



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 07:16 PM JST

PDB ID : 7WKV / pdb_00007wkv
Title : Crystal structure of human ALKBH5 in complex with 2-oxoglutarate (2OG) and m6A-containing ssRNA
Authors : Kaur, S.; McDonough, M.A.; Schofield, C.J.; Aik, W.S.
Deposited on : 2022-01-11
Resolution : 2.10 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

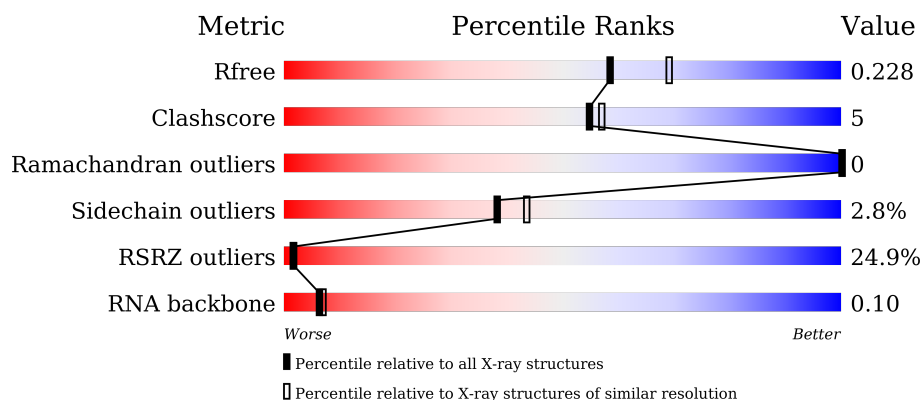
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	220	11% 85% 15%
1	C	220	28% 85% 14%
1	E	220	37% 85% 15%
2	B	8	25% 12% 12% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	8	 38%12%50%
2	F	8	 38%12%50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5527 atoms, of which 0 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 RNA demethylase ALKBH5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1732	1100	316	310	6			
1	C	219	Total	C	N	O	S	0	0	0
			1695	1075	304	310	6			
1	E	219	Total	C	N	O	S	0	0	0
			1711	1086	307	312	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	-	expression tag	UNP Q6P6C2
C	73	SER	-	expression tag	UNP Q6P6C2
E	73	SER	-	expression tag	UNP Q6P6C2

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*GP*(6MZ)P*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	P	0	0	0
			89	40	18	27	4			
2	D	4	Total	C	N	O	P	0	0	0
			89	40	18	27	4			
2	F	4	Total	C	N	O	P	0	0	0
			89	40	18	27	4			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

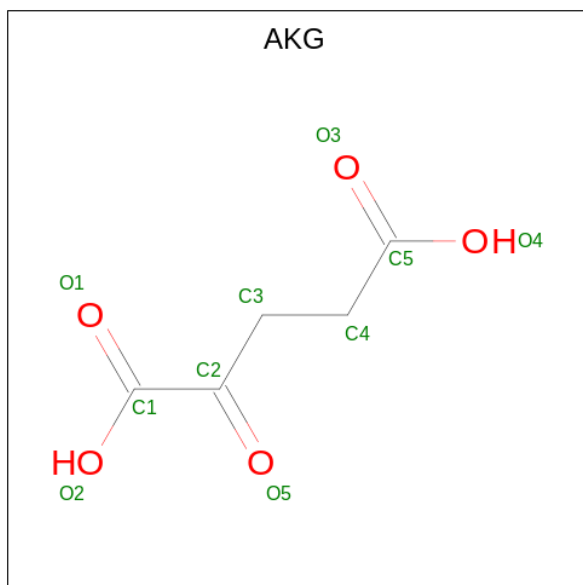
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	E	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	3	Total	O	0	0
			3	3		
5	C	19	Total	O	0	0
			19	19		
5	D	4	Total	O	0	0
			4	4		
5	E	27	Total	O	0	0
			27	27		

Continued on next page...

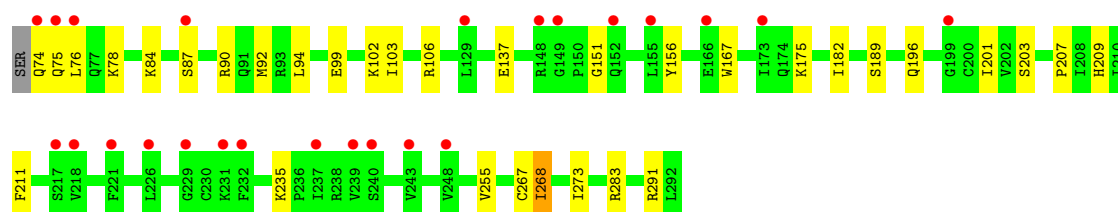
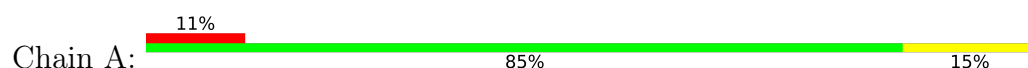
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	2	Total	O	0	0
			2	2		

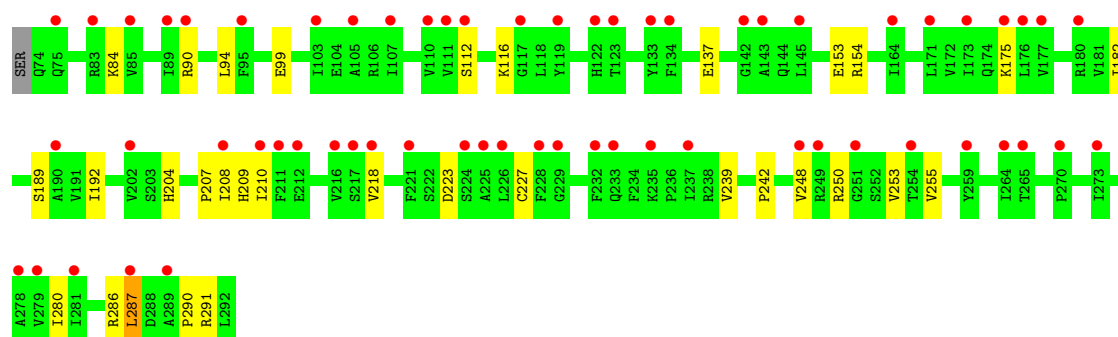
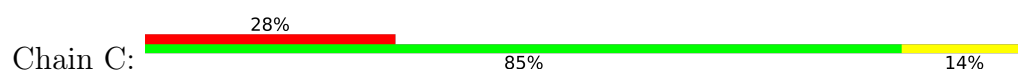
3 Residue-property plots [i](#)

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.

