



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:17 PM UTC

PDB ID : 8OOQ / pdb_00008ooq
Title : Glutamine synthetase from Methanothermococcus thermolithotrophicus in complex with 2-oxoglutarate and Mg at 2.91 Å resolution
Authors : Mueller, M.-C.; Wagner, T.
Deposited on : 2023-04-05
Resolution : 2.91 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 : 2022.3.0, CSD as543be (2022)
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

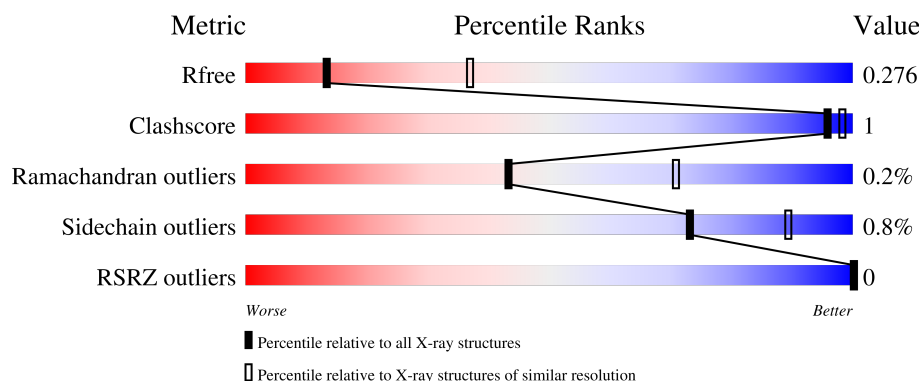
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

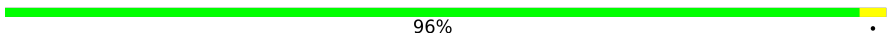
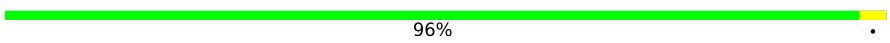
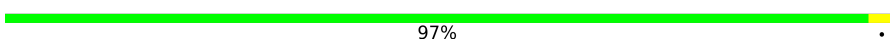
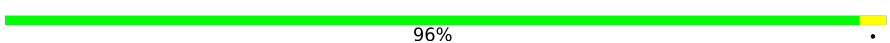
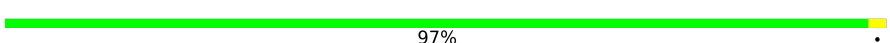
The reported resolution of this entry is 2.91 Å.

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.



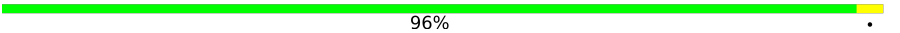
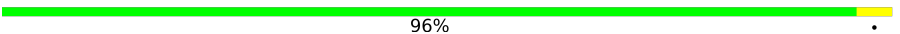
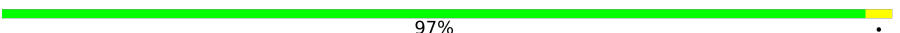
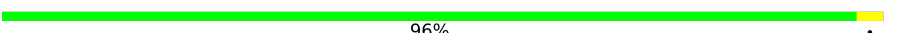
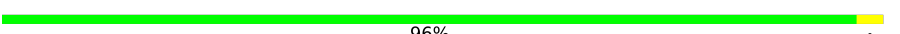
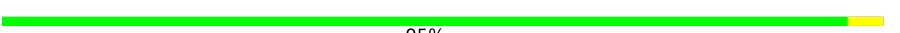
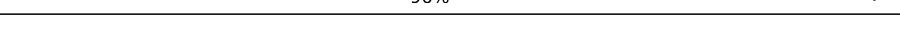
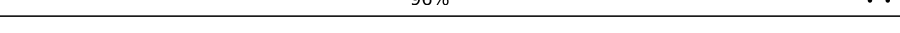
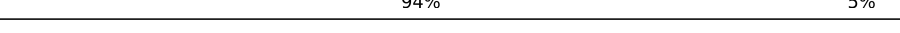
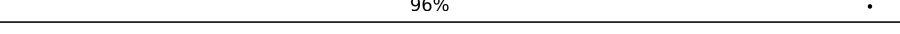
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	448	 96%
1	B	448	 96%
1	C	448	 97%
1	D	448	 96%
1	E	448	 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	448	 96% .
1	G	448	 96% .
1	H	448	 97% .
1	I	448	 96% .
1	J	448	 96% .
1	K	448	 95% .
1	L	448	 95% .
1	P	448	 95% .
1	Q	448	 96% .
1	S	448	 95% .
1	T	448	 95% . .
1	U	448	 96% .
1	V	448	 96% .
1	X	448	 96% .
1	Y	448	 96% .
1	Z	448	 96% . .
1	a	448	 94% 5%
1	b	448	 96% .
1	c	448	 96% .

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
2	EDO	X	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 85163 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 Glutamine synthetase from *Methanothermococcus thermolithotrophicus*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3528	2261	586	665	16			
1	B	446	Total	C	N	O	S	0	0	0
			3528	2261	586	665	16			
1	C	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	E	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	F	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	G	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	H	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	I	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	J	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	K	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	L	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	P	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	Q	446	Total	C	N	O	S	0	0	0
			3528	2261	586	665	16			
1	S	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	T	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	V	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	X	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	Y	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	Z	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	a	446	Total	C	N	O	S	0	0	0
			3528	2261	586	665	16			
1	b	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	c	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total 4	C 2	O 2	0	0
2	K	1	Total 4	C 2	O 2	0	0
2	P	1	Total 4	C 2	O 2	0	0
2	P	1	Total 4	C 2	O 2	0	0
2	S	1	Total 4	C 2	O 2	0	0
2	U	1	Total 4	C 2	O 2	0	0
2	U	1	Total 4	C 2	O 2	0	0
2	V	1	Total 4	C 2	O 2	0	0
2	V	1	Total 4	C 2	O 2	0	0
2	X	1	Total 4	C 2	O 2	0	0
2	X	1	Total 4	C 2	O 2	0	0
2	Y	1	Total 4	C 2	O 2	0	0
2	Y	1	Total 4	C 2	O 2	0	0
2	Z	1	Total 4	C 2	O 2	0	0
2	a	1	Total 4	C 2	O 2	0	0
2	a	1	Total 4	C 2	O 2	0	0
2	a	1	Total 4	C 2	O 2	0	0
2	b	1	Total 4	C 2	O 2	0	0
2	b	1	Total 4	C 2	O 2	0	0
2	c	1	Total 4	C 2	O 2	0	0
2	c	1	Total 4	C 2	O 2	0	0

Continued on next page...

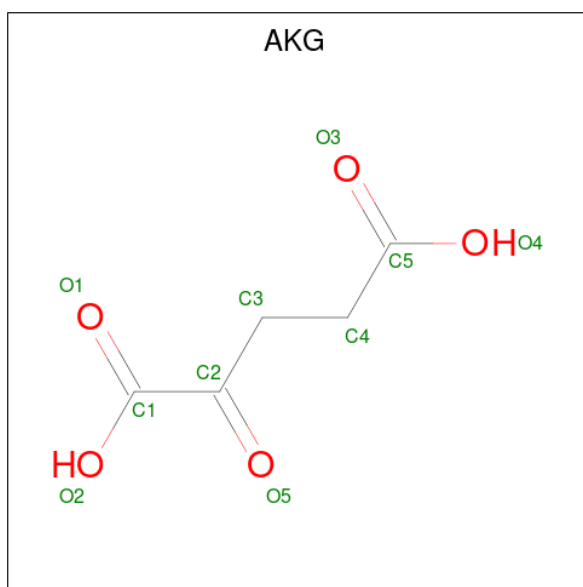
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	c	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	P	1	Total	Mg	0	0
			1	1		
3	Q	2	Total	Mg	0	0
			2	2		
3	S	1	Total	Mg	0	0
			1	1		
3	T	3	Total	Mg	0	0
			3	3		
3	Y	1	Total	Mg	0	0
			1	1		
3	b	2	Total	Mg	0	0
			2	2		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅) (labeled as "Ligand of Interest" by depositor).



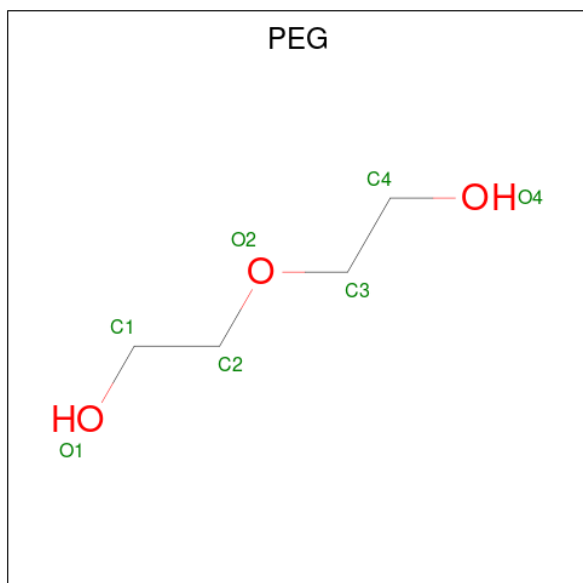
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		
4	C	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	0
			10	5	5		
4	E	1	Total	C	O	0	0
			10	5	5		
4	F	1	Total	C	O	0	0
			10	5	5		
4	G	1	Total	C	O	0	0
			10	5	5		
4	H	1	Total	C	O	0	0
			10	5	5		
4	I	1	Total	C	O	0	0
			10	5	5		
4	J	1	Total	C	O	0	0
			10	5	5		
4	K	1	Total	C	O	0	0
			10	5	5		
4	L	1	Total	C	O	0	0
			10	5	5		
4	P	1	Total	C	O	0	0
			10	5	5		
4	Q	1	Total	C	O	0	0
			10	5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	C	O	0	0
			10	5	5		
4	T	1	Total	C	O	0	0
			10	5	5		
4	U	1	Total	C	O	0	0
			10	5	5		
4	V	1	Total	C	O	0	0
			10	5	5		
4	X	1	Total	C	O	0	0
			10	5	5		
4	Y	1	Total	C	O	0	0
			10	5	5		
4	Z	1	Total	C	O	0	0
			10	5	5		
4	a	1	Total	C	O	0	0
			10	5	5		
4	b	1	Total	C	O	0	0
			10	5	5		
4	c	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

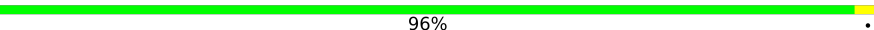
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	Z	1	7	4	3	0	0

3 Residue-property plots [i](#)

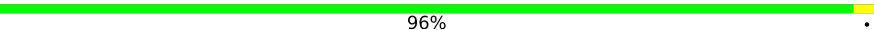
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain A:  96%

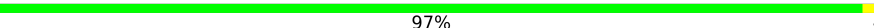


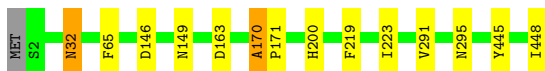
- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain B:  96%

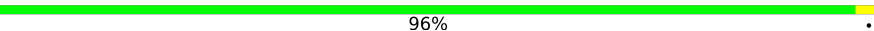


- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain C:  97%

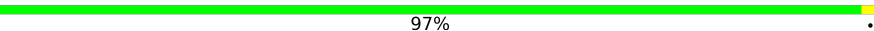


- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain D:  96%

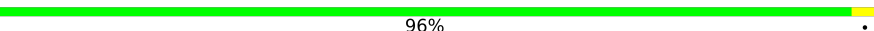


- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain E:  97%

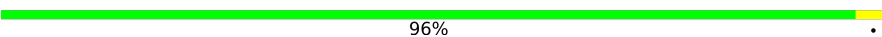


- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

Chain F:  96%

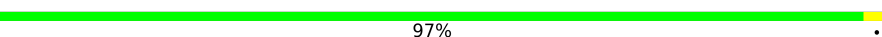


- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain G:  96%

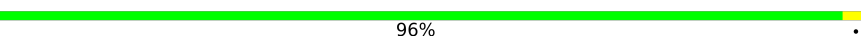


- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain H:  97%

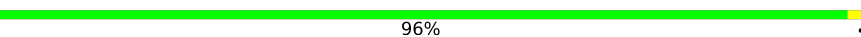


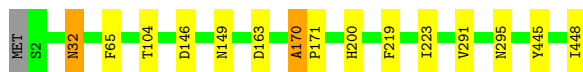
- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain I:  96%

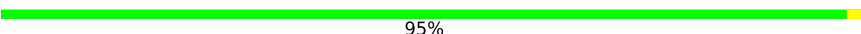


- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain J:  96%

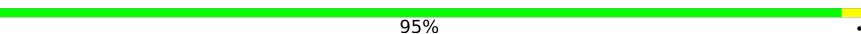


- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain K:  95%

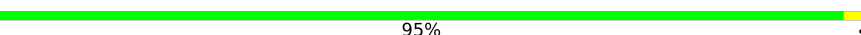


- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain L:  95%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain P:  95%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain Q: 96%



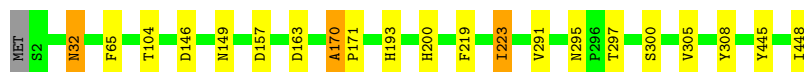
- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain S: 95%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain T: 95%



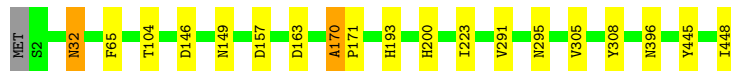
- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain U: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain V: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain X: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain Y: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain Z: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain a: 94% 5%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain b: 96%



- Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain c: 96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	131.81Å 131.93Å 203.54Å 89.95° 89.86° 60.05°	Depositor
Resolution (Å)	43.74 – 2.91 43.74 – 2.91	Depositor EDS
% Data completeness (in resolution range)	64.8 (43.74-2.91) 64.8 (43.74-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.254 , 0.278 0.255 , 0.276	Depositor DCC
R_{free} test set	8329 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 10.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.247 for k,-h+k,l 0.247 for h-k,h,l 0.246 for -h+k,-h,l 0.246 for -k,h-k,l 0.247 for h,h-k,-l 0.247 for -h+k,k,-l 0.407 for -h,-k,l 0.260 for k,h,-l 0.267 for -k,-h,-l 0.248 for -h,-h+k,-l 0.248 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	85163	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.02% 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: AKG, MG, EDO, PEG

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	0.66	1/3619 (0.0%)	0.92	1/4902 (0.0%)
1	B	0.66	1/3619 (0.0%)	0.92	2/4902 (0.0%)
1	C	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	D	0.66	1/3625 (0.0%)	0.92	2/4910 (0.0%)
1	E	0.65	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	F	0.65	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	G	0.66	1/3625 (0.0%)	0.92	2/4910 (0.0%)
1	H	0.66	1/3625 (0.0%)	0.93	1/4910 (0.0%)
1	I	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	J	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	K	0.66	1/3625 (0.0%)	0.93	2/4910 (0.0%)
1	L	0.65	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	P	0.66	1/3625 (0.0%)	0.93	1/4910 (0.0%)
1	Q	0.66	1/3619 (0.0%)	0.93	2/4902 (0.0%)
1	S	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	T	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	U	0.66	1/3625 (0.0%)	0.93	1/4910 (0.0%)
1	V	0.66	1/3625 (0.0%)	0.93	1/4910 (0.0%)
1	X	0.65	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	Y	0.66	1/3625 (0.0%)	0.93	1/4910 (0.0%)
1	Z	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
1	a	0.68	1/3619 (0.0%)	0.94	2/4902 (0.0%)
1	b	0.66	1/3625 (0.0%)	0.93	2/4910 (0.0%)
1	c	0.66	1/3625 (0.0%)	0.92	1/4910 (0.0%)
All	All	0.66	24/86976 (0.0%)	0.92	31/117808 (0.0%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	PHE	CA-C	6.63	1.56	1.52
1	K	65	PHE	CA-C	5.91	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	65	PHE	CA-C	5.81	1.55	1.52
1	Y	65	PHE	CA-C	5.79	1.55	1.52
1	Q	65	PHE	CA-C	5.78	1.55	1.52
1	L	65	PHE	CA-C	5.72	1.55	1.52
1	P	65	PHE	CA-C	5.72	1.55	1.52
1	G	65	PHE	CA-C	5.71	1.55	1.52
1	X	65	PHE	CA-C	5.71	1.55	1.52
1	C	65	PHE	CA-C	5.70	1.55	1.52
1	I	65	PHE	CA-C	5.70	1.55	1.52
1	F	65	PHE	CA-C	5.70	1.55	1.52
1	U	65	PHE	CA-C	5.69	1.55	1.52
1	a	65	PHE	CA-C	5.64	1.55	1.52
1	Z	65	PHE	CA-C	5.63	1.55	1.52
1	E	65	PHE	CA-C	5.63	1.55	1.52
1	T	65	PHE	CA-C	5.62	1.55	1.52
1	H	65	PHE	CA-C	5.62	1.55	1.52
1	S	65	PHE	CA-C	5.61	1.55	1.52
1	B	65	PHE	CA-C	5.61	1.55	1.52
1	V	65	PHE	CA-C	5.60	1.55	1.52
1	b	65	PHE	CA-C	5.58	1.55	1.52
1	D	65	PHE	CA-C	5.56	1.55	1.52
1	c	65	PHE	CA-C	5.52	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	382	GLU	CB-CG-CD	6.69	123.97	112.60
1	K	382	GLU	CB-CG-CD	6.59	123.81	112.60
1	V	32	ASN	CA-CB-CG	6.00	118.61	112.60
1	D	273	SER	CA-CB-OG	5.89	122.89	111.10
1	a	179	PHE	CA-CB-CG	5.67	119.47	113.80
1	H	32	ASN	CA-CB-CG	5.61	118.21	112.60
1	P	32	ASN	CA-CB-CG	5.52	118.12	112.60
1	Q	123	GLU	CA-CB-CG	5.51	125.13	114.10
1	A	32	ASN	CA-CB-CG	5.51	118.11	112.60
1	L	32	ASN	CA-CB-CG	5.41	118.01	112.60
1	I	32	ASN	CA-CB-CG	5.41	118.00	112.60
1	K	32	ASN	CA-CB-CG	5.39	117.99	112.60
1	c	32	ASN	CA-CB-CG	5.38	117.98	112.60
1	J	32	ASN	CA-CB-CG	5.35	117.95	112.60
1	Z	32	ASN	CA-CB-CG	5.34	117.94	112.60
1	S	32	ASN	CA-CB-CG	5.32	117.92	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	32	ASN	CA-CB-CG	5.31	117.91	112.60
1	C	32	ASN	CA-CB-CG	5.30	117.90	112.60
1	G	32	ASN	CA-CB-CG	5.29	117.89	112.60
1	Q	32	ASN	CA-CB-CG	5.29	117.89	112.60
1	a	32	ASN	CA-CB-CG	5.29	117.89	112.60
1	Y	32	ASN	CA-CB-CG	5.27	117.87	112.60
1	U	32	ASN	CA-CB-CG	5.26	117.86	112.60
1	b	32	ASN	CA-CB-CG	5.26	117.86	112.60
1	T	32	ASN	CA-CB-CG	5.25	117.86	112.60
1	E	32	ASN	CA-CB-CG	5.25	117.85	112.60
1	F	32	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	32	ASN	CA-CB-CG	5.23	117.83	112.60
1	D	32	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	179	PHE	CA-CB-CG	5.09	118.89	113.80
1	G	179	PHE	CA-CB-CG	5.04	118.84	113.80

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	3528	0	3453	9	0
1	B	3528	0	3453	6	0
1	C	3534	0	3458	7	0
1	D	3534	0	3458	7	0
1	E	3534	0	3458	5	0
1	F	3534	0	3458	9	0
1	G	3534	0	3458	8	0
1	H	3534	0	3458	5	0
1	I	3534	0	3458	7	0
1	J	3534	0	3458	6	0
1	K	3534	0	3458	9	0
1	L	3534	0	3458	8	0
1	P	3534	0	3458	9	0
1	Q	3528	0	3453	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	3534	0	3458	10	0
1	T	3534	0	3458	9	0
1	U	3534	0	3458	10	0
1	V	3534	0	3458	9	0
1	X	3534	0	3458	8	0
1	Y	3534	0	3458	8	0
1	Z	3534	0	3458	7	0
1	a	3528	0	3453	13	0
1	b	3534	0	3458	7	0
1	c	3534	0	3458	8	0
2	A	4	0	6	0	0
2	E	4	0	6	0	0
2	F	4	0	6	3	0
2	G	4	0	6	1	0
2	K	4	0	6	0	0
2	P	8	0	12	1	0
2	S	4	0	6	0	0
2	U	8	0	12	2	0
2	V	8	0	12	2	0
2	X	8	0	12	4	0
2	Y	8	0	12	0	0
2	Z	4	0	6	1	0
2	a	12	0	18	2	0
2	b	8	0	12	0	0
2	c	12	0	18	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	2	0	0	0	0
3	S	1	0	0	0	0
3	T	3	0	0	0	0
3	Y	1	0	0	0	0
3	b	2	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
4	C	10	0	4	0	0
4	D	10	0	4	0	0
4	E	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	10	0	4	0	0
4	G	10	0	4	0	0
4	H	10	0	4	0	0
4	I	10	0	4	0	0
4	J	10	0	4	0	0
4	K	10	0	4	0	0
4	L	10	0	4	0	0
4	P	10	0	4	0	0
4	Q	10	0	4	0	0
4	S	10	0	4	0	0
4	T	10	0	4	0	0
4	U	10	0	4	0	0
4	V	10	0	4	0	0
4	X	10	0	4	0	0
4	Y	10	0	4	0	0
4	Z	10	0	4	0	0
4	a	10	0	4	0	0
4	b	10	0	4	0	0
4	c	10	0	4	0	0
5	P	7	0	10	0	0
5	Z	7	0	10	0	0
All	All	85163	0	83238	190	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 1.

