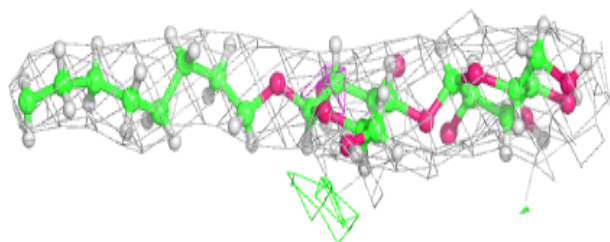
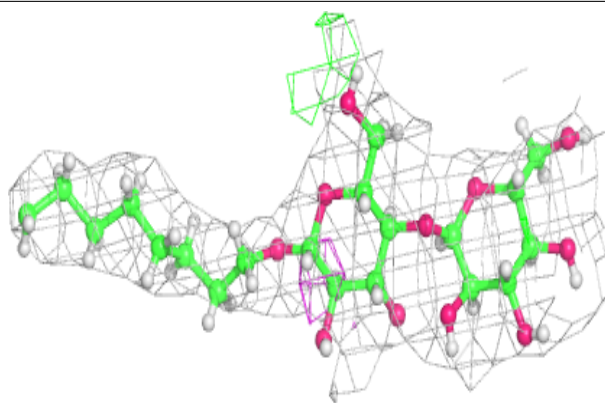
**Electron density around UMQ B 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

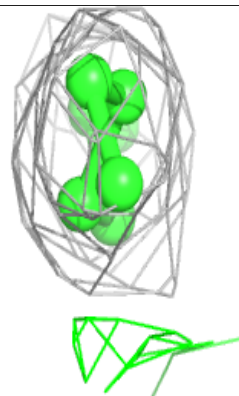
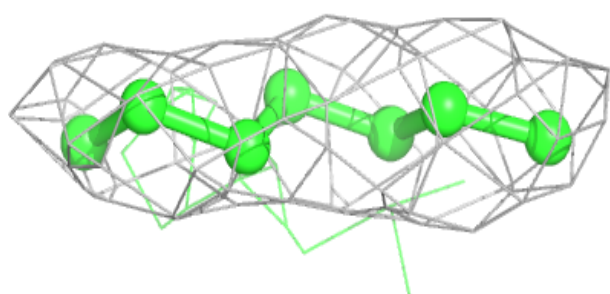
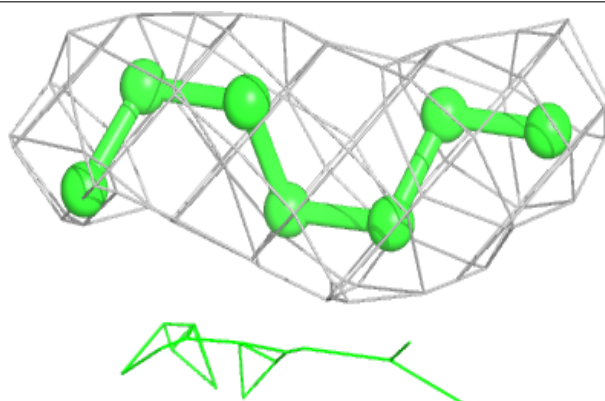


Electron density around UMQ A 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

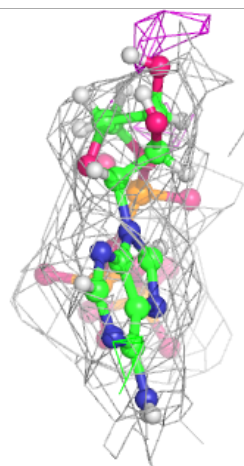
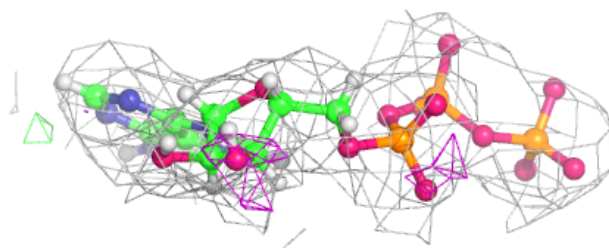
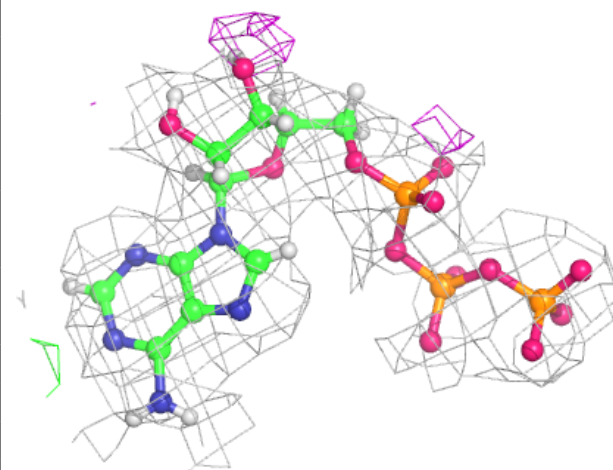
**Electron density around UMQ B 407:**