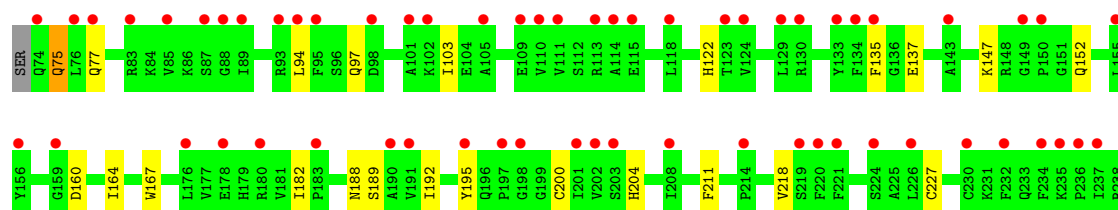
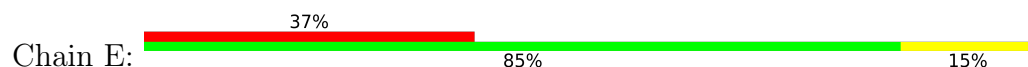
- Molecule 1: RNA demethylase ALKBH5



- Molecule 1: RNA demethylase ALKBH5

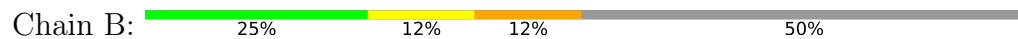


- Molecule 1: RNA demethylase ALKBH5

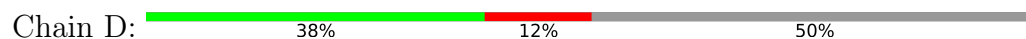




- Molecule 2: RNA (5'-R(P*GP*GP*(6MZ)P*C)-3')



- Molecule 2: RNA (5'-R(P*GP*GP*(6MZ)P*C)-3')



- Molecule 2: RNA (5'-R(P*GP*GP*(6MZ)P*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	78.36Å 78.36Å 106.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.26 – 2.10 57.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.26-2.10) 99.7 (57.26-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.188 , 0.228 0.189 , 0.228	Depositor DCC
R_{free} test set	2133 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.080 for -h,-k,l 0.093 for h,-h-k,-l 0.386 for -k,-h,-l	Xtriage
Reported twinning fraction	0.400 for -k,-h,-l	Depositor
Outliers	0 of 42646 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, AKG, 6MZ

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	0.18	0/1770	0.40	0/2394
1	C	0.14	0/1733	0.39	0/2354
1	E	0.21	0/1749	0.43	1/2371 (0.0%)
2	B	0.19	0/72	0.36	0/108
2	D	0.11	0/72	0.22	0/108
2	F	0.14	0/72	0.38	0/108
All	All	0.18	0/5468	0.40	1/7443 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	211	PHE	N-CA-C	6.38	119.86	109.59

There are no chirality outliers.

There are no planarity outliers.

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	1732	0	1728	21	0
1	C	1695	0	1639	15	0
1	E	1711	0	1676	16	0
2	B	89	0	47	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	89	0	47	1	0
2	F	89	0	47	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	10	0	4	0	0
4	C	10	0	4	0	0
4	E	10	0	4	1	0
5	A	34	0	0	1	0
5	B	3	0	0	0	0
5	C	19	0	0	0	0
5	D	4	0	0	0	0
5	E	27	0	0	0	0
5	F	2	0	0	0	0
All	All	5527	0	5196	51	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 5.

All (51) 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:A:268:ILE:HD11	1:A:273:ILE:HG12	1.61	0.81
1:A:75:GLN:HA	1:A:78:LYS:HE3	1.69	0.75
1:A:201:ILE:HG22	1:A:268:ILE:HG23	1.74	0.70
1:A:90:ARG:HB2	1:A:255:VAL:HB	1.76	0.66
1:C:99:GLU:OE1	1:C:175:LYS:NZ	2.33	0.62
1:A:196:GLN:HB3	1:E:75:GLN:HE22	1.66	0.59
1:C:112:SER:OG	1:C:116:LYS:NZ	2.35	0.59
1:E:227:CYS:HB3	1:E:242:PRO:HB3	1.85	0.57
1:A:99:GLU:OE1	1:A:175:LYS:NZ	2.37	0.56
1:A:92:MET:N	1:A:92:MET:SD	2.79	0.56
1:C:137:GLU:OE1	1:C:291:ARG:NH2	2.41	0.53
1:E:239:VAL:HG11	1:E:269:ARG:HG2	1.92	0.52
1:C:287:LEU:HD23	1:C:287:LEU:H	1.77	0.50
1:A:102:LYS:O	1:A:106:ARG:HG2	2.12	0.50
1:A:268:ILE:HD11	1:A:273:ILE:CG1	2.36	0.50
1:A:74:GLN:N	5:A:407:HOH:O	2.45	0.49
1:E:137:GLU:HB2	1:E:189:SER:HB2	1.94	0.49
1:C:90:ARG:HB2	1:C:255:VAL:HB	1.95	0.49
1:E:103:ILE:HG23	1:E:167:TRP:HZ3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:PHE:HB3	1:E:164:ILE:HA	1.95	0.48
1:C:137:GLU:HB2	1:C:189:SER:HB2	1.96	0.47
1:E:283:ARG:HH12	2:F:4:6MZ:H9C1	1.80	0.47
1:E:188:ASN:OD1	1:E:284:LYS:HA	2.15	0.46
1:A:151:GLY:HA2	1:A:209:HIS:CE1	2.51	0.46
1:E:122:HIS:ND1	1:E:160:ASP:OD2	2.31	0.45
1:A:103:ILE:HG23	1:A:167:TRP:HZ3	1.82	0.45
1:E:204:HIS:HB3	2:F:4:6MZ:O2'	2.17	0.45
1:A:137:GLU:HB2	1:A:189:SER:HB2	1.99	0.45
1:E:192:ILE:HG12	1:E:280:ILE:HG12	1.99	0.45
1:E:281:ILE:HD11	4:E:302:AKG:H32	1.99	0.44
1:C:227:CYS:HB3	1:C:242:PRO:HB3	2.00	0.44
1:A:235:LYS:HE3	2:B:3:G:O6	2.17	0.44
1:A:211:PHE:CD1	1:A:283:ARG:HD3	2.53	0.44
1:A:84:LYS:O	1:A:87:SER:OG	2.31	0.43
1:A:156:TYR:O	1:A:291:ARG:NH2	2.51	0.43
1:A:207:PRO:HB3	1:A:209:HIS:CE1	2.53	0.43
1:A:76:LEU:H	1:A:76:LEU:HD12	1.85	0.42
1:A:201:ILE:HG22	1:A:268:ILE:CG2	2.48	0.42
1:E:195:TYR:CZ	1:E:268:ILE:HD12	2.55	0.42
1:C:153:GLU:O	1:C:209:HIS:HE1	2.02	0.41
1:C:192:ILE:HG12	1:C:280:ILE:HG12	2.02	0.41
1:C:208:ILE:O	1:C:286:ARG:HD2	2.19	0.41
1:C:223:ASP:OD1	1:C:250:ARG:N	2.43	0.41
1:E:147:LYS:O	1:E:152:GLN:HG3	2.20	0.41
1:C:207:PRO:HG2	1:C:210:ILE:HB	2.03	0.41
1:E:200:CYS:HB2	1:E:268:ILE:O	2.20	0.41
1:C:218:VAL:HG22	1:C:253:VAL:HG22	2.02	0.41
1:A:203:SER:HA	1:A:267:CYS:HB3	2.03	0.41
1:C:204:HIS:HB3	2:D:4:6MZ:O2'	2.21	0.40
1:C:154:ARG:CD	1:C:290:PRO:HB2	2.52	0.40
1:E:218:VAL:HG22	1:E:253:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	217/220 (99%)	213 (98%)	4 (2%)	0	100	100
1	C	217/220 (99%)	214 (99%)	3 (1%)	0	100	100
1	E	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
All	All	651/660 (99%)	639 (98%)	12 (2%)	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	185/194 (95%)	182 (98%)	3 (2%)	55	64
1	C	177/194 (91%)	171 (97%)	6 (3%)	32	35
1	E	181/194 (93%)	175 (97%)	6 (3%)	33	37
All	All	543/582 (93%)	528 (97%)	15 (3%)	38	43