All (190) 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:c:170:ALA:HB3	1:c:200:HIS:CE1	2.35	0.62
1:I:170:ALA:HB3	1:I:200:HIS:CE1	2.34	0.62
1:B:170:ALA:HB3	1:B:200:HIS:CE1	2.34	0.62
1:U:170:ALA:HB3	1:U:200:HIS:CE1	2.35	0.62
1:X:170:ALA:HB3	1:X:200:HIS:CE1	2.35	0.62
1:E:170:ALA:HB3	1:E:200:HIS:CE1	2.34	0.62
1:P:170:ALA:HB3	1:P:200:HIS:CE1	2.35	0.62
1:Q:170:ALA:HB3	1:Q:200:HIS:CE1	2.35	0.62
1:V:170:ALA:HB3	1:V:200:HIS:CE1	2.34	0.62
1:Z:170:ALA:HB3	1:Z:200:HIS:CE1	2.35	0.62
1:H:170:ALA:HB3	1:H:200:HIS:CE1	2.35	0.62
1:J:170:ALA:HB3	1:J:200:HIS:CE1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:170:ALA:HB3	1:S:200:HIS:CE1	2.35	0.62
1:K:170:ALA:HB3	1:K:200:HIS:CE1	2.34	0.62
1:b:170:ALA:HB3	1:b:200:HIS:CE1	2.35	0.62
1:C:170:ALA:HB3	1:C:200:HIS:CE1	2.34	0.61
1:F:170:ALA:HB3	1:F:200:HIS:CE1	2.35	0.61
1:Y:170:ALA:HB3	1:Y:200:HIS:CE1	2.35	0.61
1:G:170:ALA:HB3	1:G:200:HIS:CE1	2.34	0.61
1:D:170:ALA:HB3	1:D:200:HIS:CE1	2.35	0.61
1:T:170:ALA:HB3	1:T:200:HIS:CE1	2.35	0.61
1:a:170:ALA:HB3	1:a:200:HIS:CE1	2.35	0.61
1:L:170:ALA:HB3	1:L:200:HIS:CE1	2.35	0.61
1:U:88:ARG:NH1	2:X:601:EDO:H12	2.16	0.60
1:a:252:HIS:NE2	1:a:338:GLU:OE1	2.37	0.58
1:A:170:ALA:HB3	1:A:200:HIS:CE1	2.42	0.55
1:A:170:ALA:N	1:A:171:PRO:HD3	2.22	0.55
1:Z:445:TYR:O	1:Z:448:ILE:HG12	2.09	0.53
1:C:445:TYR:O	1:C:448:ILE:HG12	2.09	0.53
1:I:445:TYR:O	1:I:448:ILE:HG12	2.09	0.53
1:J:445:TYR:O	1:J:448:ILE:HG12	2.09	0.53
1:X:172:ASP:OD2	2:X:601:EDO:H21	2.09	0.53
1:X:445:TYR:O	1:X:448:ILE:HG12	2.09	0.53
1:c:445:TYR:O	1:c:448:ILE:HG12	2.09	0.53
1:H:445:TYR:O	1:H:448:ILE:HG12	2.09	0.53
1:B:445:TYR:O	1:B:448:ILE:HG12	2.09	0.53
1:F:445:TYR:O	1:F:448:ILE:HG12	2.09	0.53
1:K:445:TYR:O	1:K:448:ILE:HG12	2.09	0.53
1:P:445:TYR:O	1:P:448:ILE:HG12	2.09	0.53
1:U:66:VAL:HG11	2:U:502:EDO:H11	1.90	0.53
1:D:445:TYR:O	1:D:448:ILE:HG12	2.08	0.52
1:V:445:TYR:O	1:V:448:ILE:HG12	2.09	0.52
1:Y:445:TYR:O	1:Y:448:ILE:HG12	2.09	0.52
1:a:445:TYR:O	1:a:448:ILE:HG12	2.09	0.52
1:b:445:TYR:O	1:b:448:ILE:HG12	2.09	0.52
1:a:50:VAL:HG13	1:a:55:LEU:HG	1.91	0.52
1:E:445:TYR:O	1:E:448:ILE:HG12	2.09	0.52
1:Q:445:TYR:O	1:Q:448:ILE:HG12	2.09	0.52
1:S:445:TYR:O	1:S:448:ILE:HG12	2.09	0.52
1:L:445:TYR:O	1:L:448:ILE:HG12	2.09	0.52
1:T:445:TYR:O	1:T:448:ILE:HG12	2.09	0.52
1:U:252:HIS:NE2	1:U:338:GLU:OE2	2.42	0.51
1:G:445:TYR:O	1:G:448:ILE:HG12	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:219:PHE:O	1:Q:223:ILE:HG12	2.10	0.51
1:A:330:ALA:HB3	1:A:336:ARG:HH21	1.75	0.50
1:F:171:PRO:HD2	2:F:501:EDO:O2	2.11	0.50
1:A:305:VAL:HG13	1:A:308:TYR:HB2	1.93	0.50
1:A:330:ALA:HB3	1:A:336:ARG:NH2	2.27	0.50
1:F:172:ASP:OD2	2:F:501:EDO:C2	2.60	0.49
1:X:71:SER:OG	1:Y:321:ARG:NH1	2.44	0.48
1:B:219:PHE:O	1:B:223:ILE:HG12	2.13	0.48
1:Z:396:ASN:HB3	2:Z:501:EDO:H22	1.94	0.48
1:P:66:VAL:HA	2:P:503:EDO:H22	1.94	0.48
1:S:170:ALA:N	1:S:171:PRO:HD3	2.29	0.48
1:T:170:ALA:N	1:T:171:PRO:HD3	2.29	0.48
1:b:291:VAL:O	1:b:295:ASN:HB2	2.14	0.47
1:K:170:ALA:N	1:K:171:PRO:HD3	2.29	0.47
1:X:171:PRO:HG2	2:X:601:EDO:H22	1.95	0.47
1:B:170:ALA:N	1:B:171:PRO:HD3	2.29	0.47
1:G:170:ALA:N	1:G:171:PRO:HD3	2.29	0.47
1:H:170:ALA:N	1:H:171:PRO:HD3	2.29	0.47
1:V:170:ALA:N	1:V:171:PRO:HD3	2.29	0.47
1:a:170:ALA:N	1:a:171:PRO:HD3	2.29	0.47
1:P:170:ALA:N	1:P:171:PRO:HD3	2.29	0.47
1:D:170:ALA:N	1:D:171:PRO:HD3	2.29	0.47
1:E:170:ALA:N	1:E:171:PRO:HD3	2.29	0.47
1:U:170:ALA:N	1:U:171:PRO:HD3	2.29	0.47
1:a:219:PHE:O	1:a:223:ILE:HG12	2.15	0.47
1:b:219:PHE:O	1:b:223:ILE:HG12	2.15	0.47
1:G:219:PHE:O	1:G:223:ILE:HD13	2.15	0.47
1:J:170:ALA:N	1:J:171:PRO:HD3	2.29	0.47
1:Q:170:ALA:N	1:Q:171:PRO:HD3	2.29	0.47
1:Z:170:ALA:N	1:Z:171:PRO:HD3	2.29	0.47
1:L:170:ALA:N	1:L:171:PRO:HD3	2.29	0.47
1:X:170:ALA:N	1:X:171:PRO:HD3	2.29	0.47
1:F:170:ALA:N	1:F:171:PRO:HD3	2.29	0.47
1:F:172:ASP:OD2	2:F:501:EDO:H22	2.15	0.47
1:G:88:ARG:NH1	2:G:501:EDO:H11	2.29	0.47
1:I:170:ALA:N	1:I:171:PRO:HD3	2.29	0.47
1:C:170:ALA:N	1:C:171:PRO:HD3	2.29	0.46
1:a:302:LYS:CE	2:a:502:EDO:H12	2.46	0.46
1:Y:170:ALA:N	1:Y:171:PRO:HD3	2.29	0.46
1:b:170:ALA:N	1:b:171:PRO:HD3	2.29	0.46
1:c:170:ALA:N	1:c:171:PRO:HD3	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:HIS:NE2	1:I:338:GLU:OE2	2.49	0.46
1:F:291:VAL:O	1:F:295:ASN:HB2	2.17	0.45
1:S:297:THR:OG1	1:S:300:SER:OG	2.31	0.45
1:Q:291:VAL:O	1:Q:295:ASN:HB2	2.17	0.45
1:D:291:VAL:O	1:D:295:ASN:HB2	2.17	0.45
1:X:291:VAL:O	1:X:295:ASN:HB2	2.17	0.45
1:Y:291:VAL:O	1:Y:295:ASN:HB2	2.17	0.45
1:C:291:VAL:O	1:C:295:ASN:HB2	2.17	0.45
1:I:291:VAL:O	1:I:295:ASN:HB2	2.17	0.45
1:P:291:VAL:O	1:P:295:ASN:HB2	2.17	0.45
1:B:291:VAL:O	1:B:295:ASN:HB2	2.17	0.44
1:c:219:PHE:O	1:c:223:ILE:HD13	2.18	0.44
1:c:291:VAL:O	1:c:295:ASN:HB2	2.17	0.44
1:J:291:VAL:O	1:J:295:ASN:HB2	2.17	0.44
1:U:88:ARG:HH11	2:X:601:EDO:H12	1.82	0.44
1:A:142:LEU:HD12	1:A:200:HIS:CD2	2.53	0.44
1:A:142:LEU:HD12	1:A:200:HIS:NE2	2.33	0.44
1:H:291:VAL:O	1:H:295:ASN:HB2	2.17	0.44
1:Z:291:VAL:O	1:Z:295:ASN:HB2	2.17	0.44
1:S:252:HIS:HB3	1:S:336:ARG:HD2	1.99	0.44
1:V:291:VAL:O	1:V:295:ASN:HB2	2.17	0.44
1:E:291:VAL:O	1:E:295:ASN:HB2	2.17	0.43
1:A:445:TYR:O	1:A:448:ILE:HG12	2.18	0.43
1:G:291:VAL:O	1:G:295:ASN:HB2	2.17	0.43
1:U:291:VAL:O	1:U:295:ASN:HB2	2.17	0.43
1:V:396:ASN:HB2	2:V:501:EDO:H12	2.00	0.43
1:T:291:VAL:O	1:T:295:ASN:HB2	2.17	0.43
1:K:252:HIS:NE2	1:K:338:GLU:OE2	2.52	0.43
1:L:291:VAL:O	1:L:295:ASN:HB2	2.17	0.43
1:S:291:VAL:O	1:S:295:ASN:HB2	2.17	0.43
1:D:97:VAL:O	1:D:97:VAL:HG13	2.19	0.43
1:S:219:PHE:CE1	1:S:223:ILE:HD11	2.53	0.43
1:a:48:ARG:O	1:a:52:GLU:HG3	2.18	0.43
1:I:157:ASP:OD1	1:I:193:HIS:NE2	2.48	0.43
1:F:157:ASP:OD1	1:F:193:HIS:NE2	2.48	0.43
1:Y:157:ASP:OD1	1:Y:193:HIS:NE2	2.48	0.43
1:U:146:ASP:HB3	1:U:149:ASN:O	2.20	0.42
1:a:334:GLY:O	1:a:336:ARG:HD3	2.20	0.42
1:A:176:ASP:OD2	1:A:230:HIS:NE2	2.51	0.42
1:I:146:ASP:HB3	1:I:149:ASN:O	2.20	0.42
1:Z:146:ASP:HB3	1:Z:149:ASN:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:219:PHE:O	1:Z:223:ILE:HD13	2.19	0.42
1:J:146:ASP:HB3	1:J:149:ASN:O	2.20	0.42
1:K:157:ASP:OD1	1:K:193:HIS:NE2	2.48	0.42
1:K:291:VAL:O	1:K:295:ASN:HB2	2.20	0.42
1:L:15:ASN:O	1:L:92:LYS:HA	2.20	0.42
1:D:146:ASP:HB3	1:D:149:ASN:O	2.20	0.41
1:F:146:ASP:HB3	1:F:149:ASN:O	2.20	0.41
1:H:146:ASP:HB3	1:H:149:ASN:O	2.20	0.41
1:Y:146:ASP:HB3	1:Y:149:ASN:O	2.20	0.41
1:c:146:ASP:HB3	1:c:149:ASN:O	2.20	0.41
1:L:157:ASP:OD1	1:L:193:HIS:NE2	2.48	0.41
1:T:297:THR:OG1	1:T:300:SER:OG	2.30	0.41
1:C:219:PHE:CE1	1:C:223:ILE:HD11	2.56	0.41
1:L:146:ASP:HB3	1:L:149:ASN:O	2.20	0.41
1:T:219:PHE:O	1:T:223:ILE:HD13	2.20	0.41
1:B:146:ASP:HB3	1:B:149:ASN:O	2.20	0.41
1:C:146:ASP:HB3	1:C:149:ASN:O	2.20	0.41
1:E:146:ASP:HB3	1:E:149:ASN:O	2.20	0.41
1:P:146:ASP:HB3	1:P:149:ASN:O	2.20	0.41
1:Q:146:ASP:HB3	1:Q:149:ASN:O	2.20	0.41
1:S:146:ASP:HB3	1:S:149:ASN:O	2.20	0.41
1:b:146:ASP:HB3	1:b:149:ASN:O	2.20	0.41
1:b:219:PHE:CE1	1:b:223:ILE:HD11	2.56	0.41
1:G:297:THR:OG1	1:G:300:SER:OG	2.33	0.41
1:c:157:ASP:OD1	1:c:193:HIS:NE2	2.49	0.41
1:X:146:ASP:HB3	1:X:149:ASN:O	2.20	0.41
1:D:157:ASP:OD1	1:D:193:HIS:NE2	2.48	0.41
1:S:219:PHE:O	1:S:223:ILE:HG12	2.21	0.41
1:S:305:VAL:HG13	1:S:308:TYR:HB2	2.03	0.41
1:T:146:ASP:HB3	1:T:149:ASN:O	2.20	0.41
1:T:305:VAL:HG13	1:T:308:TYR:HB2	2.03	0.41
1:U:103:THR:HG22	2:U:502:EDO:H12	2.03	0.41
1:V:146:ASP:HB3	1:V:149:ASN:O	2.20	0.41
1:V:396:ASN:CB	2:V:501:EDO:H12	2.51	0.41
1:a:146:ASP:HB3	1:a:149:ASN:O	2.20	0.41
1:a:157:ASP:OD1	1:a:193:HIS:NE2	2.48	0.41
1:a:305:VAL:HG13	1:a:308:TYR:HB2	2.03	0.41
1:K:146:ASP:HB3	1:K:149:ASN:O	2.20	0.41
1:P:41:GLU:O	1:P:45:GLU:HG2	2.21	0.41
1:a:302:LYS:HE3	2:a:502:EDO:H12	2.03	0.41
1:L:305:VAL:HG13	1:L:308:TYR:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:434:ARG:HB2	2:c:501:EDO:H11	2.02	0.40
1:G:305:VAL:HG13	1:G:308:TYR:HB2	2.03	0.40
1:K:305:VAL:HG13	1:K:308:TYR:HB2	2.03	0.40
1:T:157:ASP:OD1	1:T:193:HIS:NE2	2.49	0.40
1:J:219:PHE:O	1:J:223:ILE:HG12	2.22	0.40
1:P:305:VAL:HG13	1:P:308:TYR:HB2	2.03	0.40
1:Q:157:ASP:OD1	1:Q:193:HIS:NE2	2.49	0.40
1:V:157:ASP:OD1	1:V:193:HIS:NE2	2.48	0.40
1:P:157:ASP:OD1	1:P:193:HIS:NE2	2.48	0.40
1:V:305:VAL:HG13	1:V:308:TYR:HB2	2.03	0.40
1:C:219:PHE:O	1:C:223:ILE:HG12	2.21	0.40
1:K:219:PHE:CE1	1:K:223:ILE:HD11	2.56	0.40
1:U:157:ASP:OD1	1:U:193:HIS:NE2	2.48	0.40
1:Y:305:VAL:HG13	1:Y:308:TYR:HB2	2.03	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	444/448 (99%)	419 (94%)	24 (5%)	1 (0%)	43	71
1	B	444/448 (99%)	429 (97%)	13 (3%)	2 (0%)	24	53
1	C	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	D	445/448 (99%)	430 (97%)	14 (3%)	1 (0%)	43	71
1	E	445/448 (99%)	430 (97%)	14 (3%)	1 (0%)	43	71
1	F	445/448 (99%)	427 (96%)	17 (4%)	1 (0%)	43	71
1	G	445/448 (99%)	430 (97%)	14 (3%)	1 (0%)	43	71
1	H	445/448 (99%)	429 (96%)	14 (3%)	2 (0%)	30	58
1	I	445/448 (99%)	428 (96%)	16 (4%)	1 (0%)	43	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	445/448 (99%)	428 (96%)	16 (4%)	1 (0%)	43	71
1	K	445/448 (99%)	427 (96%)	17 (4%)	1 (0%)	43	71
1	L	445/448 (99%)	427 (96%)	17 (4%)	1 (0%)	43	71
1	P	445/448 (99%)	428 (96%)	16 (4%)	1 (0%)	43	71
1	Q	444/448 (99%)	428 (96%)	15 (3%)	1 (0%)	43	71
1	S	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	T	445/448 (99%)	430 (97%)	14 (3%)	1 (0%)	43	71
1	U	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	V	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	X	445/448 (99%)	430 (97%)	14 (3%)	1 (0%)	43	71
1	Y	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	Z	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	a	444/448 (99%)	425 (96%)	18 (4%)	1 (0%)	43	71
1	b	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
1	c	445/448 (99%)	429 (96%)	15 (3%)	1 (0%)	43	71
All	All	10676/10752 (99%)	10277 (96%)	373 (4%)	26 (0%)	43	71

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLU
1	B	309	GLU
1	H	309	GLU
1	B	170	ALA
1	C	170	ALA
1	D	170	ALA
1	E	170	ALA
1	F	170	ALA
1	G	170	ALA
1	H	170	ALA
1	I	170	ALA
1	J	170	ALA
1	K	170	ALA
1	L	170	ALA
1	P	170	ALA
1	Q	170	ALA
1	S	170	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	170	ALA
1	U	170	ALA
1	V	170	ALA
1	X	170	ALA
1	Y	170	ALA
1	Z	170	ALA
1	a	170	ALA
1	b	170	ALA
1	c	170	ALA

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	381/383 (100%)	380 (100%)	1 (0%)	86	95
1	B	381/383 (100%)	378 (99%)	3 (1%)	73	89
1	C	382/383 (100%)	380 (100%)	2 (0%)	81	93
1	D	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	E	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	F	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	G	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	H	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	I	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	J	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	K	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	L	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	P	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	Q	381/383 (100%)	378 (99%)	3 (1%)	73	89
1	S	382/383 (100%)	380 (100%)	2 (0%)	81	93
1	T	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	U	382/383 (100%)	379 (99%)	3 (1%)	73	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	X	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	Y	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	Z	382/383 (100%)	378 (99%)	4 (1%)	68	87
1	a	381/383 (100%)	379 (100%)	2 (0%)	81	93
1	b	382/383 (100%)	379 (99%)	3 (1%)	73	89
1	c	382/383 (100%)	380 (100%)	2 (0%)	81	93
All	All	9164/9192 (100%)	9092 (99%)	72 (1%)	73	89