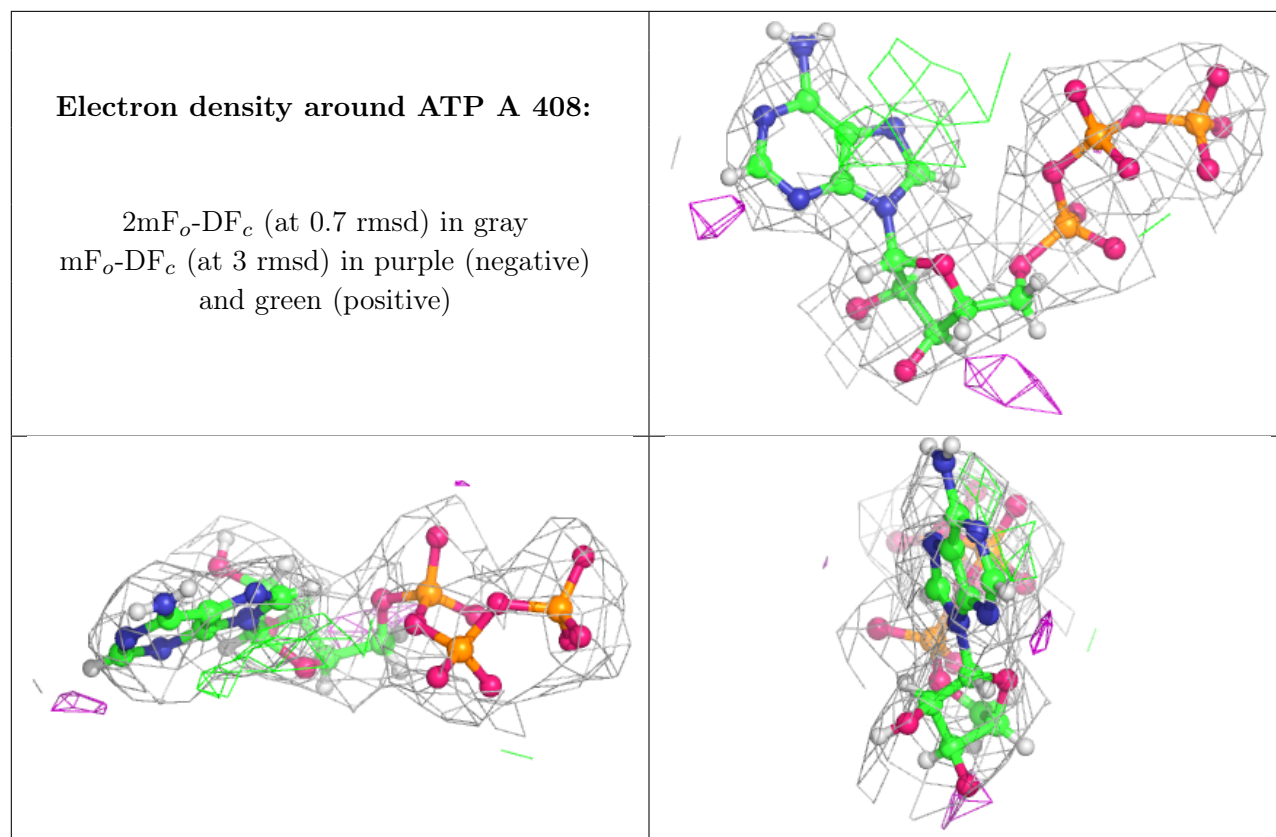
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP B 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.