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	182	ILE
1	A	268	ILE
1	C	84	LYS
1	C	94	LEU
1	C	182	ILE
1	C	239	VAL
1	C	248	VAL
1	C	287	LEU
1	E	75	GLN
1	E	77	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	94	LEU
1	E	97	GLN
1	E	182	ILE
1	E	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	179	HIS
1	C	169	HIS
1	C	179	HIS
1	C	209	HIS
1	E	75	GLN
1	E	77	GLN
1	E	169	HIS
1	E	170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	3/8 (37%)	1 (33%)	0
2	D	3/8 (37%)	1 (33%)	0
2	F	3/8 (37%)	1 (33%)	0
All	All	9/24 (37%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	6MZ
2	D	4	6MZ
2	F	4	6MZ

There are no RNA pucker outliers to report.

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

3 non-standard protein/DNA/RNA residues 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
2	6MZ	F	4	2	22,25,26	0.97	2 (9%)	30,36,39	1.53	5 (16%)
2	6MZ	B	4	2	22,25,26	0.97	2 (9%)	30,36,39	1.67	7 (23%)
2	6MZ	D	4	2	22,25,26	0.98	2 (9%)	30,36,39	1.48	4 (13%)

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
2	6MZ	F	4	2	-	2/9/27/28	0/3/3/3
2	6MZ	B	4	2	-	2/9/27/28	0/3/3/3
2	6MZ	D	4	2	-	2/9/27/28	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	6MZ	C8-N7	2.56	1.36	1.31
2	F	4	6MZ	C8-N7	2.50	1.36	1.31
2	B	4	6MZ	C8-N7	2.45	1.36	1.31
2	F	4	6MZ	C5-N7	-2.20	1.34	1.39
2	D	4	6MZ	C5-N7	-2.20	1.34	1.39
2	B	4	6MZ	C5-N7	-2.17	1.34	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	6MZ	C5-C4-N3	-4.94	120.30	126.75
2	F	4	6MZ	C5-C4-N3	-4.66	120.66	126.75
2	D	4	6MZ	C5-C4-N3	-4.40	121.01	126.75
2	B	4	6MZ	N3-C4-N9	3.79	133.33	127.08
2	F	4	6MZ	N3-C4-N9	3.34	132.58	127.08
2	D	4	6MZ	N3-C4-N9	3.23	132.40	127.08
2	B	4	6MZ	N9-C8-N7	-2.93	109.90	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	6MZ	N9-C8-N7	-2.76	110.14	113.91
2	F	4	6MZ	N9-C8-N7	-2.72	110.19	113.91
2	B	4	6MZ	C5-C6-N1	2.71	121.08	118.20
2	F	4	6MZ	C5-C6-N1	2.67	121.05	118.20
2	B	4	6MZ	C4-C5-C6	2.67	118.87	116.81
2	D	4	6MZ	C5-C6-N1	2.62	120.99	118.20
2	F	4	6MZ	C4-C5-C6	2.37	118.64	116.81
2	B	4	6MZ	C4-N9-C8	2.21	108.12	105.73
2	B	4	6MZ	C5-N7-C8	2.07	106.45	103.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	6MZ	O4'-C4'-C5'-O5'
2	F	4	6MZ	O4'-C4'-C5'-O5'
2	B	4	6MZ	O4'-C4'-C5'-O5'
2	D	4	6MZ	C3'-C4'-C5'-O5'
2	B	4	6MZ	C3'-C4'-C5'-O5'
2	F	4	6MZ	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	6MZ	2	0
2	D	4	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AKG	C	302	3	9,9,9	1.00	0	11,11,11	1.39	1 (9%)
4	AKG	A	302	3	9,9,9	1.16	0	11,11,11	1.40	2 (18%)
4	AKG	E	302	3	9,9,9	1.09	0	11,11,11	1.18	1 (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
4	AKG	C	302	3	-	4/9/9/9	-
4	AKG	A	302	3	-	3/9/9/9	-
4	AKG	E	302	3	-	4/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	AKG	O1-C1-C2	-3.62	116.88	121.72
4	A	302	AKG	O1-C1-C2	-3.16	117.49	121.72
4	E	302	AKG	O1-C1-C2	-3.08	117.61	121.72
4	A	302	AKG	O4-C5-C4	2.04	120.59	114.03

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	AKG	O2-C1-C2-O5
4	E	302	AKG	O2-C1-C2-O5
4	E	302	AKG	C3-C4-C5-O3
4	E	302	AKG	C3-C4-C5-O4
4	A	302	AKG	C2-C3-C4-C5
4	C	302	AKG	C2-C3-C4-C5
4	E	302	AKG	C2-C3-C4-C5
4	C	302	AKG	C3-C4-C5-O3
4	C	302	AKG	C3-C4-C5-O4

Continued on next page...

Continued from previous page...