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	B	32	ASN
1	B	104	THR
1	B	163	ASP
1	C	32	ASN
1	C	163	ASP
1	D	32	ASN
1	D	104	THR
1	D	163	ASP
1	E	32	ASN
1	E	104	THR
1	E	163	ASP
1	F	32	ASN
1	F	104	THR
1	F	163	ASP
1	F	223	ILE
1	G	32	ASN
1	G	104	THR
1	G	163	ASP
1	H	32	ASN
1	H	104	THR
1	H	163	ASP
1	I	32	ASN
1	I	104	THR
1	I	163	ASP
1	J	32	ASN
1	J	104	THR
1	J	163	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	32	ASN
1	K	104	THR
1	K	163	ASP
1	L	32	ASN
1	L	99	CYS
1	L	104	THR
1	L	163	ASP
1	P	32	ASN
1	P	104	THR
1	P	163	ASP
1	P	223	ILE
1	Q	32	ASN
1	Q	104	THR
1	Q	163	ASP
1	S	32	ASN
1	S	163	ASP
1	T	32	ASN
1	T	104	THR
1	T	163	ASP
1	T	223	ILE
1	U	32	ASN
1	U	104	THR
1	U	163	ASP
1	V	32	ASN
1	V	104	THR
1	V	163	ASP
1	V	223	ILE
1	X	32	ASN
1	X	104	THR
1	X	163	ASP
1	Y	32	ASN
1	Y	104	THR
1	Y	163	ASP
1	Z	32	ASN
1	Z	104	THR
1	Z	163	ASP
1	Z	223	ILE
1	a	32	ASN
1	a	163	ASP
1	b	9	GLU
1	b	32	ASN
1	b	163	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	32	ASN
1	c	163	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	22	GLN
1	A	245	ASN
1	A	271	GLN
1	A	295	ASN
1	A	376	ASN
1	B	151	HIS
1	B	271	GLN
1	B	318	ASN
1	B	376	ASN
1	C	22	GLN
1	C	271	GLN
1	C	318	ASN
1	C	376	ASN
1	D	129	ASN
1	D	258	ASN
1	D	271	GLN
1	D	318	ASN
1	D	376	ASN
1	E	151	HIS
1	E	271	GLN
1	E	318	ASN
1	E	376	ASN
1	F	129	ASN
1	F	151	HIS
1	F	258	ASN
1	F	271	GLN
1	F	278	ASN
1	F	318	ASN
1	F	376	ASN
1	G	22	GLN
1	G	271	GLN
1	G	318	ASN
1	G	376	ASN
1	H	22	GLN
1	H	271	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	318	ASN
1	H	376	ASN
1	I	14	ASN
1	I	22	GLN
1	I	318	ASN
1	I	376	ASN
1	J	129	ASN
1	J	151	HIS
1	J	258	ASN
1	J	271	GLN
1	J	318	ASN
1	J	376	ASN
1	K	14	ASN
1	K	22	GLN
1	K	151	HIS
1	K	271	GLN
1	K	295	ASN
1	K	318	ASN
1	K	376	ASN
1	L	14	ASN
1	L	151	HIS
1	L	271	GLN
1	L	318	ASN
1	L	376	ASN
1	P	14	ASN
1	P	271	GLN
1	P	295	ASN
1	P	318	ASN
1	P	376	ASN
1	Q	151	HIS
1	Q	271	GLN
1	Q	318	ASN
1	Q	376	ASN
1	S	6	GLN
1	S	129	ASN
1	S	258	ASN
1	S	271	GLN
1	S	318	ASN
1	S	376	ASN
1	T	22	GLN
1	T	271	GLN
1	T	318	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	376	ASN
1	U	22	GLN
1	U	151	HIS
1	U	271	GLN
1	U	318	ASN
1	U	376	ASN
1	V	151	HIS
1	V	271	GLN
1	V	278	ASN
1	V	318	ASN
1	V	376	ASN
1	X	271	GLN
1	X	318	ASN
1	X	376	ASN
1	Y	271	GLN
1	Y	318	ASN
1	Y	376	ASN
1	Z	129	ASN
1	Z	258	ASN
1	Z	271	GLN
1	Z	318	ASN
1	Z	376	ASN
1	a	151	HIS
1	a	271	GLN
1	a	376	ASN
1	b	14	ASN
1	b	271	GLN
1	b	295	ASN
1	b	318	ASN
1	b	376	ASN
1	c	14	ASN
1	c	22	GLN
1	c	129	ASN
1	c	151	HIS
1	c	258	ASN
1	c	271	GLN
1	c	318	ASN
1	c	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 17 are monoatomic - leaving 51 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	b	505	-	9,9,9	1.89	1 (11%)	11,11,11	1.08	0
2	EDO	a	501	-	3,3,3	0.16	0	2,2,2	0.23	0
4	AKG	L	501	-	9,9,9	1.87	1 (11%)	11,11,11	1.12	0
4	AKG	V	503	-	9,9,9	1.87	1 (11%)	11,11,11	1.38	2 (18%)
4	AKG	B	503	-	9,9,9	1.87	1 (11%)	11,11,11	1.13	0
4	AKG	D	501	-	9,9,9	1.85	1 (11%)	11,11,11	1.15	1 (9%)
4	AKG	Z	503	-	9,9,9	1.86	1 (11%)	11,11,11	1.15	0
4	AKG	I	501	-	9,9,9	1.84	1 (11%)	11,11,11	1.39	3 (27%)
2	EDO	a	502	-	3,3,3	0.15	0	2,2,2	0.22	0
2	EDO	X	601	-	3,3,3	0.16	0	2,2,2	0.23	0
4	AKG	S	603	-	9,9,9	1.80	1 (11%)	11,11,11	1.19	1 (9%)
2	EDO	U	501	-	3,3,3	0.15	0	2,2,2	0.24	0
2	EDO	Y	601	-	3,3,3	0.15	0	2,2,2	0.23	0
2	EDO	b	502	-	3,3,3	0.16	0	2,2,2	0.23	0
2	EDO	U	502	-	3,3,3	0.15	0	2,2,2	0.24	0
2	EDO	b	501	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	J	502	-	9,9,9	1.88	1 (11%)	11,11,11	1.35	2 (18%)
2	EDO	A	501	-	3,3,3	0.16	0	2,2,2	0.22	0
2	EDO	X	602	-	3,3,3	0.15	0	2,2,2	0.23	0
2	EDO	F	501	-	3,3,3	0.16	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AKG	U	503	-	9,9,9	1.84	1 (11%)	11,11,11	1.38	3 (27%)
5	PEG	P	502	-	6,6,6	0.12	0	5,5,5	0.07	0
2	EDO	P	501	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	H	502	-	9,9,9	1.85	1 (11%)	11,11,11	1.43	4 (36%)
4	AKG	C	501	-	9,9,9	1.85	1 (11%)	11,11,11	1.35	2 (18%)
2	EDO	c	503	-	3,3,3	0.15	0	2,2,2	0.22	0
4	AKG	K	503	-	9,9,9	1.88	1 (11%)	11,11,11	1.35	3 (27%)
4	AKG	a	504	-	9,9,9	1.88	1 (11%)	11,11,11	1.12	2 (18%)
2	EDO	c	501	-	3,3,3	0.14	0	2,2,2	0.24	0
4	AKG	X	603	-	9,9,9	1.87	1 (11%)	11,11,11	1.35	2 (18%)
2	EDO	c	502	-	3,3,3	0.15	0	2,2,2	0.22	0
4	AKG	P	505	-	9,9,9	1.86	1 (11%)	11,11,11	1.25	2 (18%)
2	EDO	K	501	-	3,3,3	0.14	0	2,2,2	0.23	0
4	AKG	A	503	-	9,9,9	1.87	1 (11%)	11,11,11	1.30	1 (9%)
4	AKG	Q	503	-	9,9,9	1.83	1 (11%)	11,11,11	1.41	3 (27%)
5	PEG	Z	502	-	6,6,6	0.11	0	5,5,5	0.09	0
2	EDO	G	501	-	3,3,3	0.16	0	2,2,2	0.24	0
2	EDO	Y	602	-	3,3,3	0.15	0	2,2,2	0.23	0
2	EDO	V	501	-	3,3,3	0.15	0	2,2,2	0.24	0
2	EDO	Z	501	-	3,3,3	0.16	0	2,2,2	0.23	0
4	AKG	Y	604	-	9,9,9	1.87	1 (11%)	11,11,11	1.41	3 (27%)
2	EDO	V	502	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	F	503	-	9,9,9	1.84	1 (11%)	11,11,11	1.14	2 (18%)
2	EDO	E	501	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	E	502	-	9,9,9	1.85	1 (11%)	11,11,11	1.17	2 (18%)
2	EDO	P	503	-	3,3,3	0.15	0	2,2,2	0.21	0
2	EDO	a	503	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	T	504	-	9,9,9	1.84	1 (11%)	11,11,11	1.35	1 (9%)
2	EDO	S	601	-	3,3,3	0.15	0	2,2,2	0.23	0
4	AKG	c	504	-	9,9,9	1.83	1 (11%)	11,11,11	1.44	3 (27%)
4	AKG	G	502	-	9,9,9	1.85	1 (11%)	11,11,11	1.19	2 (18%)

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	b	505	-	-	4/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	a	501	-	-	0/1/1/1	-
4	AKG	L	501	-	-	3/9/9/9	-
4	AKG	V	503	-	-	1/9/9/9	-
4	AKG	B	503	-	-	2/9/9/9	-
4	AKG	D	501	-	-	4/9/9/9	-
4	AKG	Z	503	-	-	4/9/9/9	-
4	AKG	I	501	-	-	3/9/9/9	-
2	EDO	a	502	-	-	1/1/1/1	-
2	EDO	X	601	-	-	0/1/1/1	-
4	AKG	S	603	-	-	4/9/9/9	-
2	EDO	U	501	-	-	1/1/1/1	-
2	EDO	Y	601	-	-	1/1/1/1	-
2	EDO	b	502	-	-	1/1/1/1	-
2	EDO	U	502	-	-	1/1/1/1	-
2	EDO	b	501	-	-	1/1/1/1	-
4	AKG	J	502	-	-	3/9/9/9	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	X	602	-	-	1/1/1/1	-
2	EDO	F	501	-	-	0/1/1/1	-
4	AKG	U	503	-	-	3/9/9/9	-
5	PEG	P	502	-	-	2/4/4/4	-
2	EDO	P	501	-	-	1/1/1/1	-
4	AKG	H	502	-	-	4/9/9/9	-
4	AKG	C	501	-	-	1/9/9/9	-
2	EDO	c	503	-	-	1/1/1/1	-
4	AKG	K	503	-	-	2/9/9/9	-
4	AKG	a	504	-	-	1/9/9/9	-
2	EDO	c	501	-	-	1/1/1/1	-
4	AKG	X	603	-	-	3/9/9/9	-
2	EDO	c	502	-	-	1/1/1/1	-
4	AKG	P	505	-	-	4/9/9/9	-
2	EDO	K	501	-	-	0/1/1/1	-
4	AKG	A	503	-	-	3/9/9/9	-
4	AKG	Q	503	-	-	3/9/9/9	-
5	PEG	Z	502	-	-	1/4/4/4	-
2	EDO	G	501	-	-	1/1/1/1	-
2	EDO	Y	602	-	-	0/1/1/1	-
2	EDO	V	501	-	-	0/1/1/1	-
2	EDO	Z	501	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	Y	604	-	-	1/9/9/9	-
2	EDO	V	502	-	-	1/1/1/1	-
4	AKG	F	503	-	-	4/9/9/9	-
2	EDO	E	501	-	-	1/1/1/1	-
4	AKG	E	502	-	-	4/9/9/9	-
2	EDO	P	503	-	-	1/1/1/1	-
2	EDO	a	503	-	-	1/1/1/1	-
4	AKG	T	504	-	-	3/9/9/9	-
2	EDO	S	601	-	-	1/1/1/1	-
4	AKG	c	504	-	-	4/9/9/9	-
4	AKG	G	502	-	-	4/9/9/9	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	502	AKG	C2-C1	-4.75	1.46	1.53
4	b	505	AKG	C2-C1	-4.71	1.46	1.53
4	Y	604	AKG	C2-C1	-4.71	1.46	1.53
4	K	503	AKG	C2-C1	-4.71	1.46	1.53
4	V	503	AKG	C2-C1	-4.68	1.46	1.53
4	a	504	AKG	C2-C1	-4.67	1.46	1.53
4	A	503	AKG	C2-C1	-4.67	1.46	1.53
4	H	502	AKG	C2-C1	-4.66	1.46	1.53
4	B	503	AKG	C2-C1	-4.65	1.46	1.53
4	X	603	AKG	C2-C1	-4.64	1.46	1.53
4	P	505	AKG	C2-C1	-4.64	1.46	1.53
4	E	502	AKG	C2-C1	-4.60	1.46	1.53
4	L	501	AKG	C2-C1	-4.59	1.46	1.53
4	G	502	AKG	C2-C1	-4.59	1.46	1.53
4	U	503	AKG	C2-C1	-4.57	1.46	1.53
4	Z	503	AKG	C2-C1	-4.57	1.46	1.53
4	D	501	AKG	C2-C1	-4.57	1.46	1.53
4	c	504	AKG	C2-C1	-4.56	1.46	1.53
4	Q	503	AKG	C2-C1	-4.56	1.46	1.53
4	I	501	AKG	C2-C1	-4.55	1.46	1.53
4	F	503	AKG	C2-C1	-4.54	1.46	1.53
4	T	504	AKG	C2-C1	-4.54	1.46	1.53
4	C	501	AKG	C2-C1	-4.54	1.46	1.53
4	S	603	AKG	C2-C1	-4.39	1.46	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	505	AKG	O1-C1-C2	-2.54	118.65	121.81
4	c	504	AKG	O1-C1-C2	-2.33	118.92	121.81
4	V	503	AKG	O1-C1-C2	-2.32	118.93	121.81
4	G	502	AKG	O1-C1-C2	-2.30	118.95	121.81
4	Y	604	AKG	O4-C5-C4	2.29	121.22	114.00
4	T	504	AKG	O4-C5-C4	2.27	121.18	114.00
4	Q	503	AKG	O1-C1-C2	-2.27	118.99	121.81
4	H	502	AKG	O4-C5-C4	2.26	121.13	114.00
4	c	504	AKG	O4-C5-C4	2.25	121.11	114.00
4	A	503	AKG	O4-C5-C4	2.23	121.06	114.00
4	H	502	AKG	O1-C1-C2	-2.23	119.03	121.81
4	Q	503	AKG	O4-C5-C4	2.23	121.05	114.00
4	V	503	AKG	O4-C5-C4	2.22	121.00	114.00
4	I	501	AKG	O4-C5-C4	2.21	120.98	114.00
4	I	501	AKG	O1-C1-C2	-2.19	119.09	121.81
4	U	503	AKG	O4-C5-C4	2.19	120.91	114.00
4	J	502	AKG	O4-C5-C4	2.19	120.90	114.00
4	P	505	AKG	O2-C1-C2	2.18	119.65	113.59
4	X	603	AKG	O4-C5-C4	2.18	120.89	114.00
4	J	502	AKG	O1-C1-C2	-2.18	119.10	121.81
4	C	501	AKG	O4-C5-C4	2.17	120.86	114.00
4	F	503	AKG	O1-C1-C2	-2.17	119.11	121.81
4	K	503	AKG	O1-C1-C2	-2.16	119.12	121.81
4	Y	604	AKG	O1-C1-C2	-2.14	119.15	121.81
4	E	502	AKG	O1-C1-C2	-2.13	119.16	121.81
4	G	502	AKG	O2-C1-C2	2.11	119.43	113.59
4	Q	503	AKG	O2-C1-C2	2.09	119.40	113.59
4	S	603	AKG	O2-C1-C2	2.09	119.39	113.59
4	H	502	AKG	O2-C1-C2	2.08	119.36	113.59
4	U	503	AKG	O1-C1-C2	-2.08	119.22	121.81
4	K	503	AKG	O4-C5-C4	2.08	120.56	114.00
4	K	503	AKG	O2-C1-C2	2.08	119.35	113.59
4	c	504	AKG	O2-C1-C2	2.07	119.33	113.59
4	U	503	AKG	O2-C1-C2	2.06	119.31	113.59
4	a	504	AKG	O2-C1-C2	2.06	119.30	113.59
4	D	501	AKG	O2-C1-C2	2.05	119.28	113.59
4	F	503	AKG	O2-C1-C2	2.04	119.25	113.59
4	E	502	AKG	O2-C1-C2	2.03	119.23	113.59
4	a	504	AKG	O1-C1-C2	-2.03	119.29	121.81
4	Y	604	AKG	O2-C1-C2	2.03	119.21	113.59
4	X	603	AKG	O1-C1-C2	-2.02	119.29	121.81
4	I	501	AKG	O2-C1-C2	2.02	119.20	113.59
4	C	501	AKG	O2-C1-C2	2.01	119.17	113.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	502	AKG	O3-C5-C4	-2.00	116.74	123.09

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	AKG	O2-C1-C2-C3
4	C	501	AKG	O2-C1-C2-C3
4	D	501	AKG	O2-C1-C2-C3
4	E	502	AKG	O2-C1-C2-C3
4	F	503	AKG	O2-C1-C2-C3
4	H	502	AKG	O2-C1-C2-C3
4	I	501	AKG	O2-C1-C2-C3
4	J	502	AKG	O2-C1-C2-C3
4	K	503	AKG	O2-C1-C2-C3
4	L	501	AKG	O2-C1-C2-C3
4	P	505	AKG	O2-C1-C2-C3
4	Q	503	AKG	O2-C1-C2-C3
4	T	504	AKG	O2-C1-C2-C3
4	U	503	AKG	O2-C1-C2-C3
4	V	503	AKG	O2-C1-C2-C3
4	X	603	AKG	O2-C1-C2-C3
4	Y	604	AKG	O2-C1-C2-C3
4	Z	503	AKG	O2-C1-C2-C3
4	b	505	AKG	O2-C1-C2-C3
4	c	504	AKG	O1-C1-C2-C3
4	c	504	AKG	O2-C1-C2-O5
4	c	504	AKG	O2-C1-C2-C3
2	b	502	EDO	O1-C1-C2-O2
5	P	502	PEG	O2-C3-C4-O4
2	U	502	EDO	O1-C1-C2-O2
2	a	502	EDO	O1-C1-C2-O2
5	P	502	PEG	O1-C1-C2-O2
2	G	501	EDO	O1-C1-C2-O2
5	Z	502	PEG	C1-C2-O2-C3
4	D	501	AKG	O1-C1-C2-O5
4	F	503	AKG	O1-C1-C2-O5
4	G	502	AKG	O1-C1-C2-O5
4	L	501	AKG	O1-C1-C2-O5
4	S	603	AKG	O1-C1-C2-O5
4	Z	503	AKG	O1-C1-C2-O5
4	b	505	AKG	O1-C1-C2-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	c	504	AKG	O1-C1-C2-O5
4	D	501	AKG	O1-C1-C2-C3
4	E	502	AKG	O1-C1-C2-C3
4	F	503	AKG	O1-C1-C2-C3
4	H	502	AKG	O1-C1-C2-C3
4	L	501	AKG	O1-C1-C2-C3
4	P	505	AKG	O1-C1-C2-C3
4	Z	503	AKG	O1-C1-C2-C3
4	b	505	AKG	O1-C1-C2-C3
4	B	503	AKG	O2-C1-C2-O5
4	D	501	AKG	O2-C1-C2-O5
4	E	502	AKG	O2-C1-C2-O5
4	F	503	AKG	O2-C1-C2-O5
4	G	502	AKG	O2-C1-C2-O5
4	H	502	AKG	O2-C1-C2-O5
4	P	505	AKG	O2-C1-C2-O5
4	S	603	AKG	O2-C1-C2-O5
4	Z	503	AKG	O2-C1-C2-O5
4	a	504	AKG	O2-C1-C2-O5
4	b	505	AKG	O2-C1-C2-O5
2	Z	501	EDO	O1-C1-C2-O2
4	B	503	AKG	O2-C1-C2-C3
4	G	502	AKG	O2-C1-C2-C3
4	S	603	AKG	O2-C1-C2-C3
4	A	503	AKG	C3-C4-C5-O4
4	X	603	AKG	C3-C4-C5-O4
2	A	501	EDO	O1-C1-C2-O2
2	E	501	EDO	O1-C1-C2-O2
2	P	501	EDO	O1-C1-C2-O2
2	S	601	EDO	O1-C1-C2-O2
2	U	501	EDO	O1-C1-C2-O2
2	V	502	EDO	O1-C1-C2-O2
2	X	602	EDO	O1-C1-C2-O2
2	Y	601	EDO	O1-C1-C2-O2
2	a	503	EDO	O1-C1-C2-O2
2	b	501	EDO	O1-C1-C2-O2
2	c	501	EDO	O1-C1-C2-O2
2	c	502	EDO	O1-C1-C2-O2
2	c	503	EDO	O1-C1-C2-O2
4	T	504	AKG	C3-C4-C5-O4
4	I	501	AKG	C3-C4-C5-O4
4	E	502	AKG	O1-C1-C2-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	502	AKG	O1-C1-C2-O5
4	P	505	AKG	O1-C1-C2-O5
4	X	603	AKG	C3-C4-C5-O3
4	A	503	AKG	C3-C4-C5-O3
4	G	502	AKG	O1-C1-C2-C3
4	K	503	AKG	O1-C1-C2-C3
4	S	603	AKG	O1-C1-C2-C3
4	I	501	AKG	C3-C4-C5-O3
4	T	504	AKG	C3-C4-C5-O3
2	P	503	EDO	O1-C1-C2-O2
4	U	503	AKG	C3-C4-C5-O4
4	U	503	AKG	C3-C4-C5-O3
4	J	502	AKG	C3-C4-C5-O4
4	Q	503	AKG	C3-C4-C5-O4
4	J	502	AKG	C3-C4-C5-O3
4	Q	503	AKG	C3-C4-C5-O3