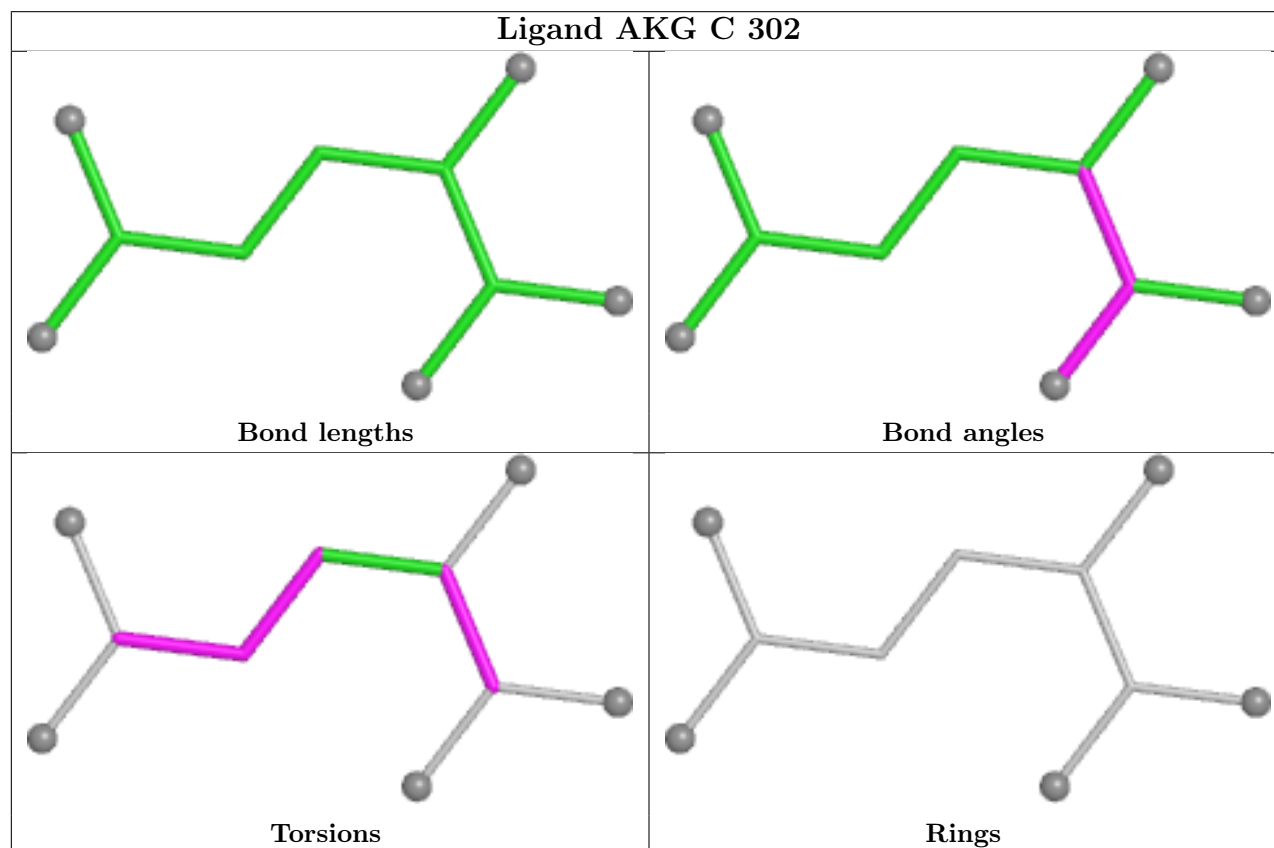
Mol	Chain	Res	Type	Atoms
4	A	302	AKG	C3-C4-C5-O3
4	A	302	AKG	C3-C4-C5-O4

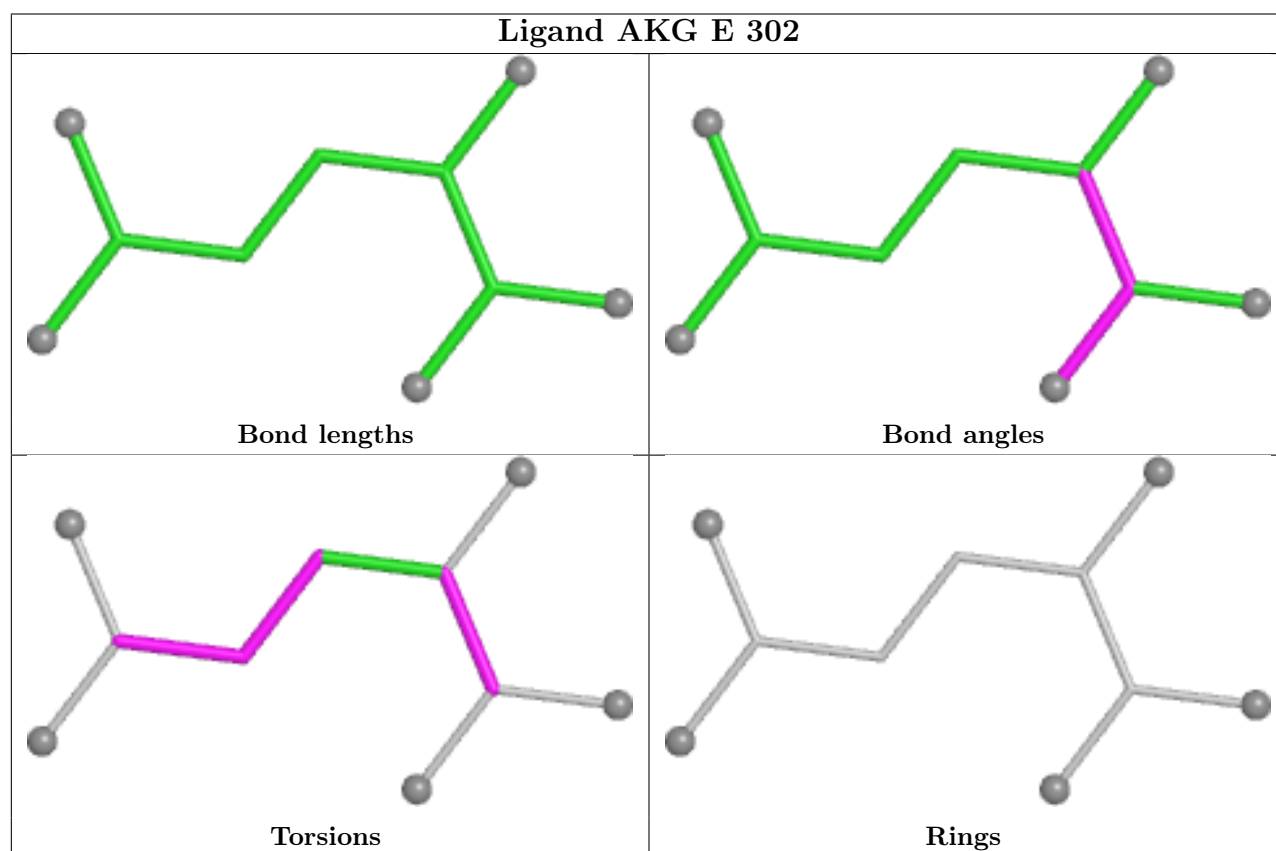
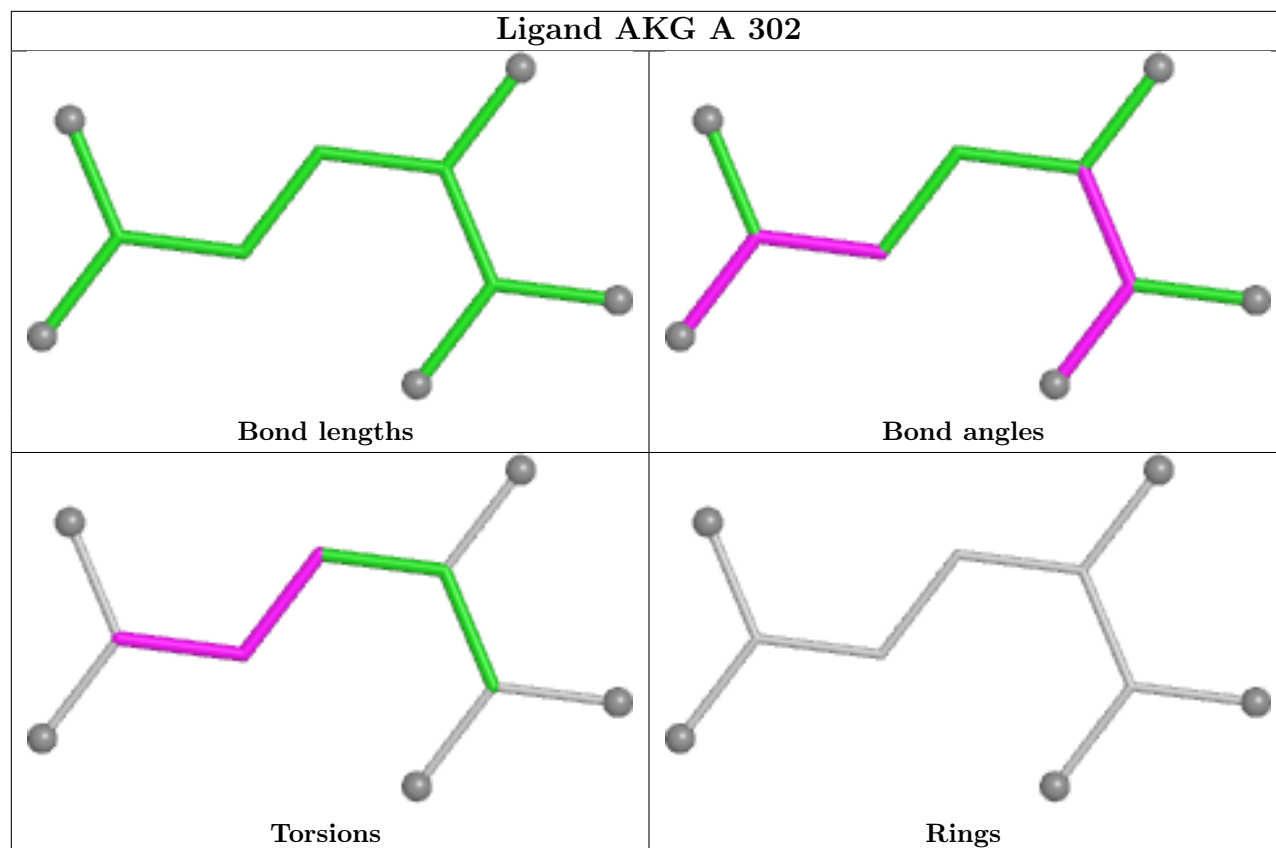
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	302	AKG	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 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	219/220 (99%)	1.04	24 (10%)	10 11	31, 42, 66, 112	0
1	C	219/220 (99%)	1.61	61 (27%)	1 1	42, 50, 65, 84	0
1	E	219/220 (99%)	1.78	81 (36%)	1 1	42, 53, 75, 104	0
2	B	3/8 (37%)	-0.03	0	100 100	44, 44, 48, 50	0
2	D	3/8 (37%)	0.71	0	100 100	56, 56, 58, 60	0
2	F	3/8 (37%)	0.82	0	100 100	60, 60, 66, 68	0
All	All	666/684 (97%)	1.46	166 (24%)	2 2	31, 50, 69, 112	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	ALA	7.0
1	E	278	ALA	5.7
1	E	235	LYS	5.0
1	E	88	GLY	4.9
1	C	103	ILE	4.8
1	E	201	ILE	4.8
1	C	133	TYR	4.6
1	C	202	VAL	4.4
1	E	111	VAL	4.4
1	E	220	PHE	4.1
1	C	164	ILE	4.1
1	E	77	GLN	4.0
1	C	273	ILE	4.0
1	E	287	LEU	3.9
1	C	226	LEU	3.8
1	E	254	THR	3.8
1	C	221	PHE	3.8
1	E	134	PHE	3.7
1	C	265	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	235	LYS	3.6
1	C	237	ILE	3.6
1	C	107	ILE	3.5
1	E	221	PHE	3.5
1	C	177	VAL	3.4
1	E	214	PRO	3.4
1	C	190	ALA	3.4
1	A	231	LYS	3.4
1	E	176	LEU	3.3
1	C	117	GLY	3.3
1	A	243	VAL	3.3
1	A	239	VAL	3.3
1	E	195	TYR	3.3
1	E	155	LEU	3.3
1	E	281	ILE	3.2
1	E	123	THR	3.2
1	C	90	ARG	3.2
1	A	76	LEU	3.2
1	C	229	GLY	3.2
1	A	226	LEU	3.2
1	C	145	LEU	3.1
1	C	83	ARG	3.1
1	C	180	ARG	3.1
1	C	218	VAL	3.1
1	E	101	ALA	3.1
1	C	208	ILE	3.1
1	C	119	TYR	3.0
1	C	232	PHE	3.0
1	E	288	ASP	3.0
1	A	129	LEU	3.0
1	E	110	VAL	3.0
1	C	249	ARG	2.9
1	E	198	GLY	2.9
1	C	105	ALA	2.9
1	E	129	LEU	2.8
1	E	232	PHE	2.8
1	A	148	ARG	2.8
1	A	221	PHE	2.8
1	E	260	ALA	2.8
1	E	244	LEU	2.8
1	A	237	ILE	2.8
1	C	228	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	166	GLU	2.7
1	C	264	ILE	2.7
1	E	74	GLN	2.7
1	E	114	ALA	2.7
1	E	93	ARG	2.7
1	E	253	VAL	2.7
1	C	281	ILE	2.7
1	A	199	GLY	2.7
1	C	211	PHE	2.6
1	C	171	LEU	2.6
1	A	240	SER	2.6
1	A	173	ILE	2.6
1	E	264	ILE	2.6
1	A	149	GLY	2.6
1	C	270	PRO	2.6
1	E	239	VAL	2.6
1	E	113	ARG	2.6
1	E	252	SER	2.6
1	A	152	GLN	2.6
1	E	89	ILE	2.6
1	E	272	ASP	2.6
1	E	135	PHE	2.5
1	A	218	VAL	2.5
1	C	279	VAL	2.5
1	E	133	TYR	2.5
1	E	251	GLY	2.5
1	A	87	SER	2.5
1	E	150	PRO	2.5
1	E	203	SER	2.5
1	C	134	PHE	2.5
1	C	251	GLY	2.5
1	E	191	VAL	2.5
1	E	156	TYR	2.5
1	E	76	LEU	2.5
1	E	226	LEU	2.5
1	A	248	VAL	2.5
1	E	197	PRO	2.5
1	E	180	ARG	2.5
1	E	276	ARG	2.5
1	C	122	HIS	2.4
1	E	130	ARG	2.4
1	C	210	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	109	GLU	2.4
1	E	95	PHE	2.4
1	E	234	PHE	2.4
1	E	98	ASP	2.4
1	C	173	ILE	2.4
1	E	115	GLU	2.4
1	E	149	GLY	2.4
1	A	74	GLN	2.3
1	C	85	VAL	2.3
1	E	85	VAL	2.3
1	E	143	ALA	2.3
1	A	155	LEU	2.3
1	C	176	LEU	2.3
1	C	287	LEU	2.3
1	E	240	SER	2.3
1	C	111	VAL	2.3
1	A	75	GLN	2.3
1	E	230	CYS	2.3
1	E	83	ARG	2.3
1	E	219	SER	2.3
1	E	102	LYS	2.3
1	E	159	GLY	2.3
1	E	224	SER	2.2
1	A	232	PHE	2.2
1	E	208	ILE	2.2
1	E	202	VAL	2.2
1	E	236	PRO	2.2
1	C	289	ALA	2.2
1	E	105	ALA	2.2
1	C	217	SER	2.2
1	C	254	THR	2.2
1	C	216	VAL	2.2
1	C	233	GLN	2.2
1	E	87	SER	2.2
1	C	175	LYS	2.2
1	C	89	ILE	2.2
1	E	237	ILE	2.2
1	C	248	VAL	2.2
1	E	124	VAL	2.2
1	E	94	LEU	2.2
1	C	112	SER	2.2
1	E	259	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	178	GLU	2.1
1	C	123	THR	2.1
1	E	268	ILE	2.1
1	E	273	ILE	2.1
1	A	229	GLY	2.1
1	E	190	ALA	2.1
1	C	224	SER	2.1
1	E	118	LEU	2.1
1	C	142	GLY	2.1
1	C	95	PHE	2.1
1	C	278	ALA	2.1
1	A	217	SER	2.1
1	C	212	GLU	2.1
1	E	242	PRO	2.1
1	C	75	GLN	2.0
1	E	267	CYS	2.0
1	C	259	TYR	2.0
1	E	258	GLY	2.0
1	C	110	VAL	2.0
1	C	225	ALA	2.0
1	E	183	PRO	2.0