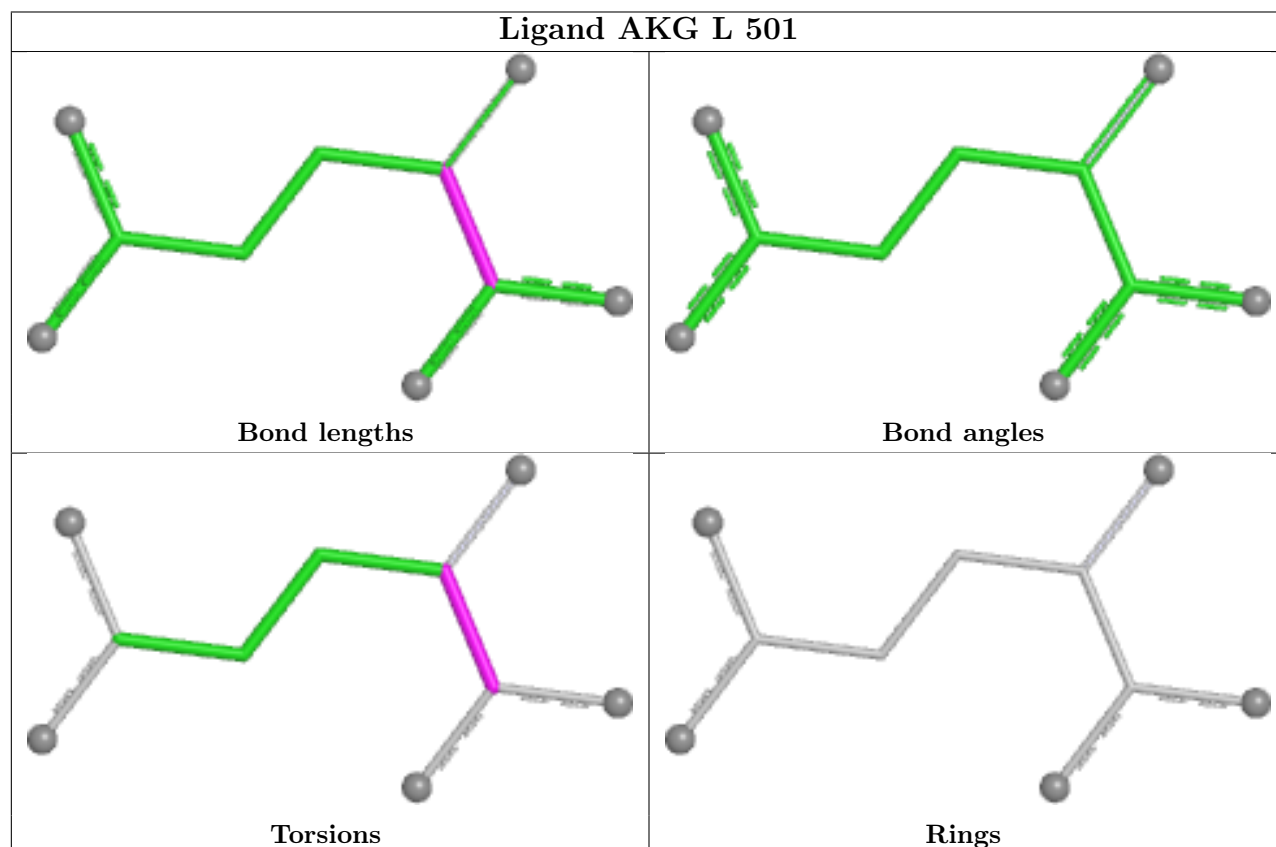
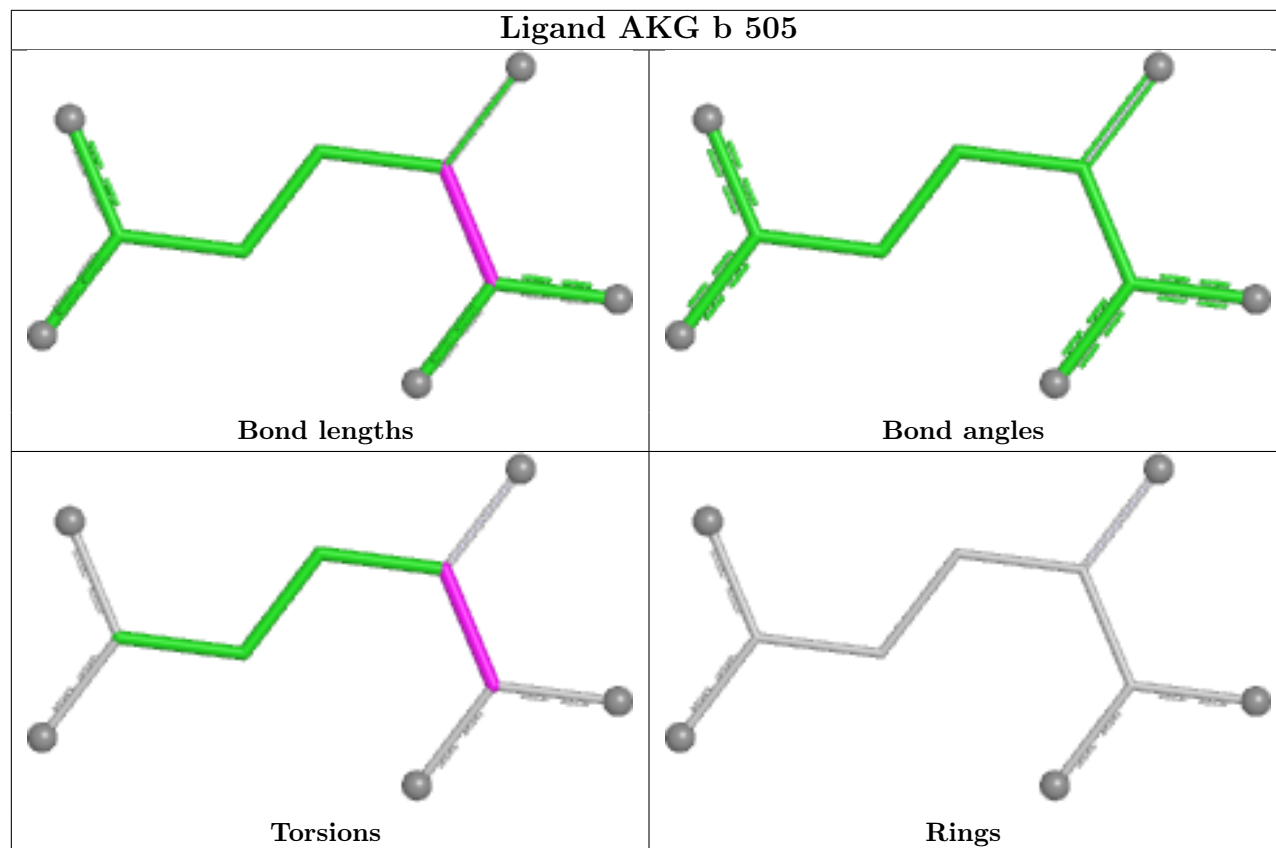
There are no ring outliers.

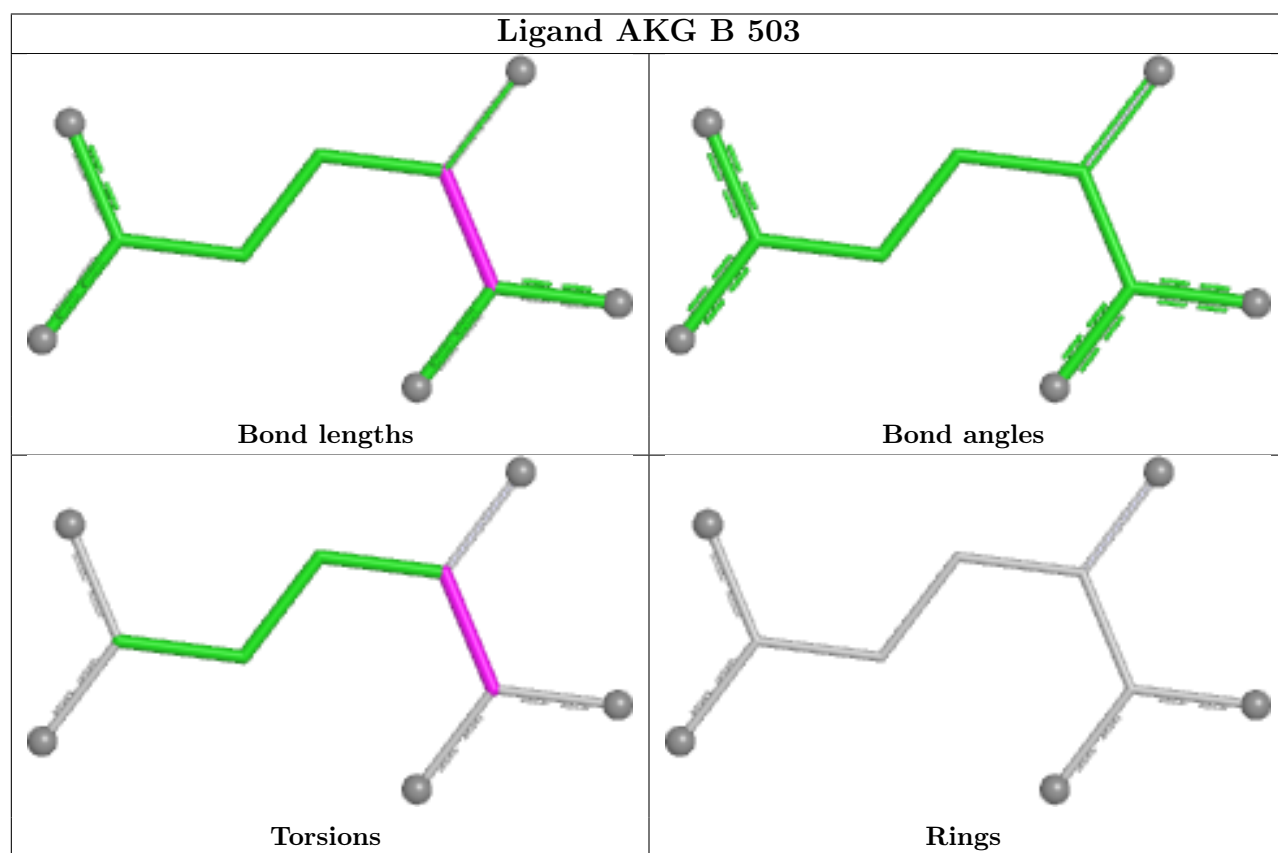
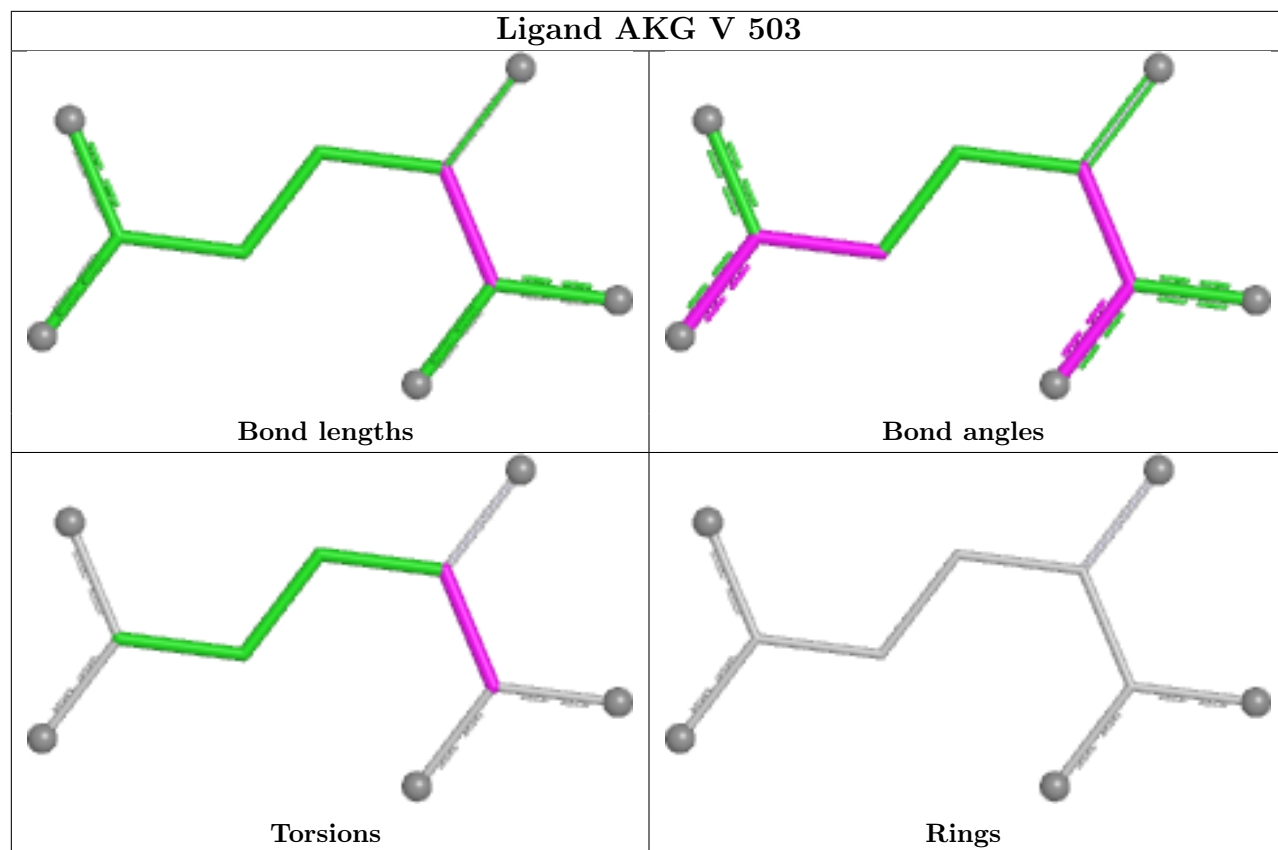
9 monomers are involved in 17 short contacts:

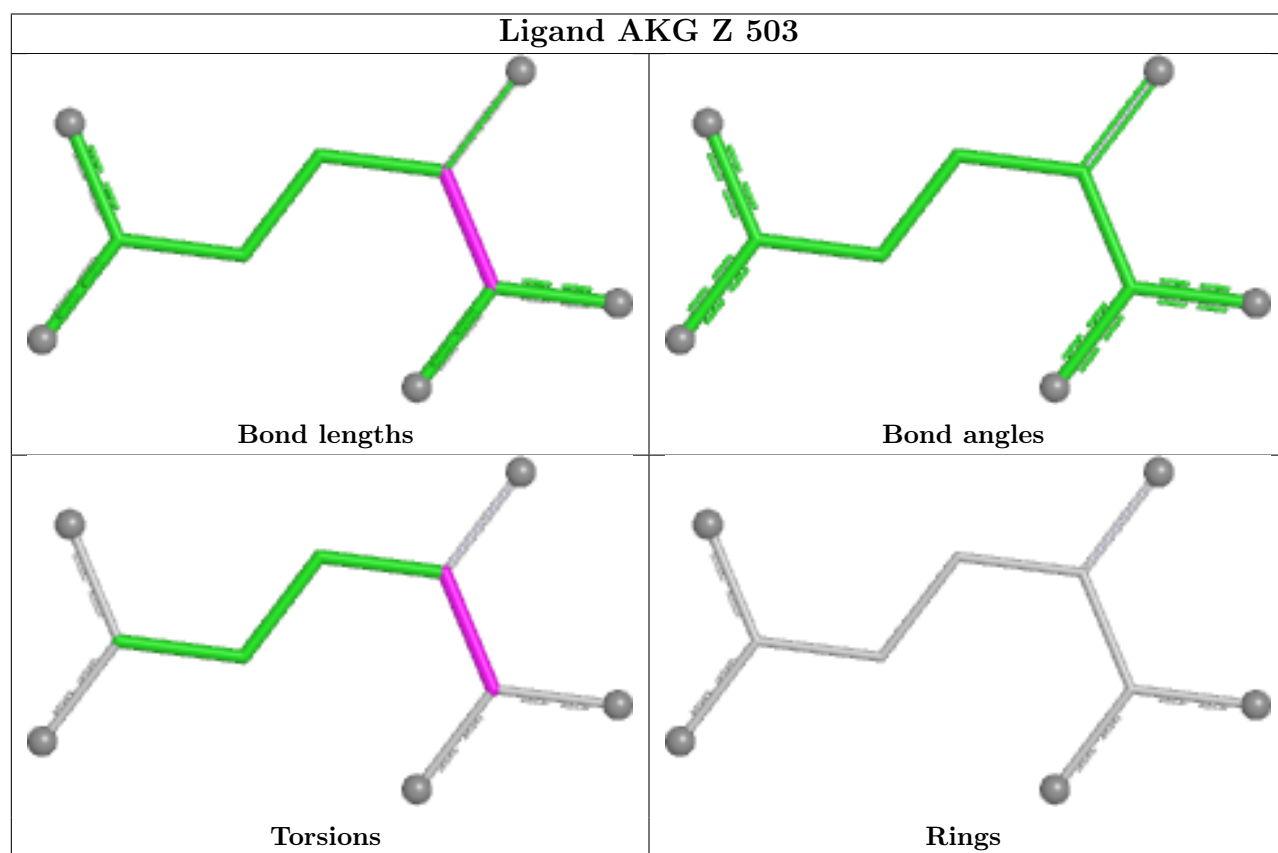
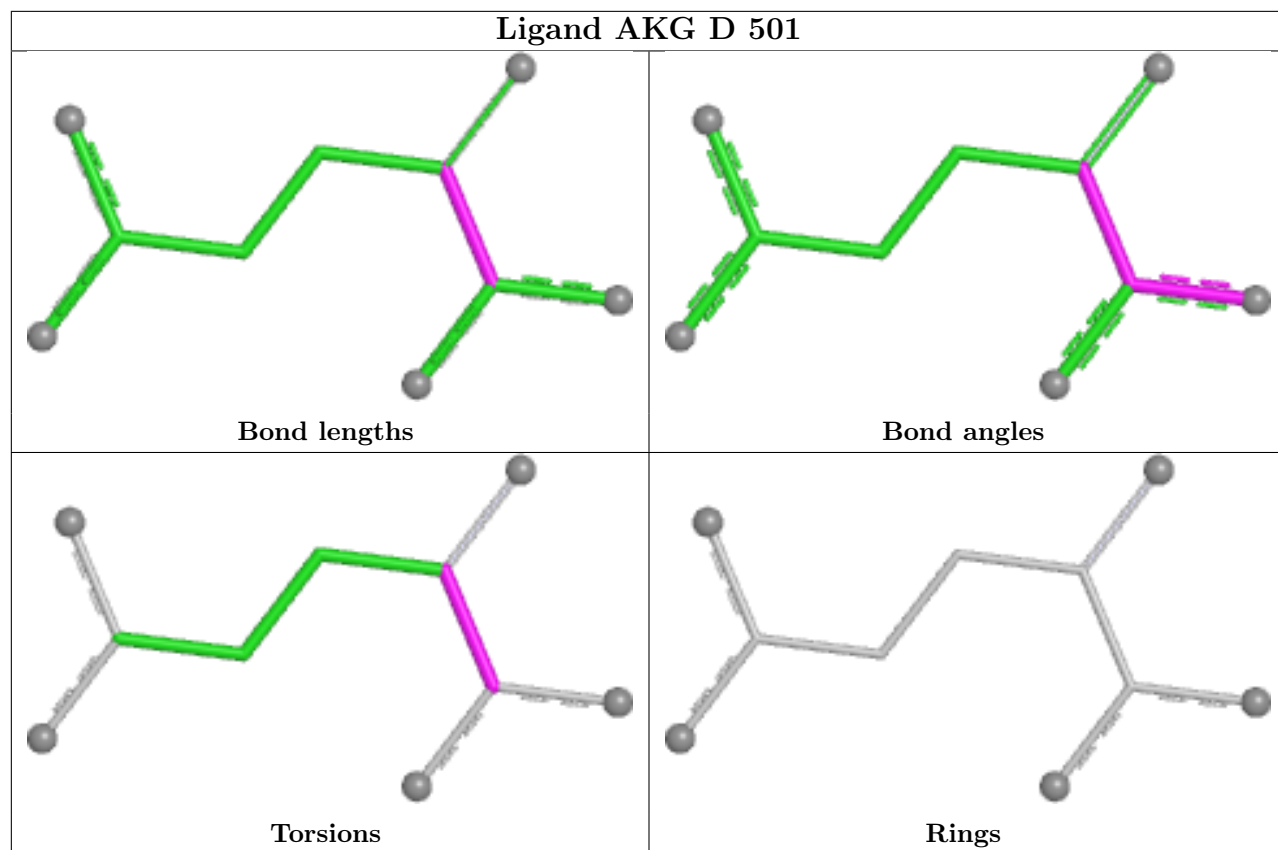
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	502	EDO	2	0
2	X	601	EDO	4	0
2	U	502	EDO	2	0
2	F	501	EDO	3	0
2	c	501	EDO	1	0
2	G	501	EDO	1	0
2	V	501	EDO	2	0
2	Z	501	EDO	1	0
2	P	503	EDO	1	0

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

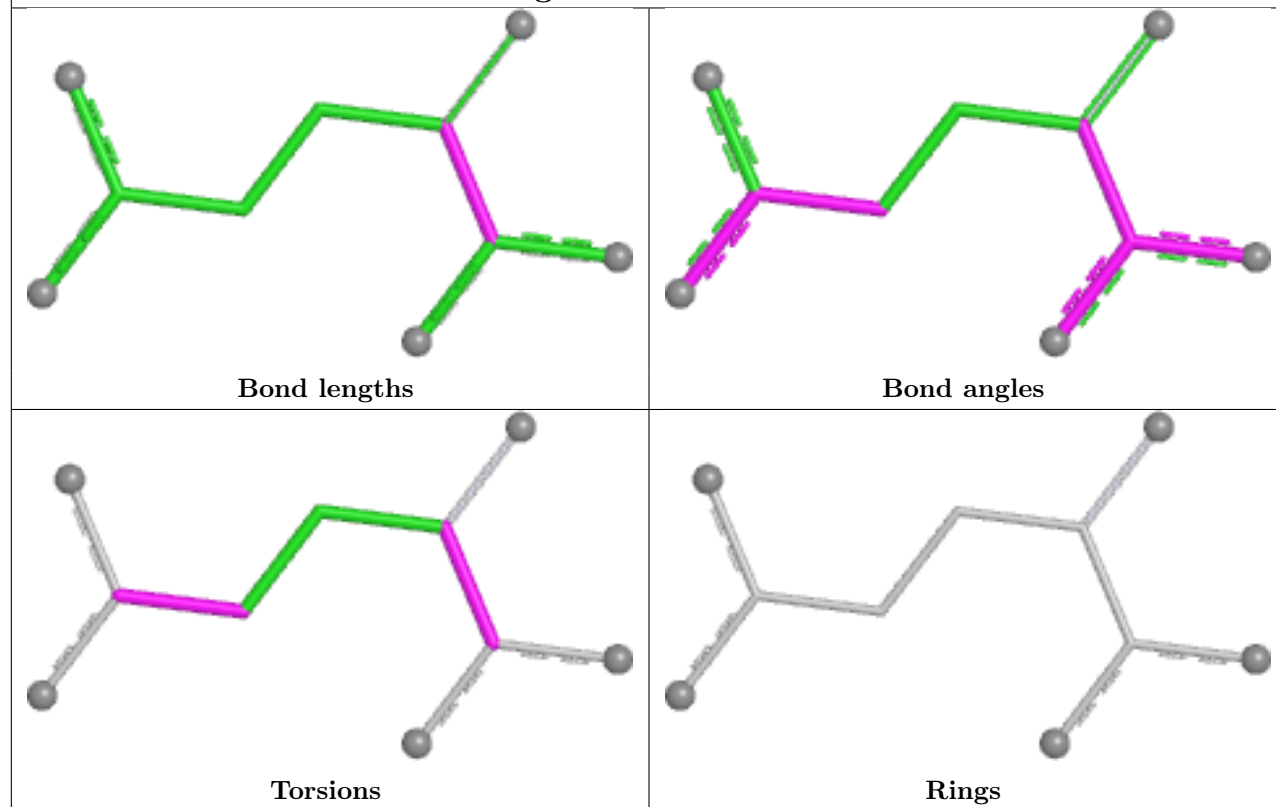
equivalents in the CSD to analyse the geometry.



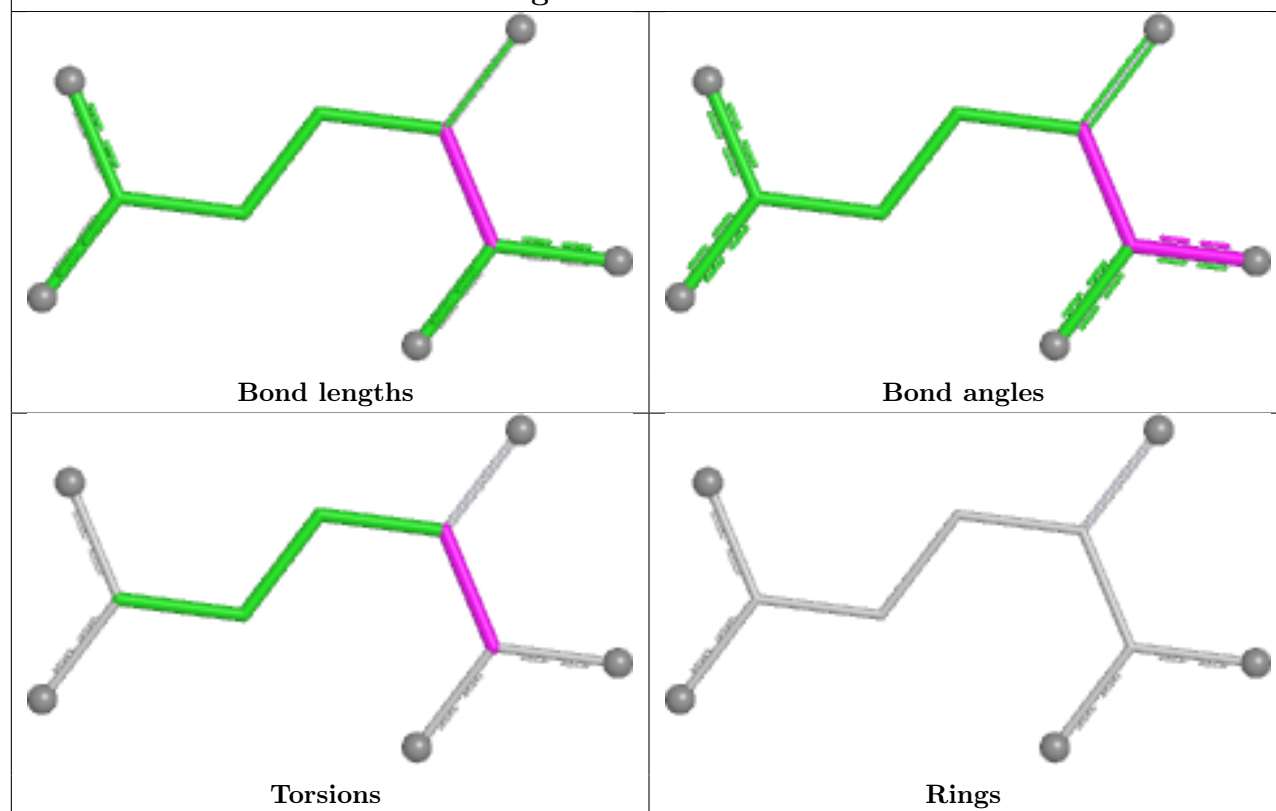




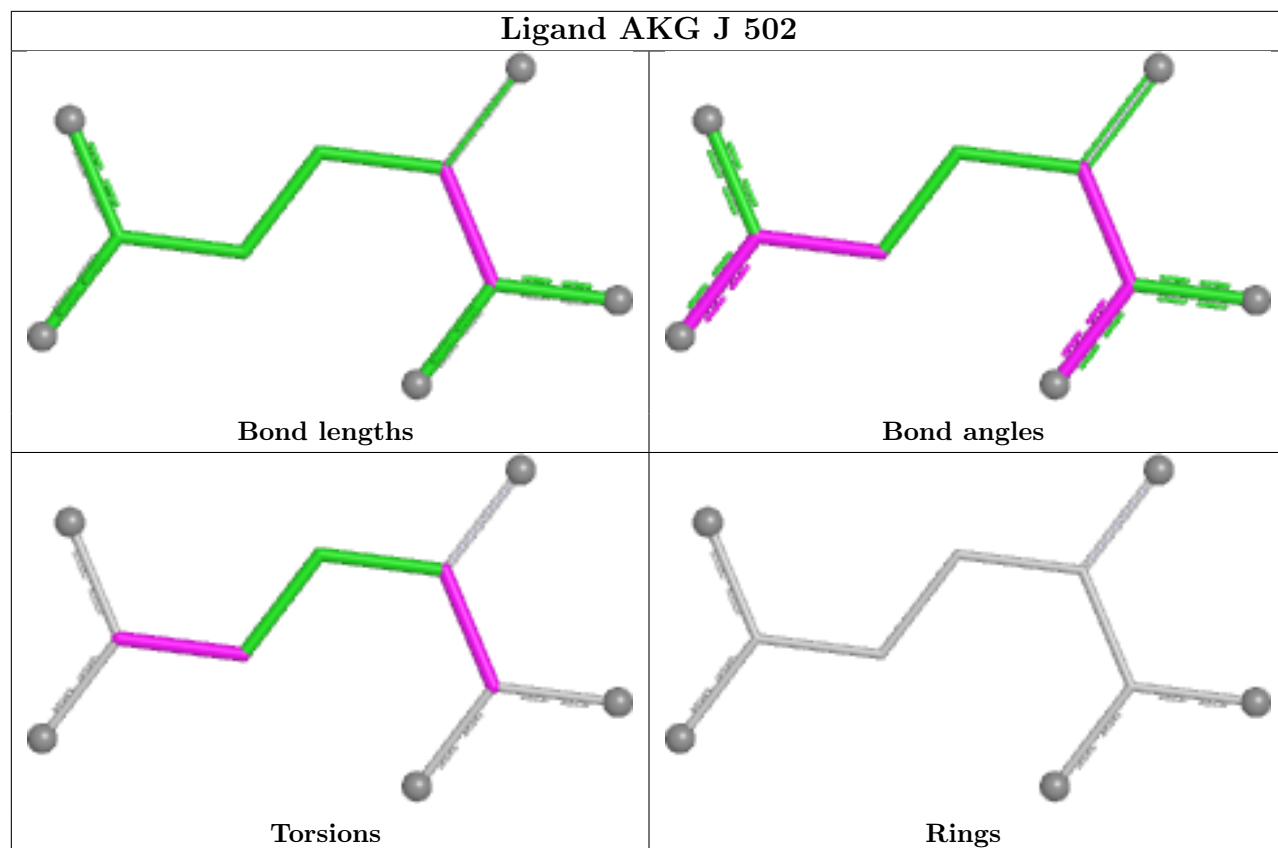
Ligand AKG I 501



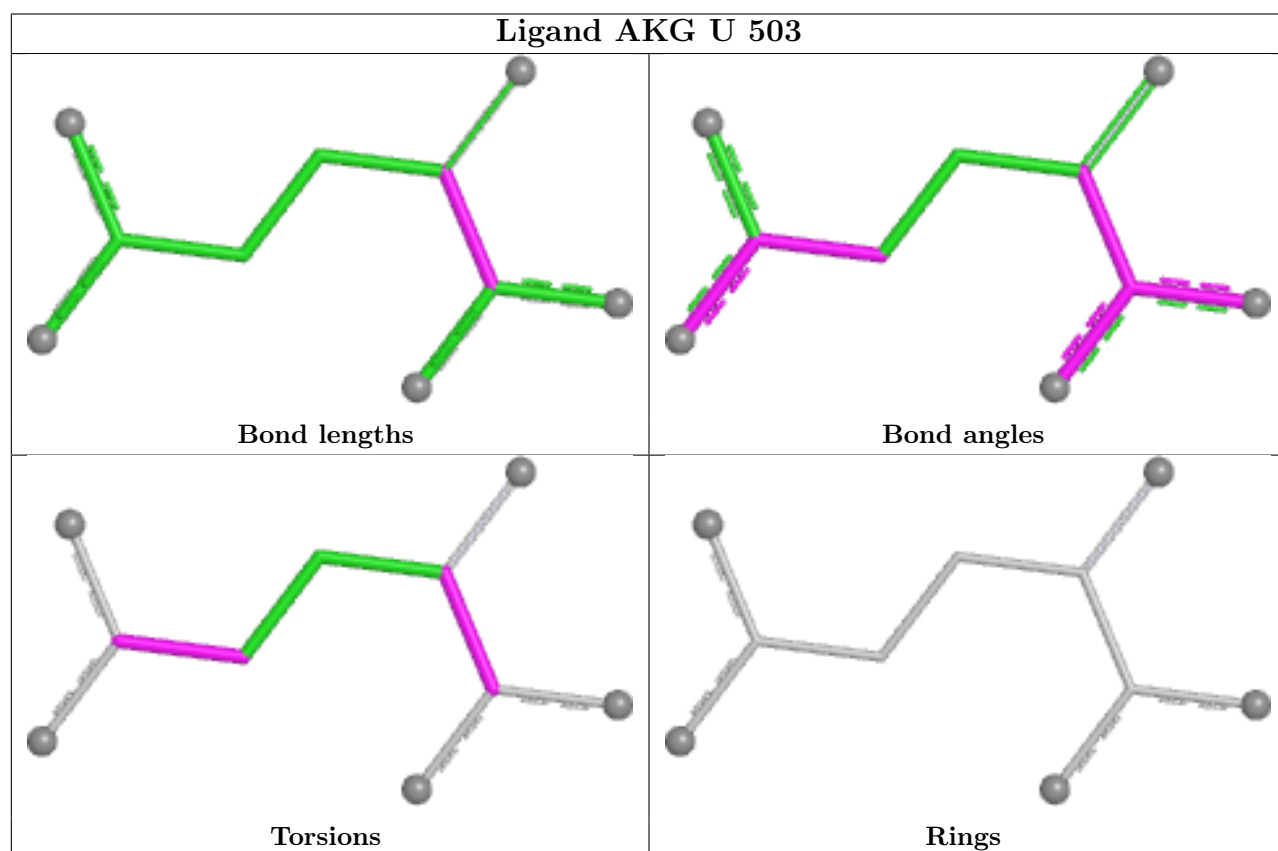
Ligand AKG S 603

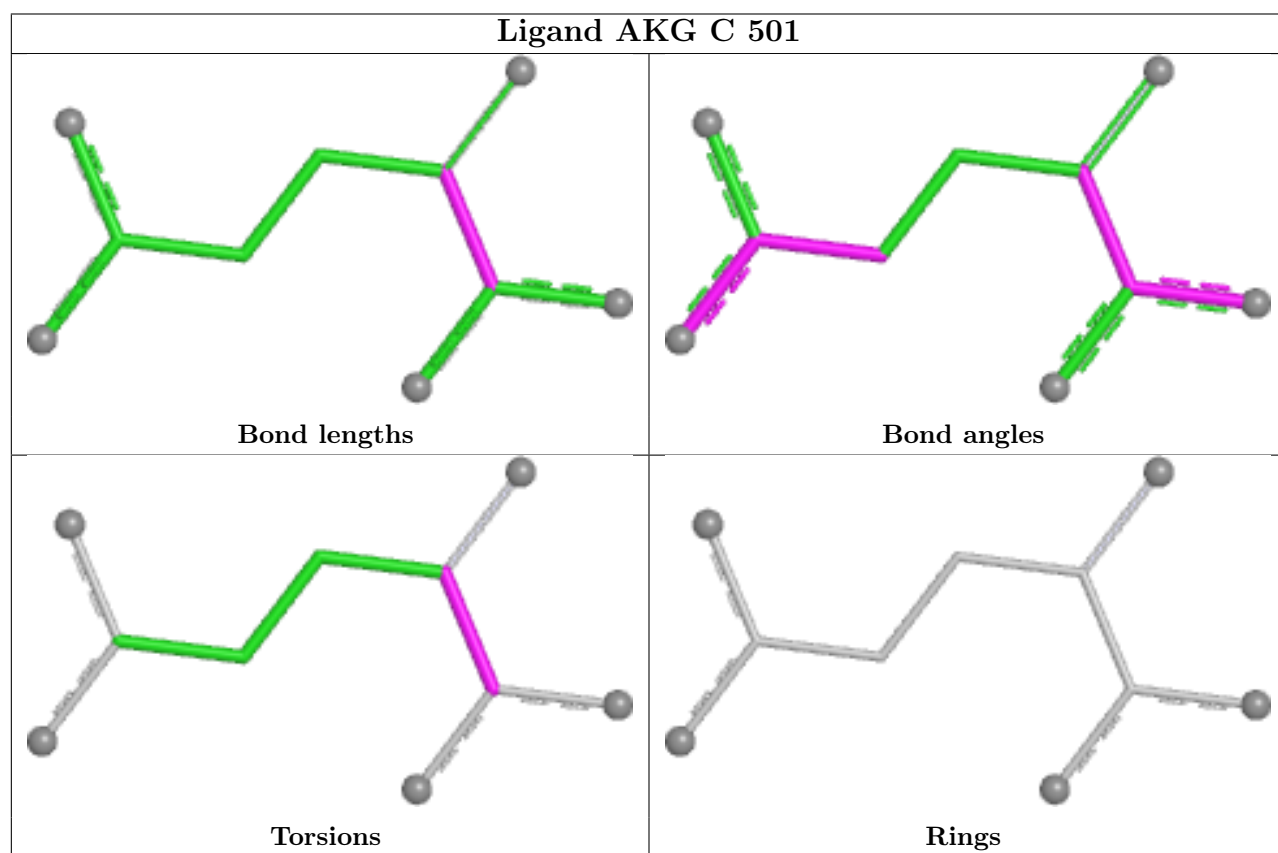
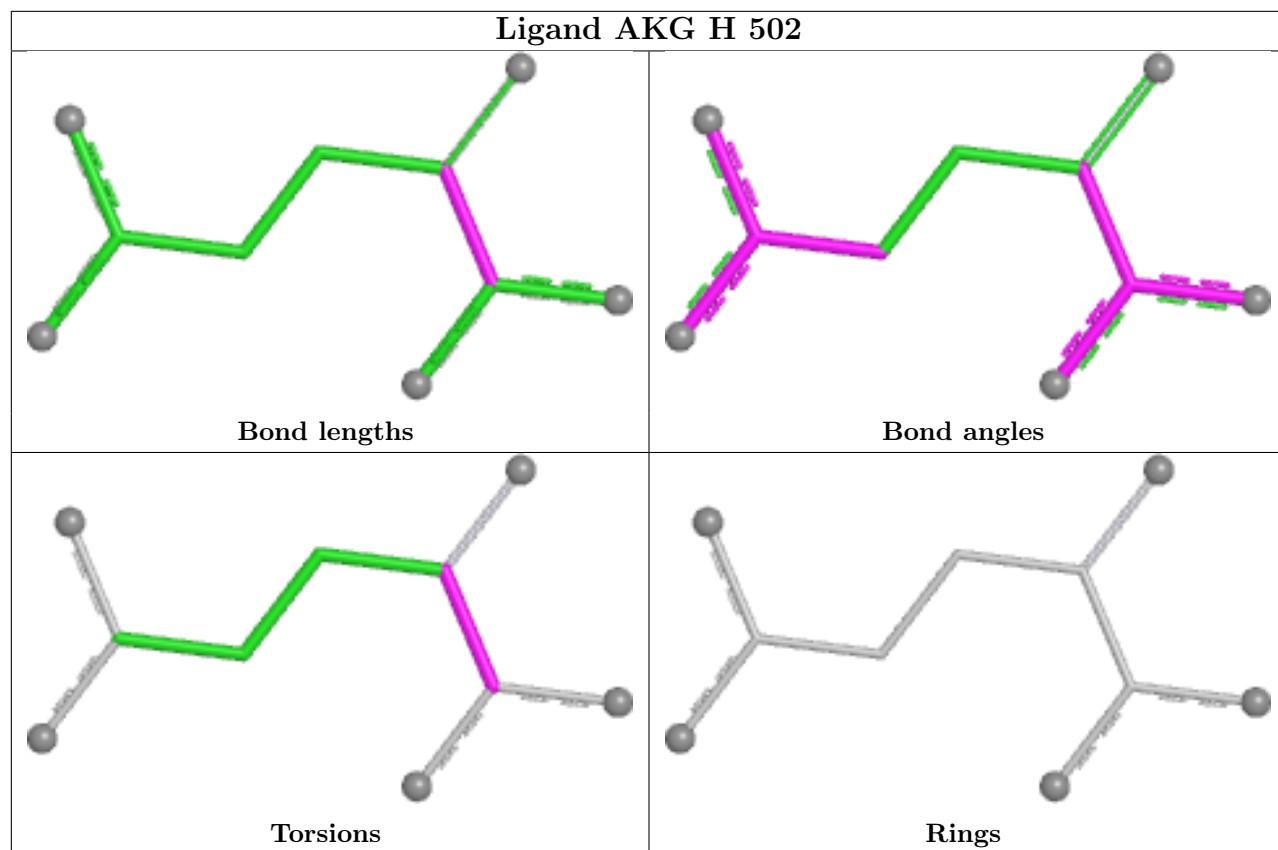