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

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	6MZ	F	4	23/24	0.91	0.15	50,52,55,57	0
2	6MZ	B	4	23/24	0.93	0.10	35,37,40,48	0
2	6MZ	D	4	23/24	0.96	0.10	45,51,54,56	0

6.3 Carbohydrates [i](#)

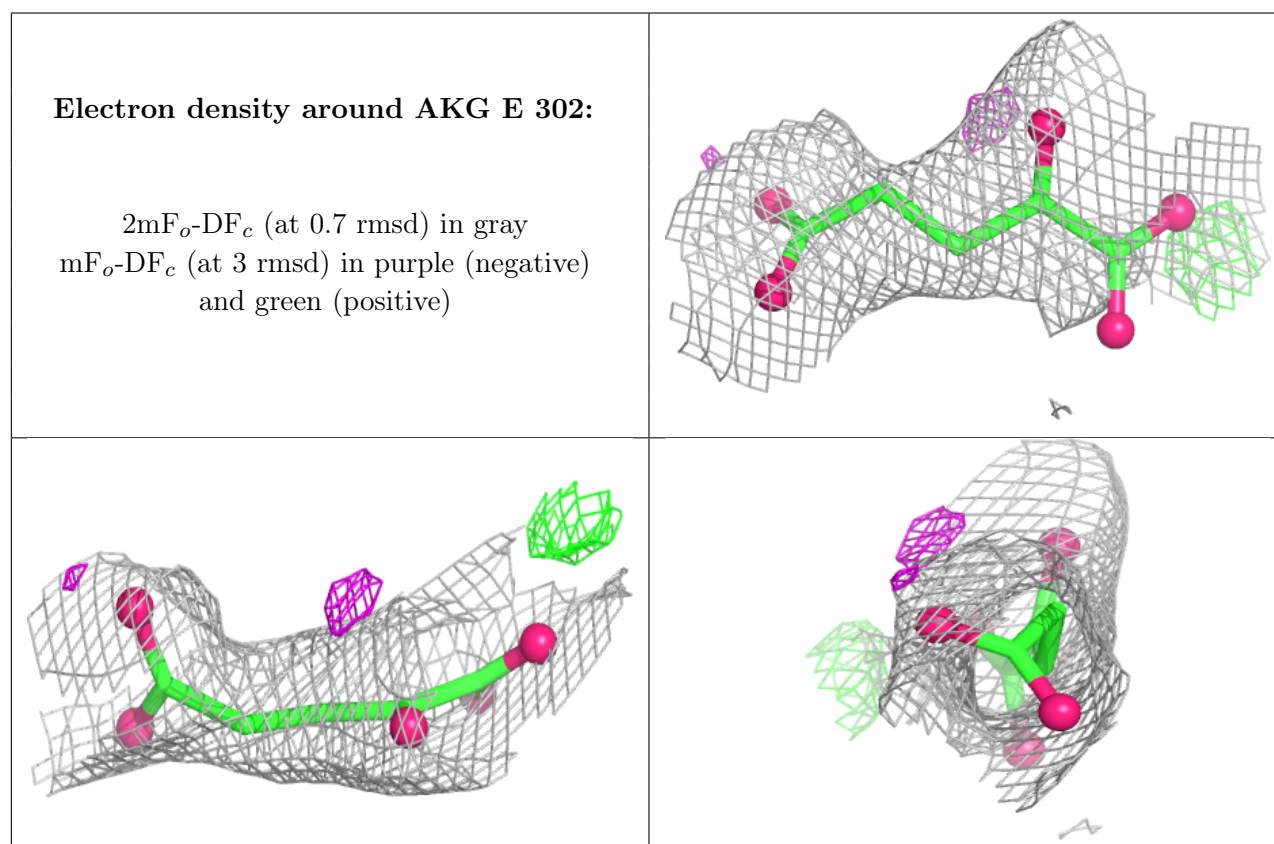
There are no oligosaccharides in this entry.

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.

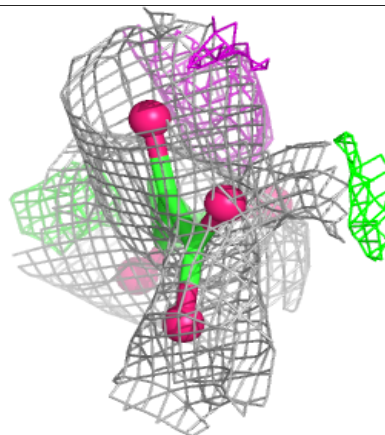
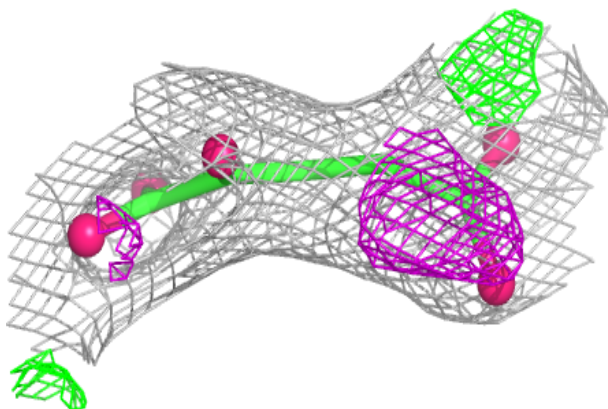
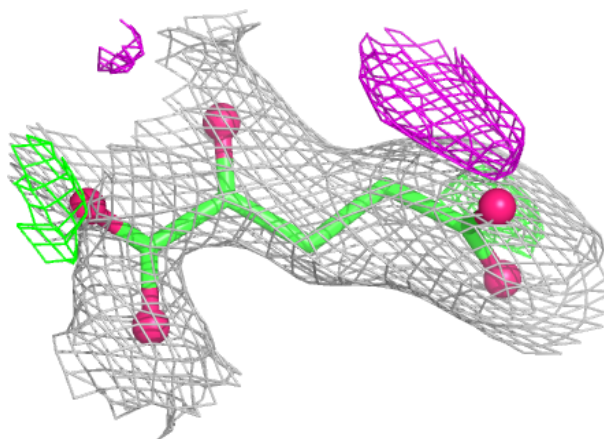
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AKG	E	302	10/10	0.94	0.13	41,48,52,62	0
4	AKG	A	302	10/10	0.96	0.12	7,31,35,39	0
4	AKG	C	302	10/10	0.97	0.09	28,37,45,47	0
3	MN	E	301	1/1	0.99	0.03	45,45,45,45	0
3	MN	A	301	1/1	0.99	0.06	19,19,19,19	0
3	MN	C	301	1/1	1.00	0.03	42,42,42,42	0

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.



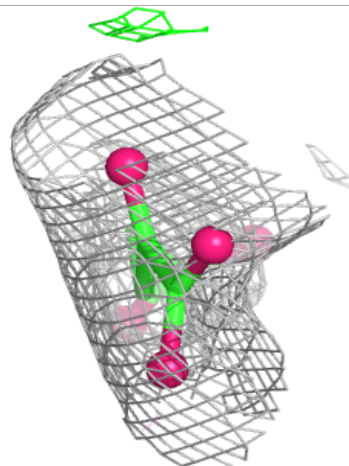
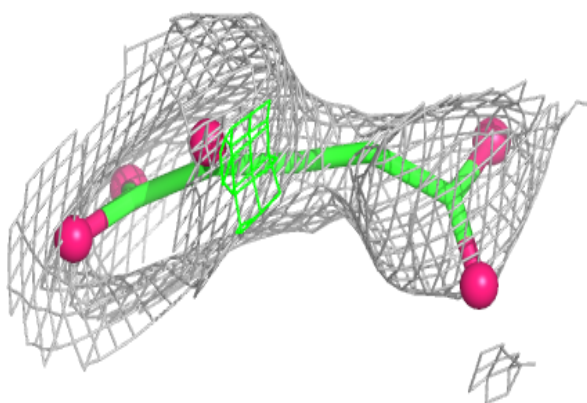
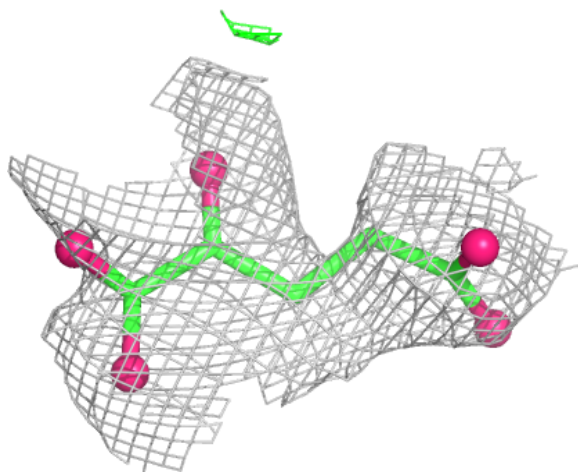
Electron density around AKG A 302:

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



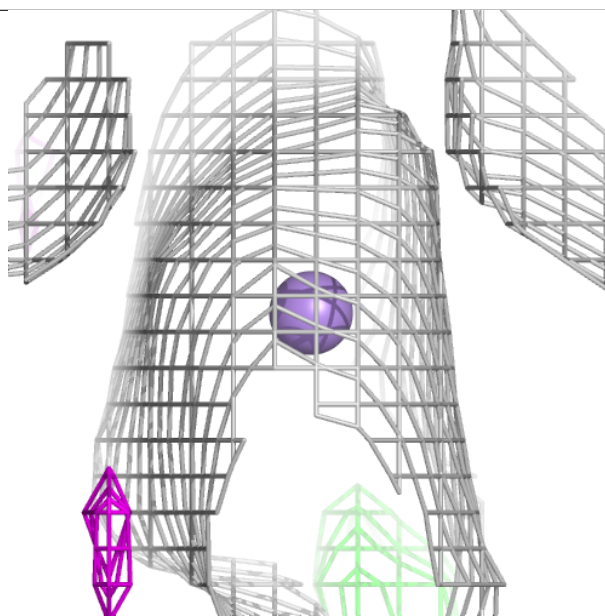
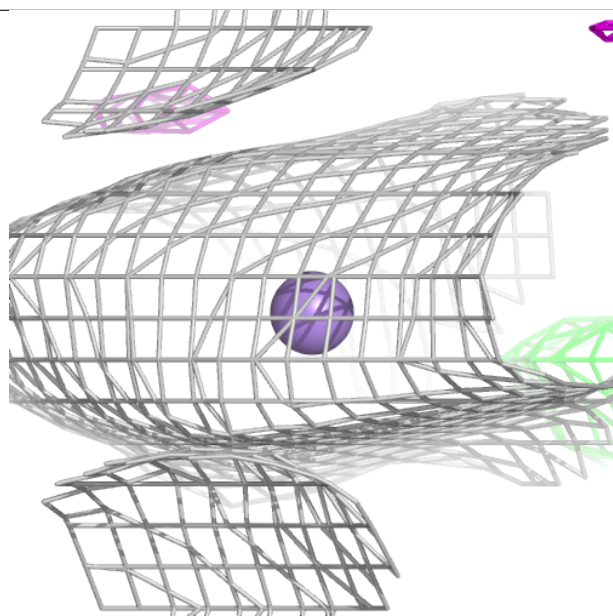
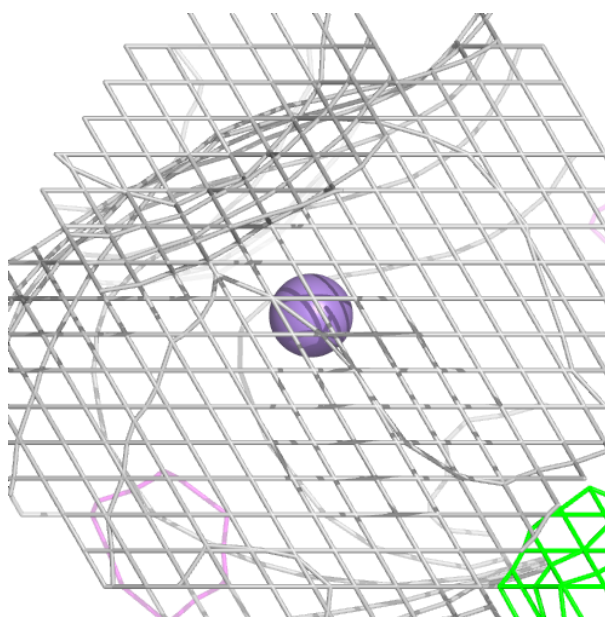
Electron density around AKG C 302:

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



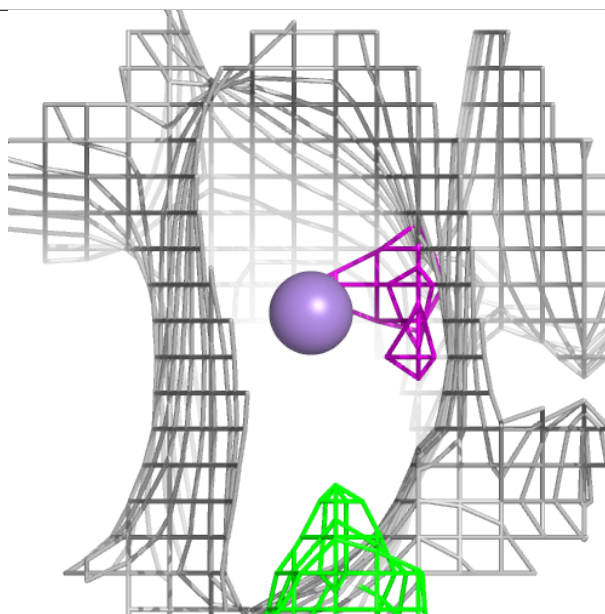
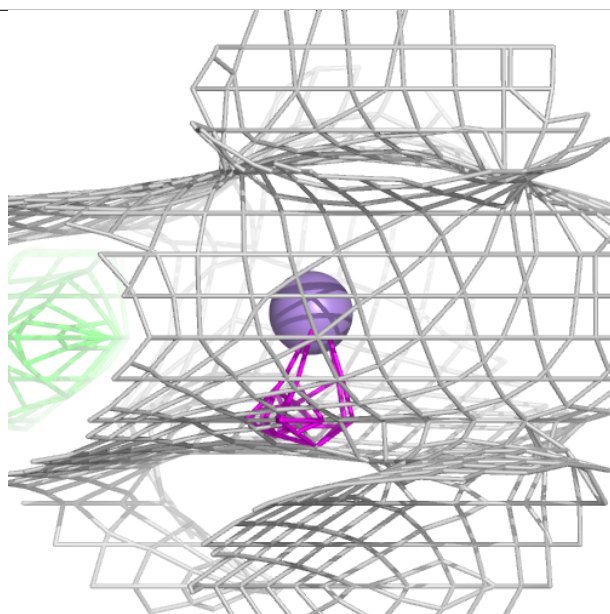
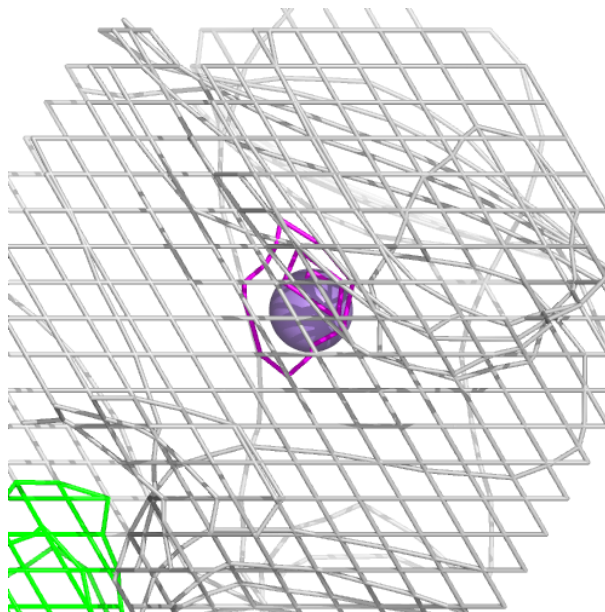
Electron density around MN E 301:

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



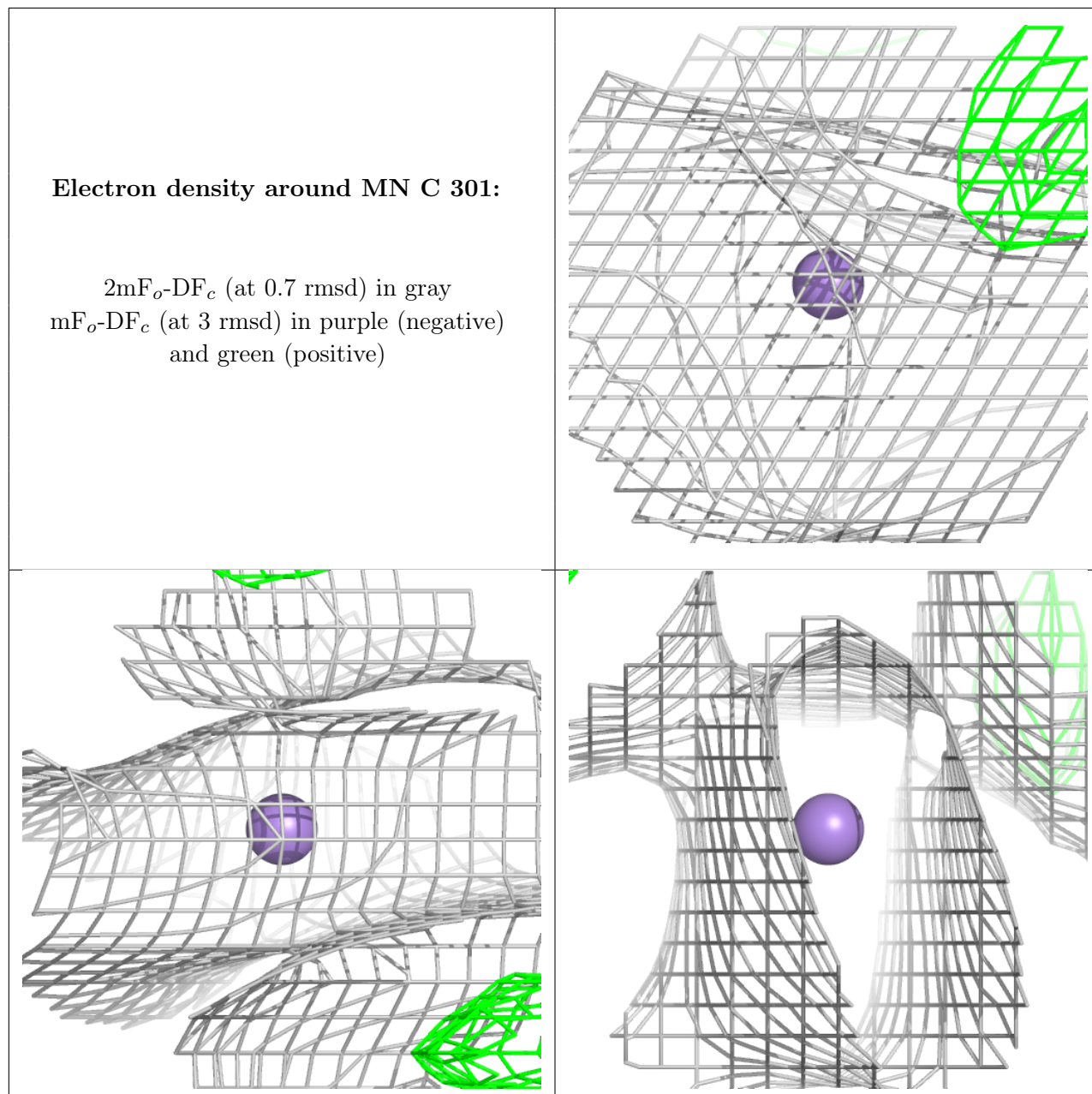
Electron density around MN A 301:

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



Electron density around MN C 301:

$2mF_o-DF_c$ (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.