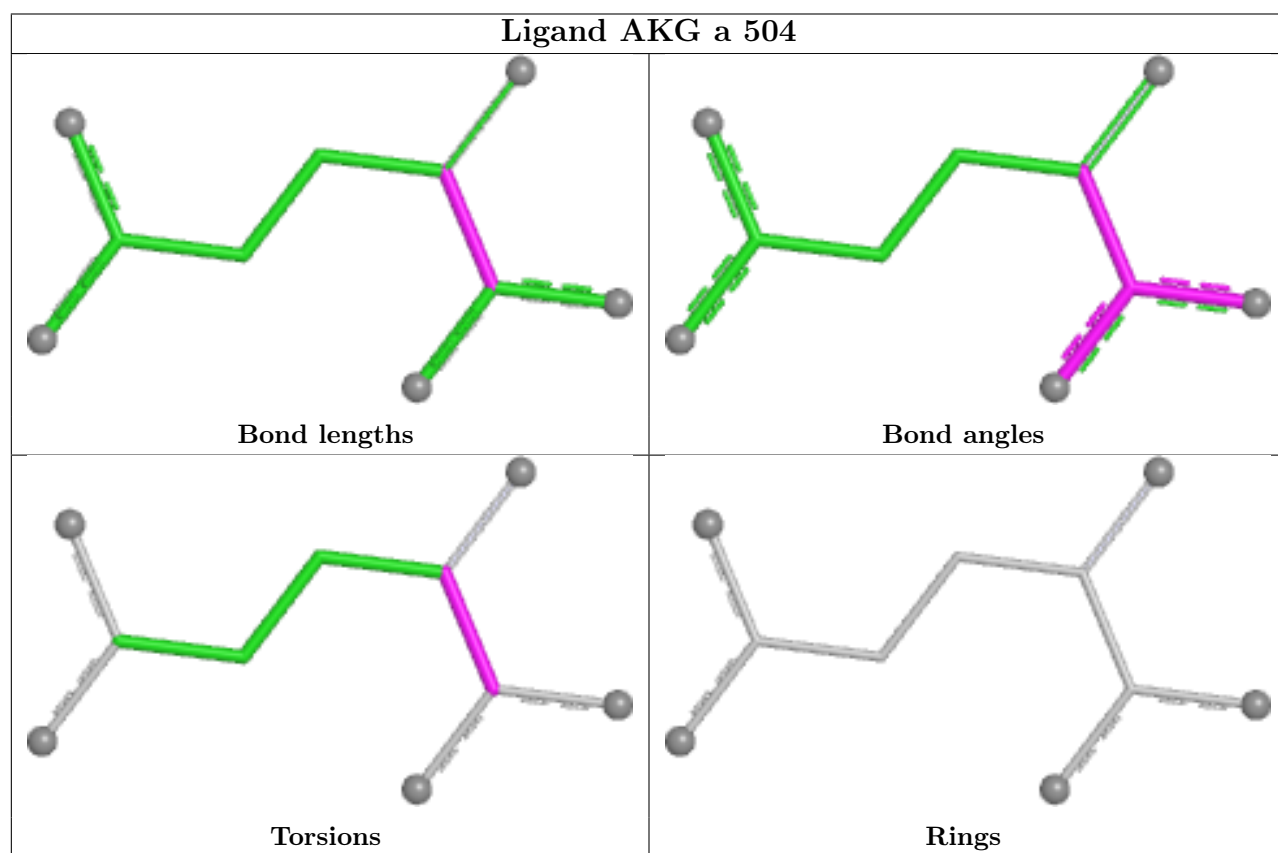
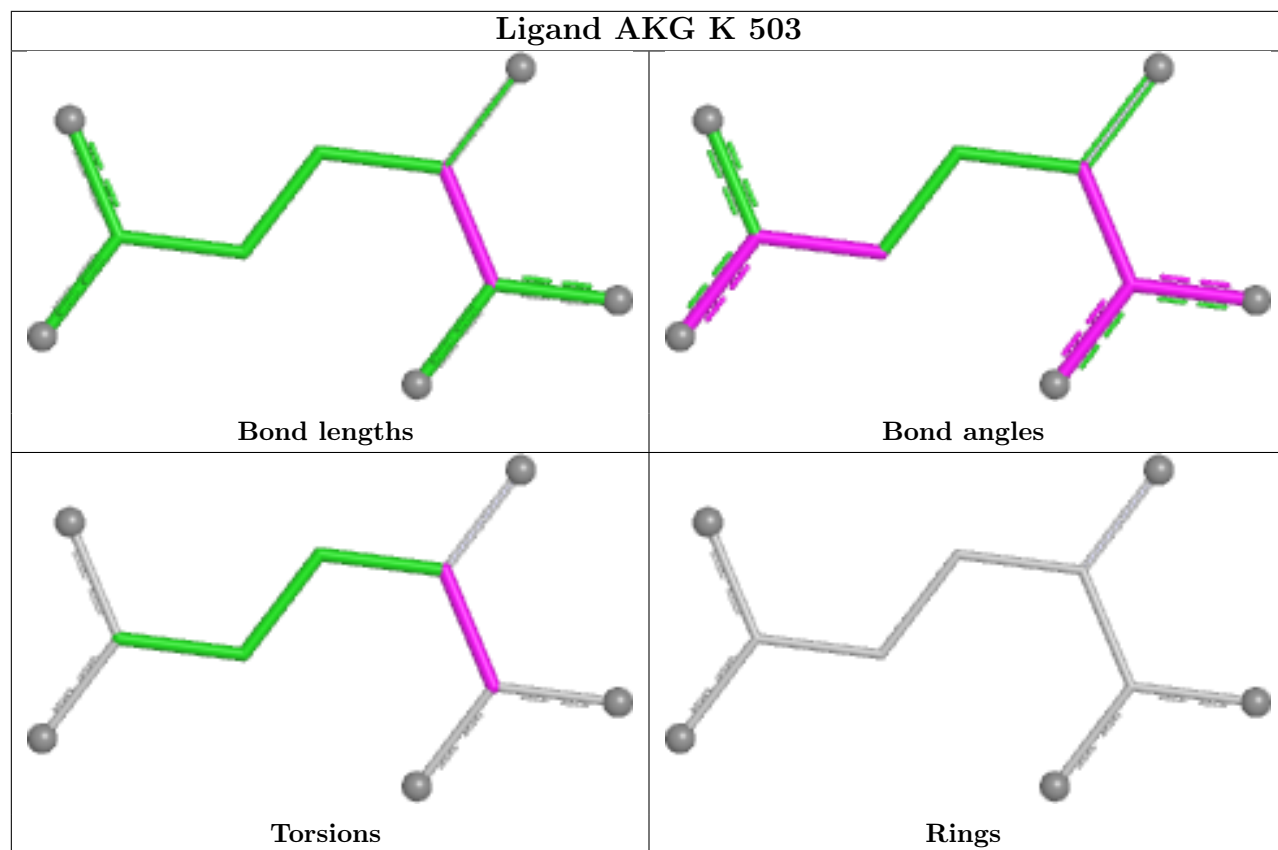
Ligand AKG J 502

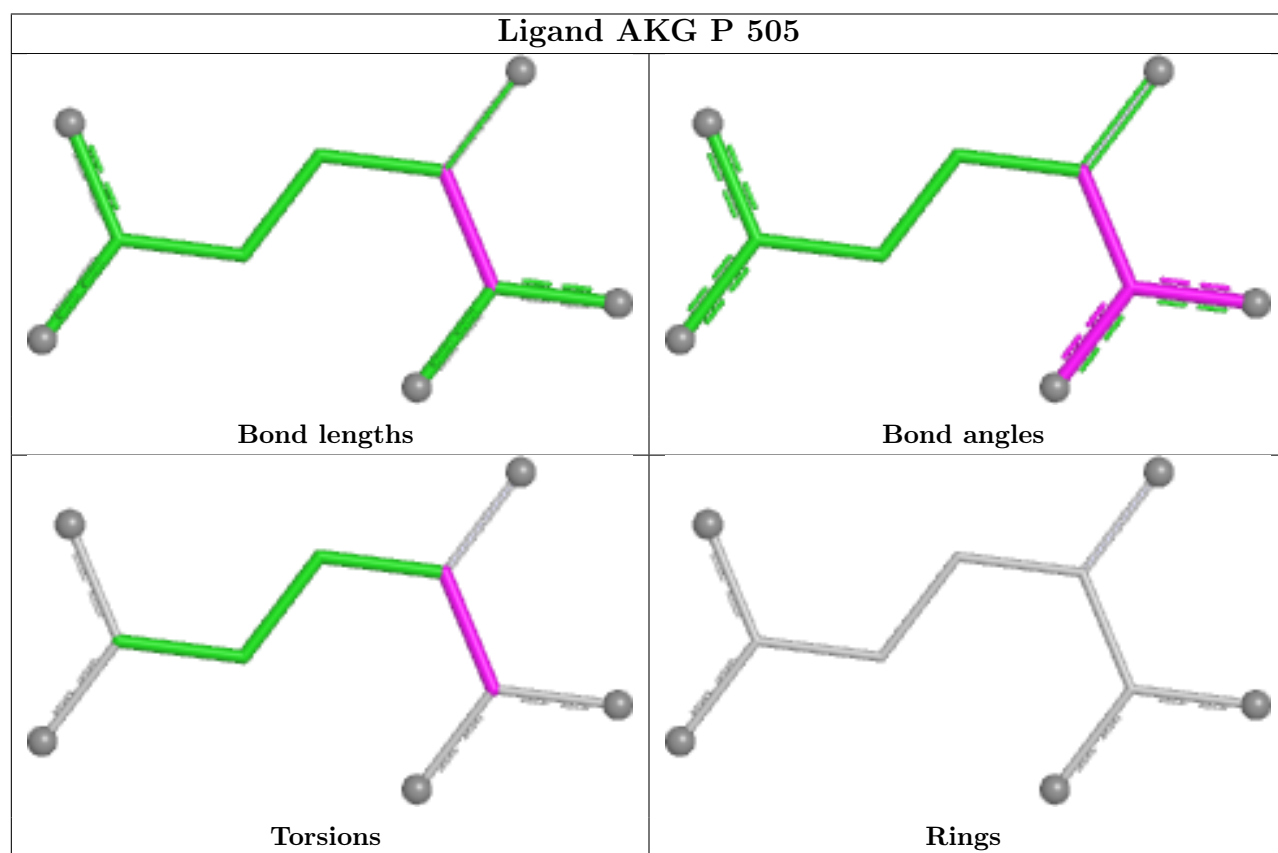
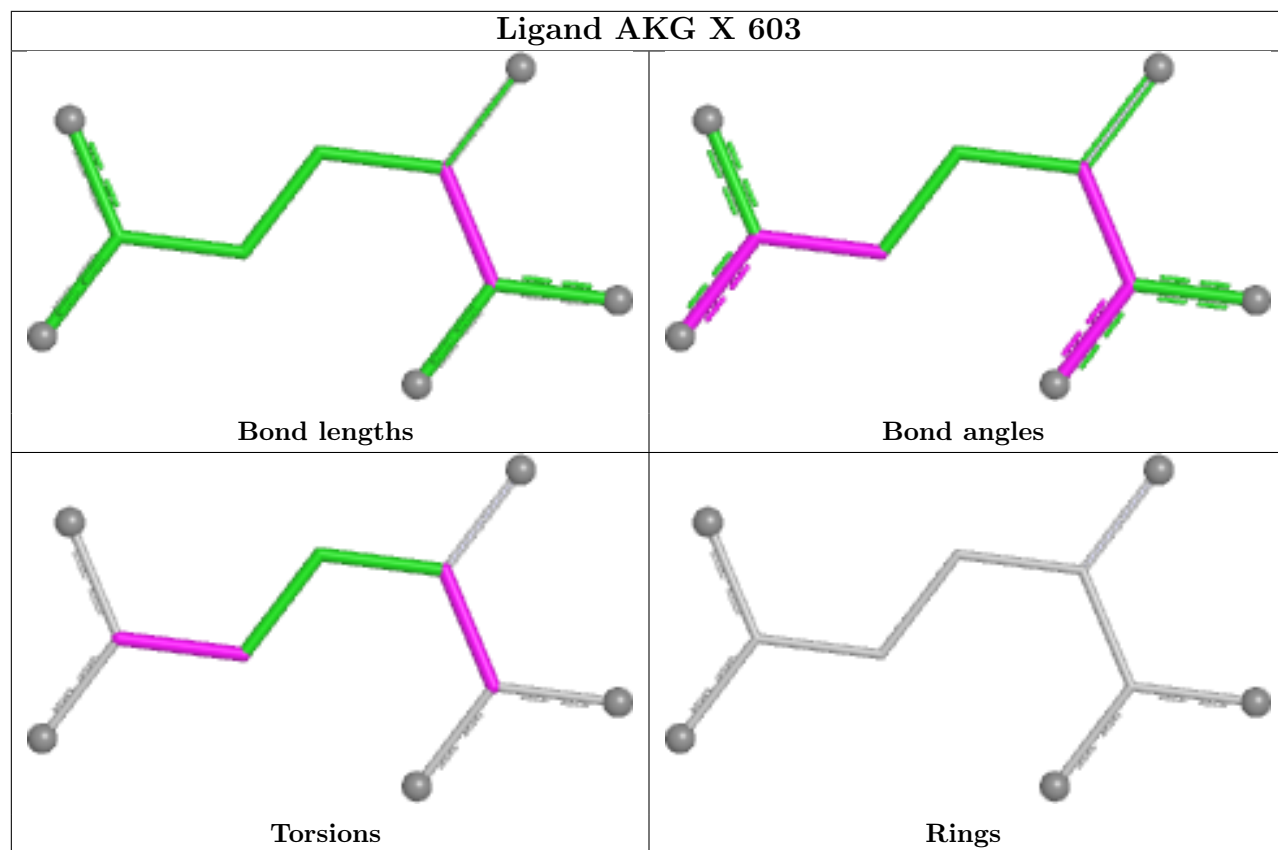


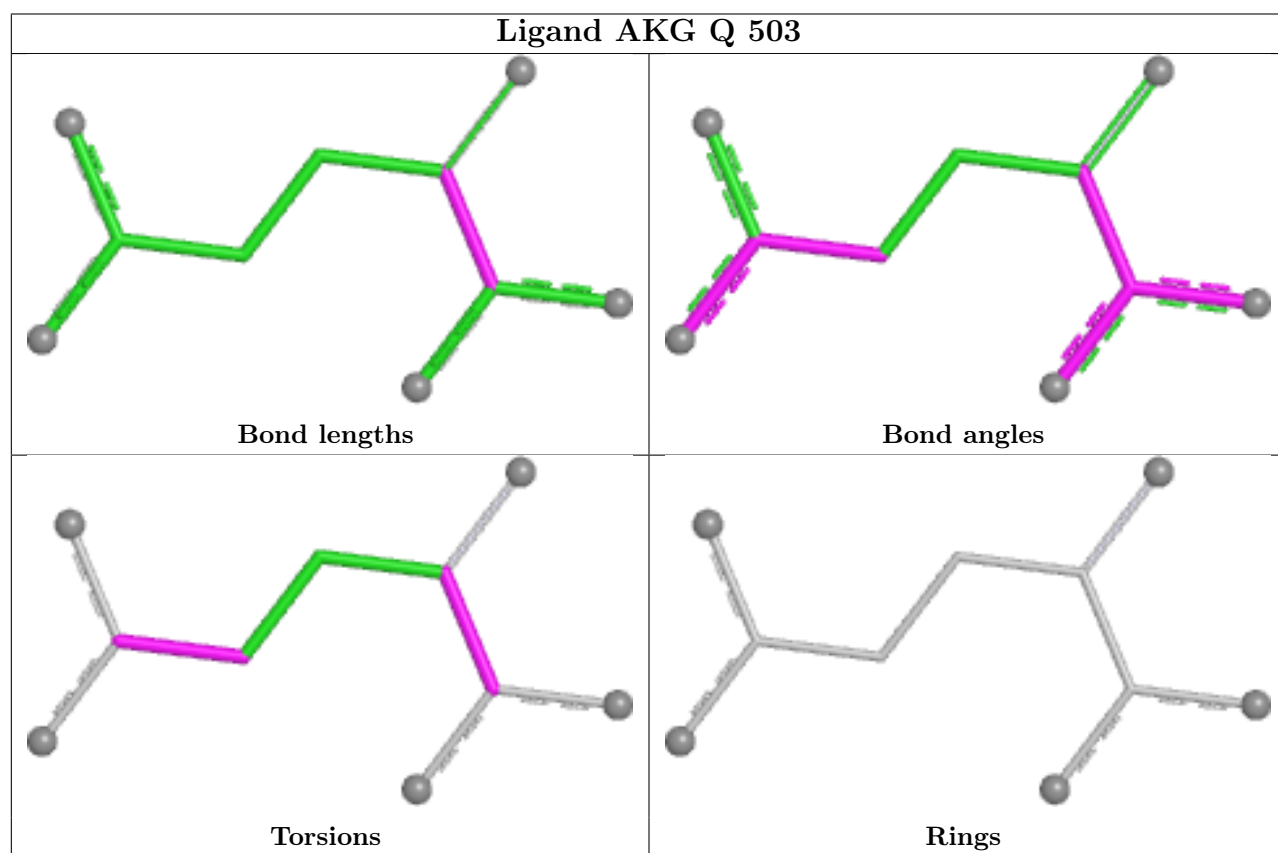
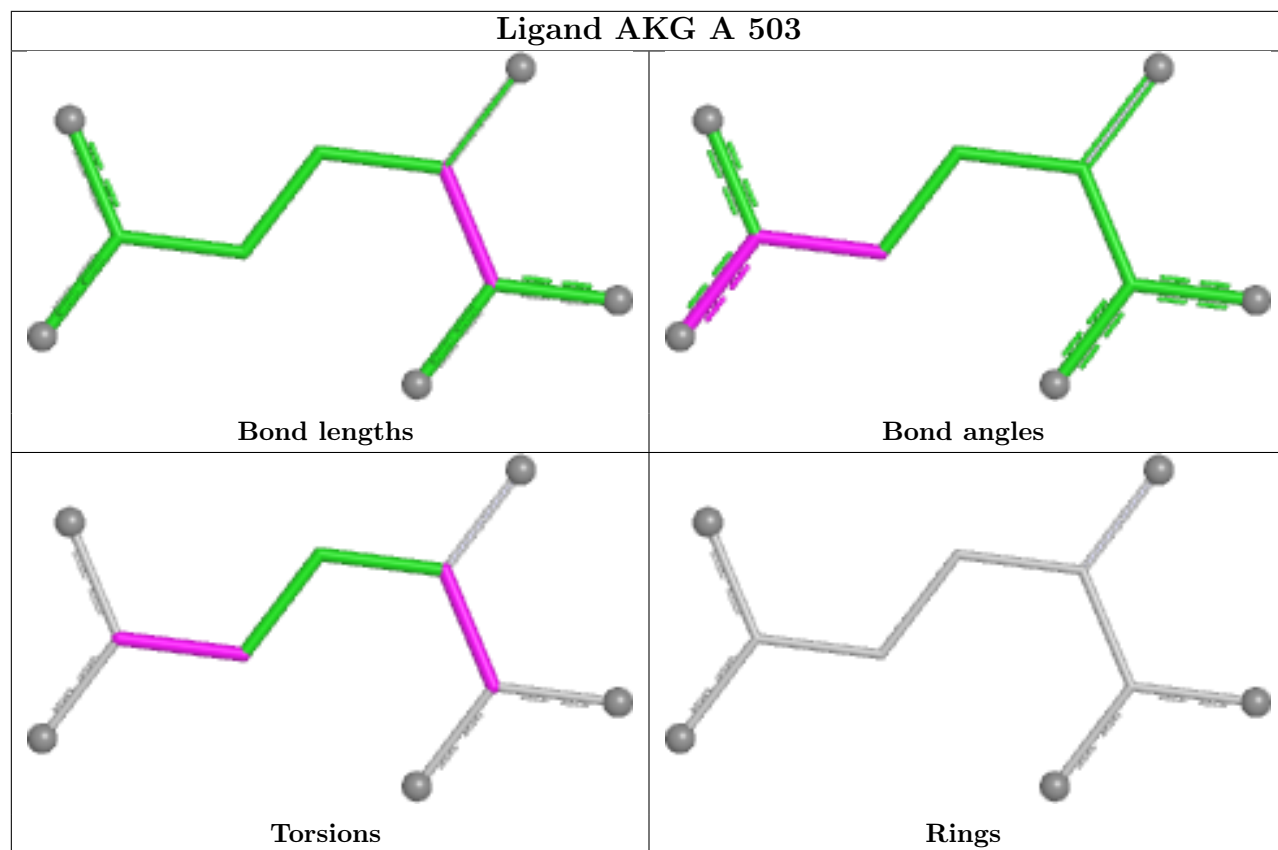
Ligand AKG U 503

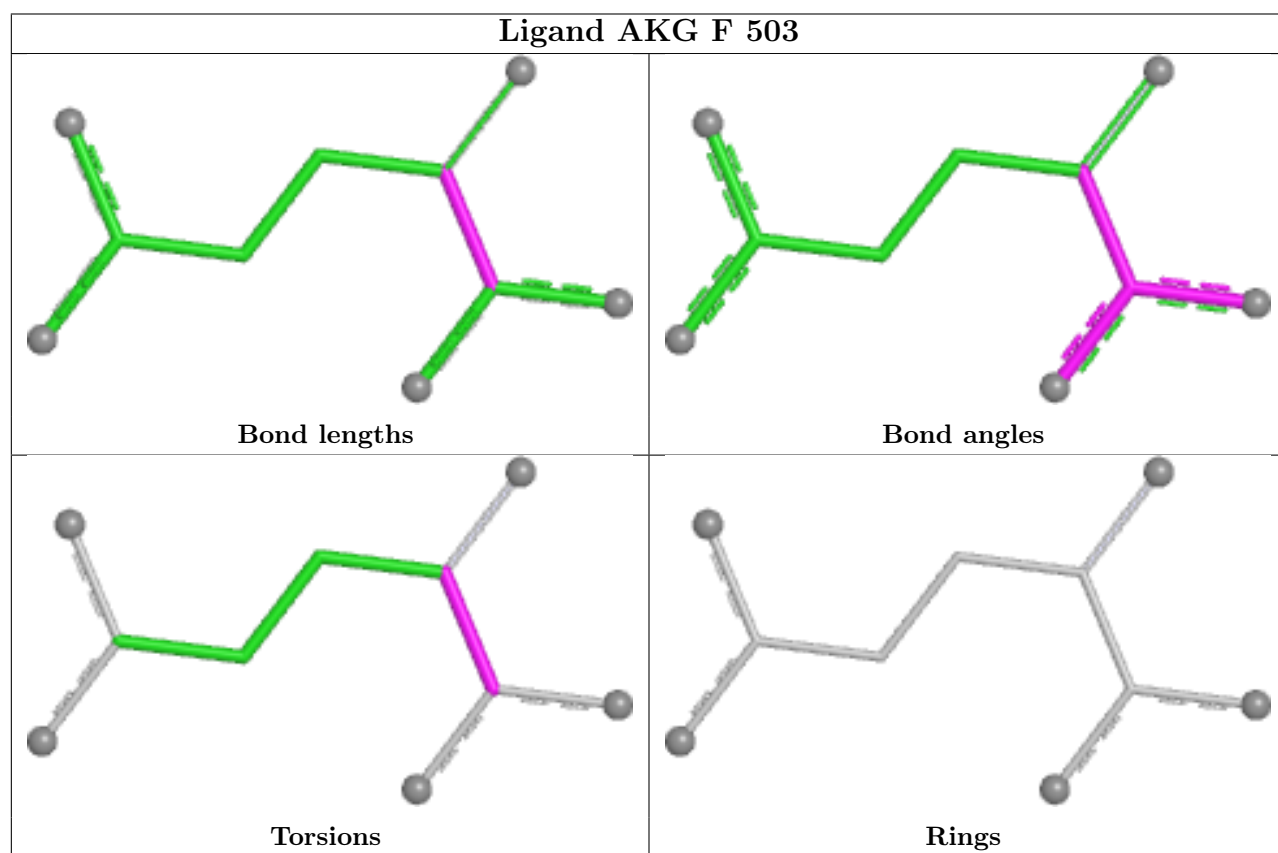
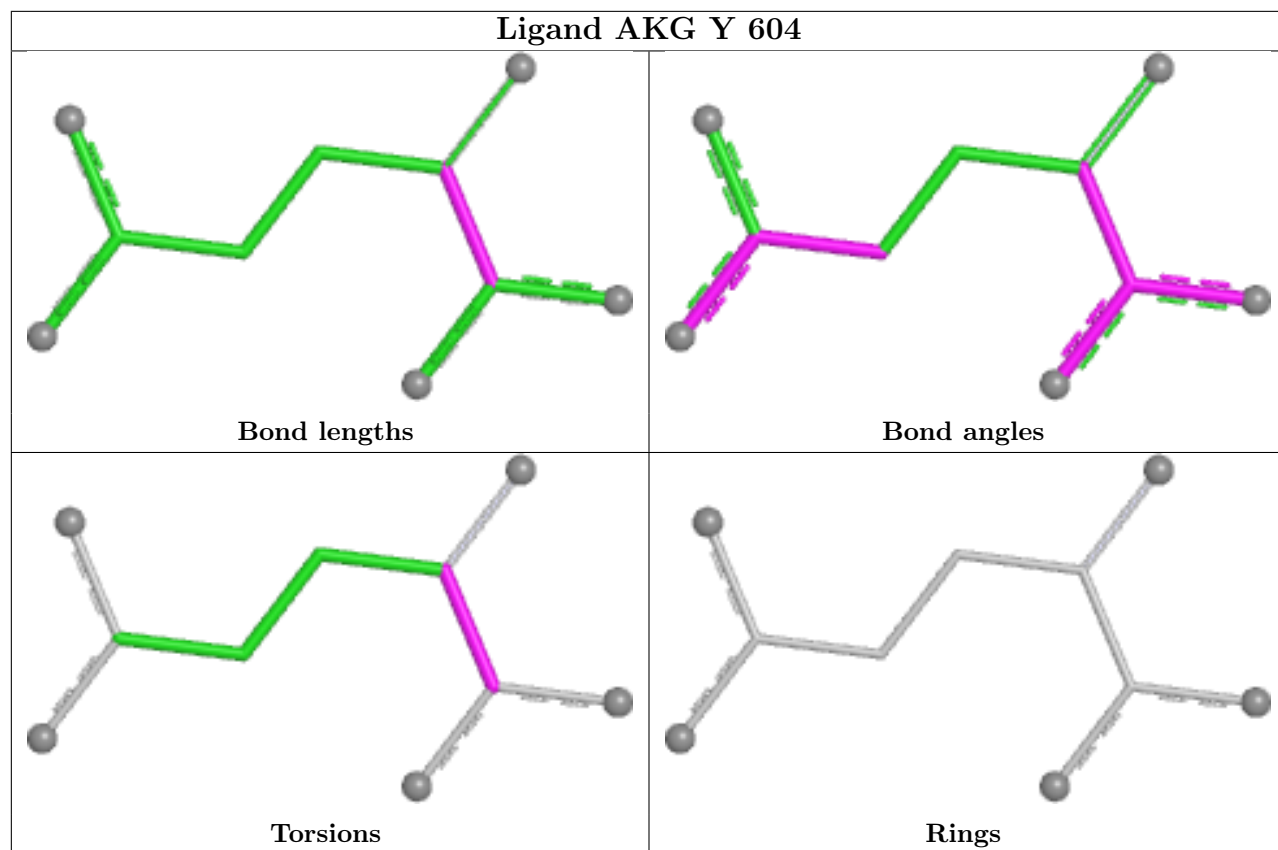


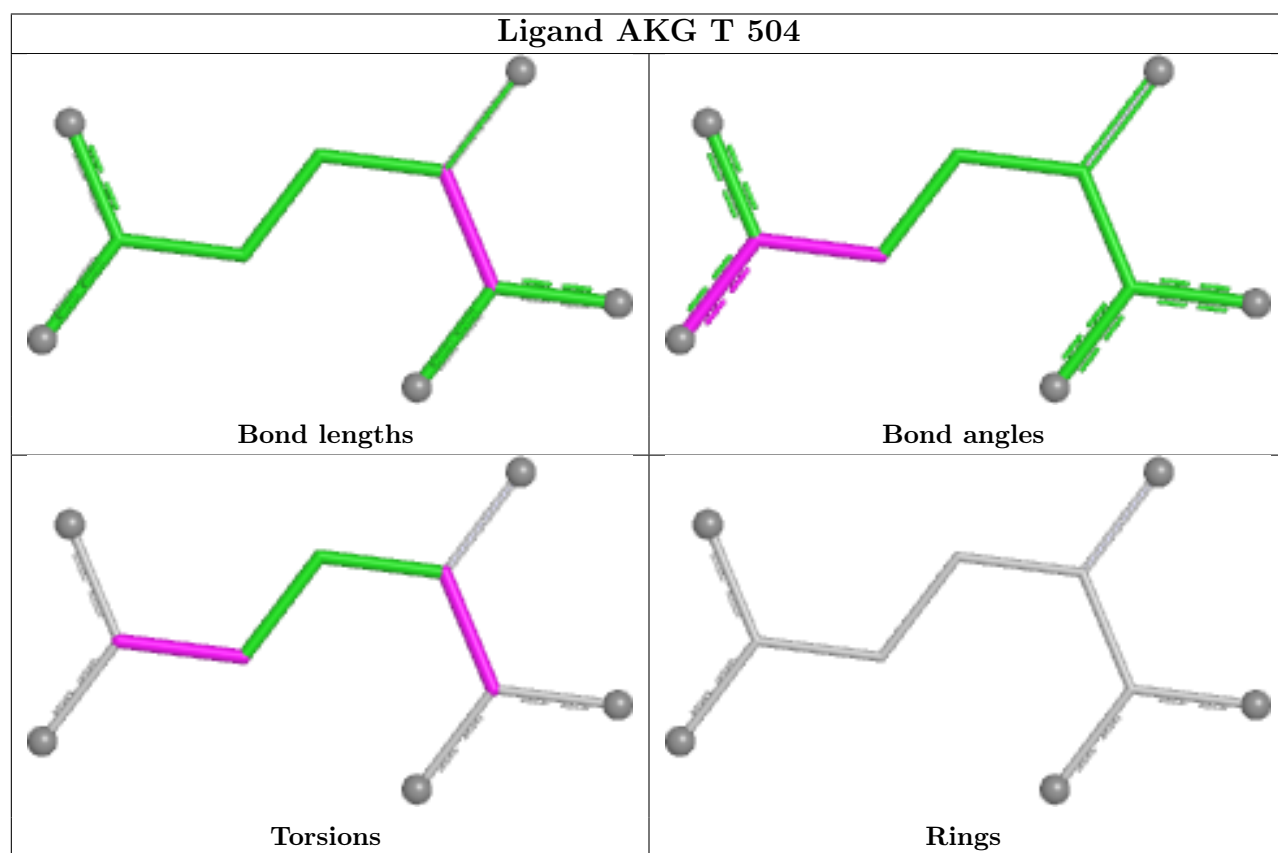
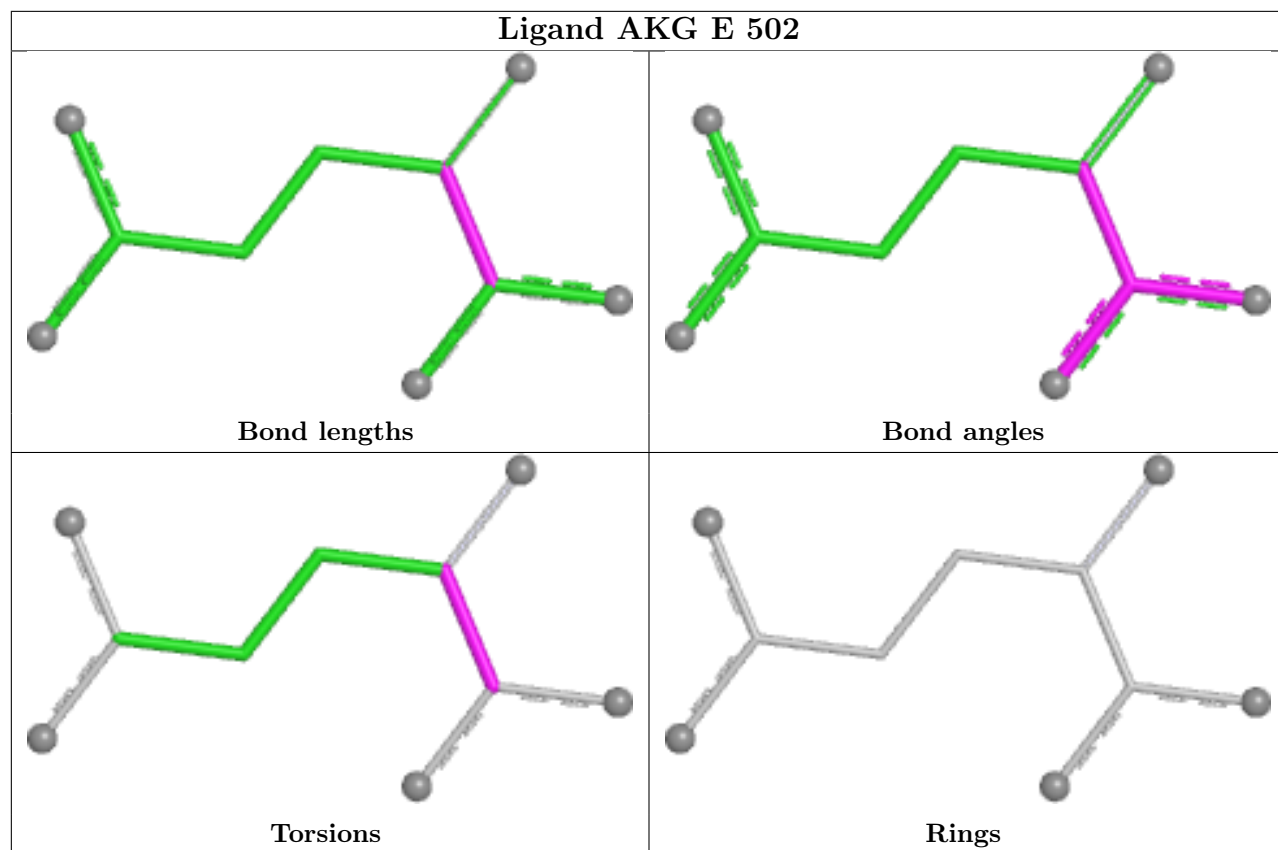




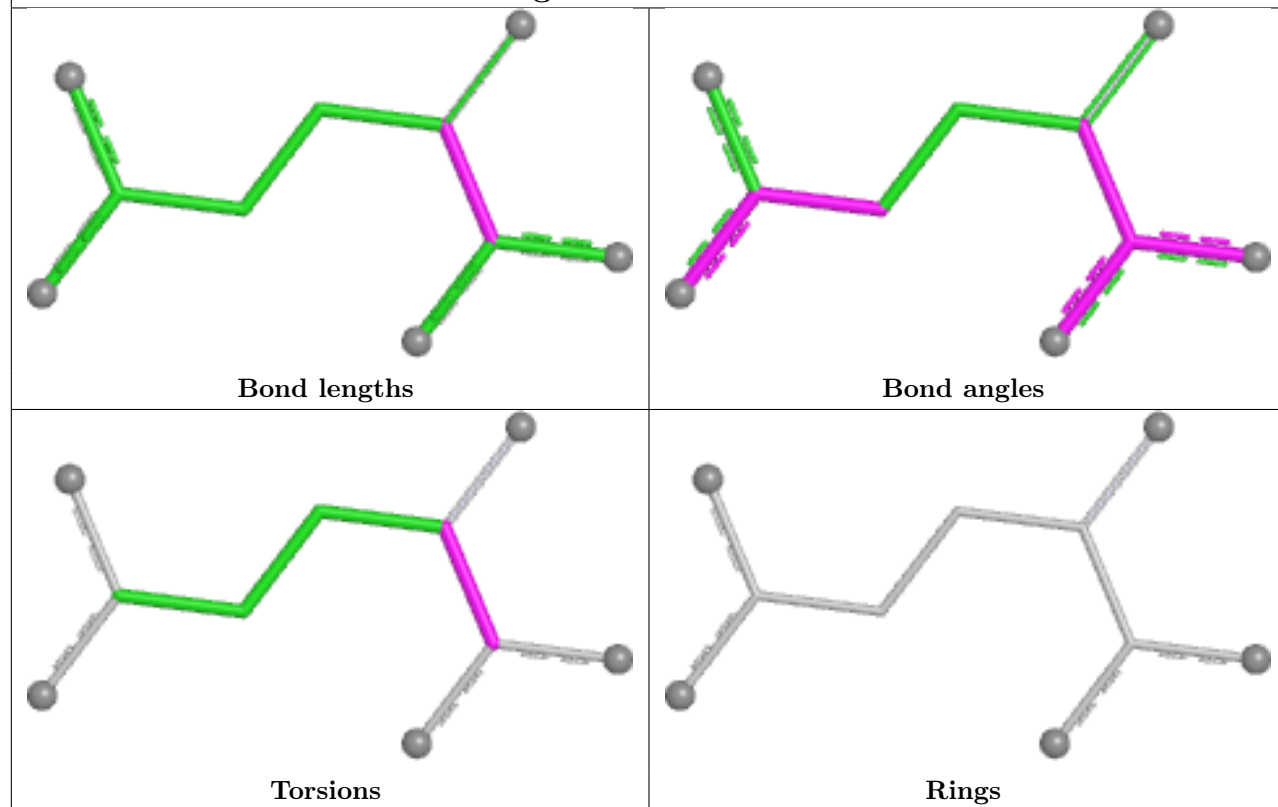




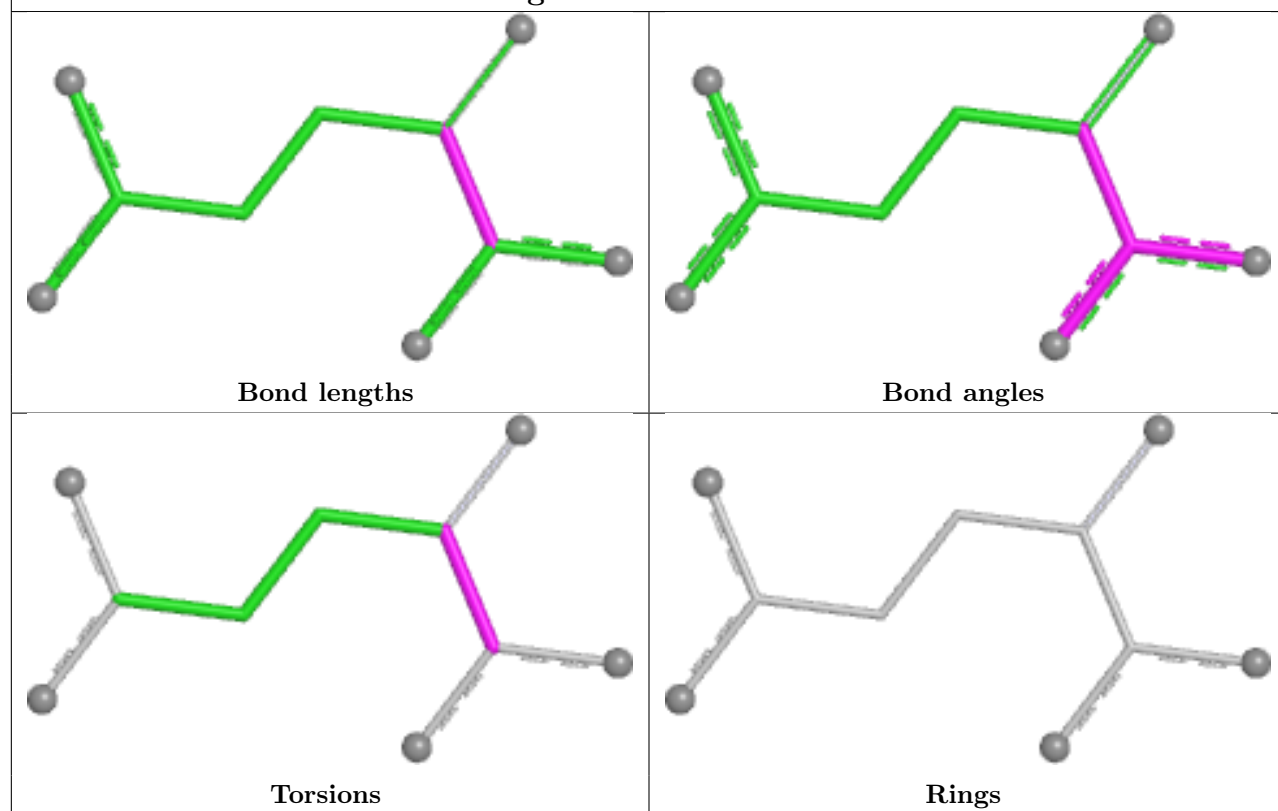




Ligand AKG c 504



Ligand AKG G 502



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	446/448 (99%)	-1.57	0 100 100	43, 66, 89, 107	0
1	B	446/448 (99%)	-1.57	0 100 100	46, 64, 101, 121	0
1	C	447/448 (99%)	-1.53	0 100 100	52, 71, 102, 125	0
1	D	447/448 (99%)	-1.47	0 100 100	51, 72, 109, 127	0
1	E	447/448 (99%)	-1.55	0 100 100	47, 67, 100, 126	0
1	F	447/448 (99%)	-1.53	0 100 100	48, 65, 98, 119	0
1	G	447/448 (99%)	-1.58	0 100 100	42, 61, 86, 104	0
1	H	447/448 (99%)	-1.54	0 100 100	46, 63, 91, 118	0
1	I	447/448 (99%)	-1.51	0 100 100	49, 72, 105, 129	0
1	J	447/448 (99%)	-1.51	0 100 100	53, 74, 112, 134	0
1	K	447/448 (99%)	-1.52	0 100 100	46, 67, 108, 143	0
1	L	447/448 (99%)	-1.53	0 100 100	47, 68, 103, 127	0
1	P	447/448 (99%)	-1.59	0 100 100	25, 48, 75, 101	0
1	Q	446/448 (99%)	-1.52	0 100 100	31, 58, 91, 112	0
1	S	447/448 (99%)	-1.56	0 100 100	31, 57, 90, 104	0
1	T	447/448 (99%)	-1.56	0 100 100	22, 52, 91, 128	0
1	U	447/448 (99%)	-1.56	0 100 100	29, 51, 89, 127	0
1	V	447/448 (99%)	-1.53	0 100 100	29, 56, 87, 114	0
1	X	447/448 (99%)	-1.57	0 100 100	26, 51, 92, 111	0
1	Y	447/448 (99%)	-1.61	0 100 100	19, 48, 80, 99	0
1	Z	447/448 (99%)	-1.54	0 100 100	27, 58, 95, 124	0
1	a	446/448 (99%)	-1.60	0 100 100	26, 48, 79, 107	0
1	b	447/448 (99%)	-1.59	0 100 100	27, 53, 84, 101	0
1	c	447/448 (99%)	-1.60	0 100 100	24, 49, 83, 106	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10724/10752 (99%)	-1.55	0 100 100	19, 62, 97, 143	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
3	MG	F	502	1/1	0.97	0.05	50,50,50,50	0
3	MG	b	504	1/1	0.97	0.04	40,40,40,40	0
2	EDO	U	502	4/4	0.98	0.05	34,37,41,42	0
3	MG	Q	501	1/1	0.98	0.08	42,42,42,42	0
3	MG	S	602	1/1	0.98	0.03	24,24,24,24	0
3	MG	b	503	1/1	0.98	0.04	39,39,39,39	0
2	EDO	b	502	4/4	0.98	0.04	24,32,37,38	0
4	AKG	E	502	10/10	0.98	0.05	44,51,60,64	0
2	EDO	V	502	4/4	0.99	0.04	31,36,37,42	0
2	EDO	X	602	4/4	0.99	0.05	26,43,44,50	0
2	EDO	Y	601	4/4	0.99	0.02	20,29,36,36	0
2	EDO	Y	602	4/4	0.99	0.04	25,35,37,43	0
2	EDO	b	501	4/4	0.99	0.04	25,26,30,34	0
2	EDO	E	501	4/4	0.99	0.05	43,51,52,52	0
2	EDO	c	501	4/4	0.99	0.03	14,18,20,22	0
2	EDO	c	502	4/4	0.99	0.04	26,28,32,36	0
2	EDO	c	503	4/4	0.99	0.05	29,30,32,46	0
3	MG	B	501	1/1	0.99	0.05	13,13,13,13	0
3	MG	B	502	1/1	0.99	0.02	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	F	501	4/4	0.99	0.02	24,29,32,49	0
3	MG	H	501	1/1	0.99	0.12	48,48,48,48	0
3	MG	K	502	1/1	0.99	0.06	61,61,61,61	0
2	EDO	K	501	4/4	0.99	0.05	39,40,43,47	0
2	EDO	P	501	4/4	0.99	0.03	21,22,23,24	0
3	MG	T	502	1/1	0.99	0.05	27,27,27,27	0
2	EDO	P	503	4/4	0.99	0.03	27,32,33,41	0
2	EDO	S	601	4/4	0.99	0.03	28,30,37,37	0
4	AKG	A	503	10/10	0.99	0.05	48,57,60,62	0
4	AKG	B	503	10/10	0.99	0.03	34,48,61,63	0
4	AKG	C	501	10/10	0.99	0.04	40,60,68,73	0
4	AKG	D	501	10/10	0.99	0.05	51,57,61,62	0
2	EDO	A	501	4/4	0.99	0.04	36,44,49,55	0
4	AKG	F	503	10/10	0.99	0.03	40,48,64,66	0
4	AKG	G	502	10/10	0.99	0.04	40,55,62,63	0
4	AKG	H	502	10/10	0.99	0.03	37,48,55,60	0
4	AKG	I	501	10/10	0.99	0.04	52,66,69,69	0
4	AKG	J	502	10/10	0.99	0.04	46,52,58,60	0
4	AKG	K	503	10/10	0.99	0.05	43,52,62,72	0
4	AKG	L	501	10/10	0.99	0.04	52,65,67,75	0
4	AKG	P	505	10/10	0.99	0.03	22,39,46,46	0
4	AKG	Q	503	10/10	0.99	0.04	21,38,46,51	0
4	AKG	S	603	10/10	0.99	0.04	28,34,45,46	0
4	AKG	T	504	10/10	0.99	0.04	35,46,51,58	0
4	AKG	U	503	10/10	0.99	0.03	27,38,42,57	0
4	AKG	V	503	10/10	0.99	0.03	31,39,51,52	0
4	AKG	X	603	10/10	0.99	0.03	27,50,55,75	0
4	AKG	Y	604	10/10	0.99	0.04	30,39,43,43	0
4	AKG	Z	503	10/10	0.99	0.03	39,50,57,82	0
4	AKG	b	505	10/10	0.99	0.03	33,38,43,46	0
4	AKG	c	504	10/10	0.99	0.04	31,43,51,62	0
5	PEG	Z	502	7/7	0.99	0.04	35,41,48,55	0
3	MG	T	501	1/1	1.00	0.02	36,36,36,36	0
2	EDO	Z	501	4/4	1.00	0.02	17,33,44,44	0
3	MG	T	503	1/1	1.00	0.05	37,37,37,37	0
3	MG	Y	603	1/1	1.00	0.02	35,35,35,35	0
3	MG	A	502	1/1	1.00	0.05	23,23,23,23	0
2	EDO	a	501	4/4	1.00	0.03	14,16,19,35	0
2	EDO	a	502	4/4	1.00	0.03	12,26,28,36	0
2	EDO	a	503	4/4	1.00	0.02	26,29,30,37	0
2	EDO	X	601	4/4	1.00	0.02	27,36,37,38	0
3	MG	J	501	1/1	1.00	0.04	34,34,34,34	0

Continued on next page...

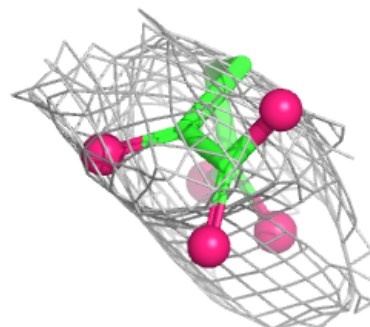
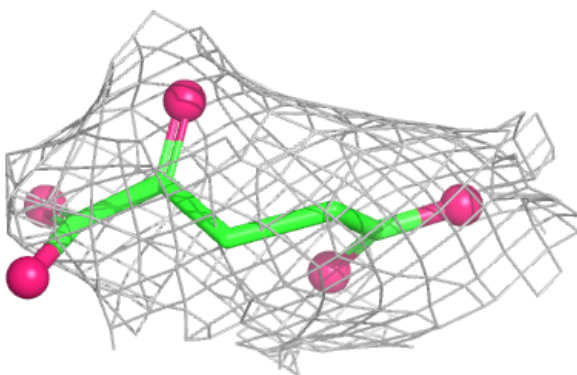
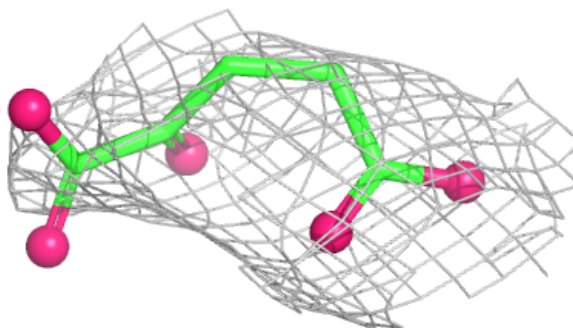
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	G	501	4/4	1.00	0.02	27,32,34,39	0
3	MG	P	504	1/1	1.00	0.02	33,33,33,33	0
4	AKG	a	504	10/10	1.00	0.05	31,35,46,51	0
2	EDO	V	501	4/4	1.00	0.02	12,40,43,55	0
3	MG	Q	502	1/1	1.00	0.03	25,25,25,25	0
5	PEG	P	502	7/7	1.00	0.02	16,33,40,48	0
2	EDO	U	501	4/4	1.00	0.02	30,34,39,50	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.

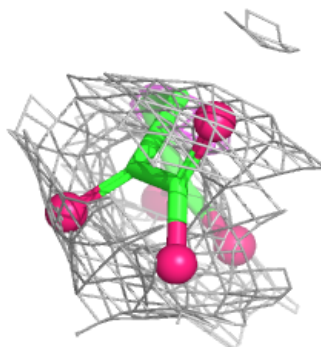
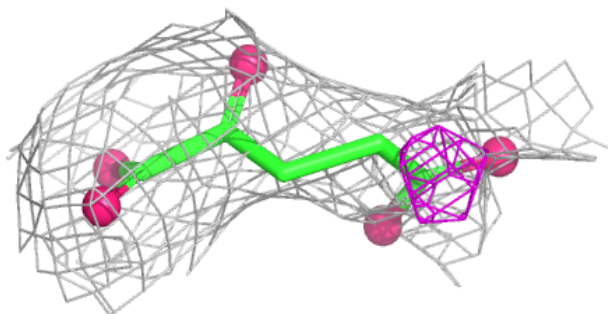
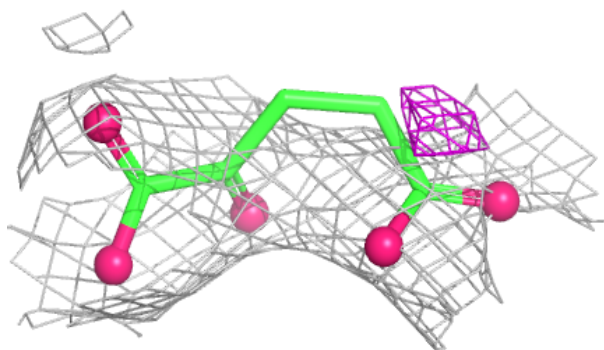
Electron density around AKG E 502:

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

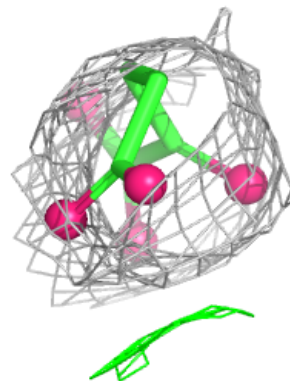
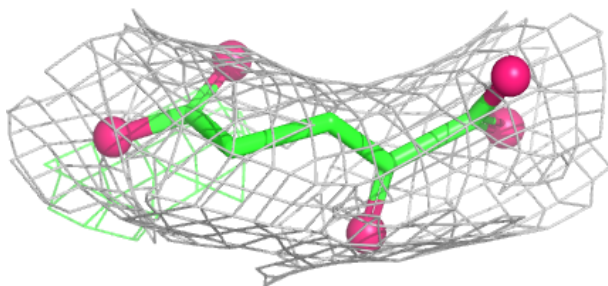
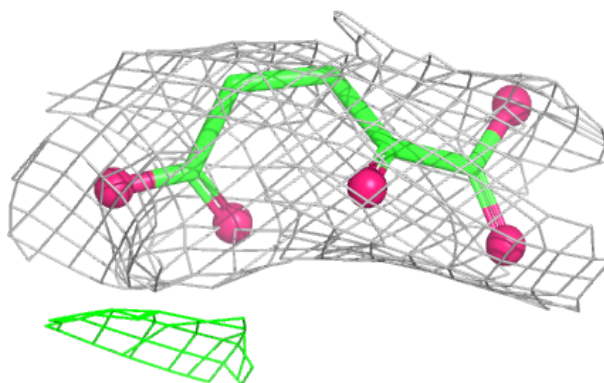


Electron density around AKG A 503:

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

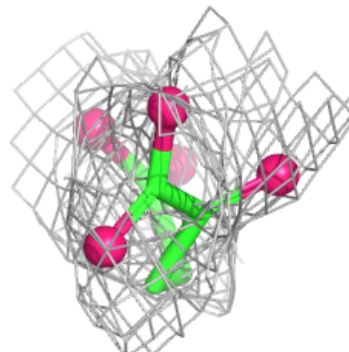
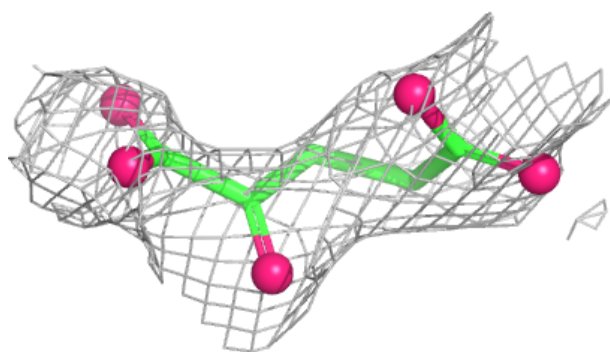
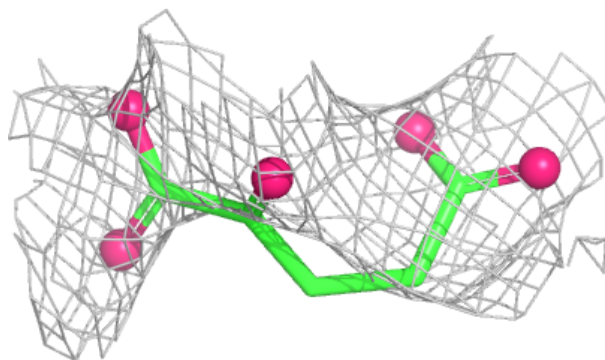
**Electron density around AKG B 503:**

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

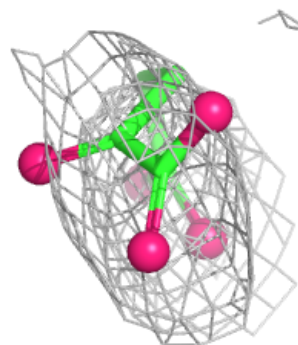
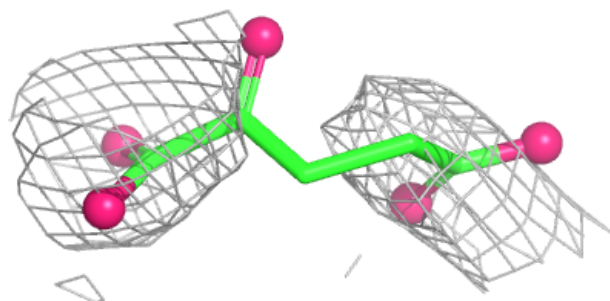
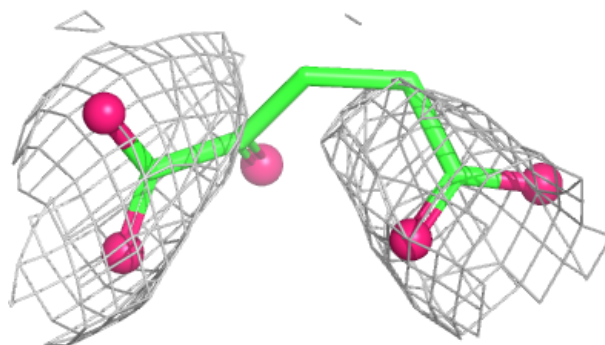


Electron density around AKG C 501:

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

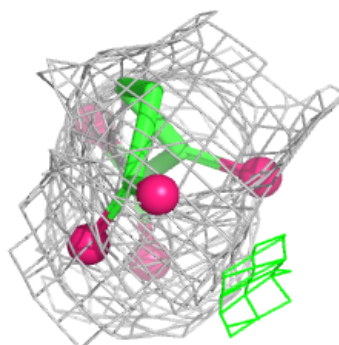
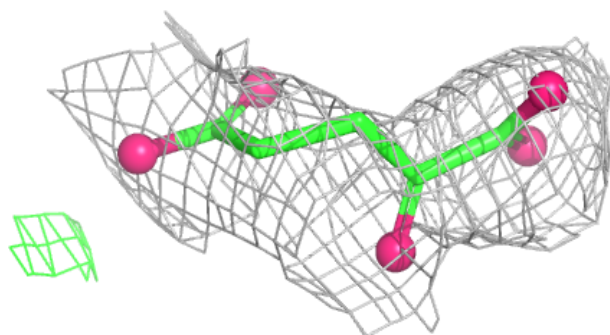
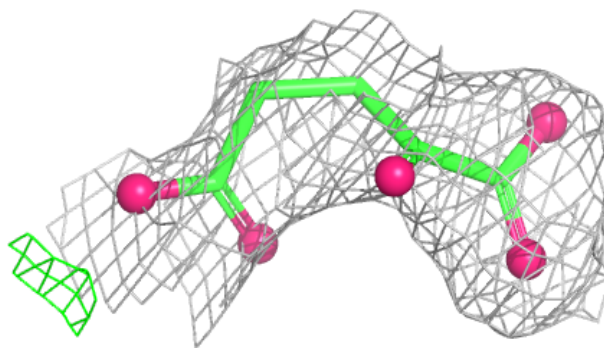
**Electron density around AKG D 501:**

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

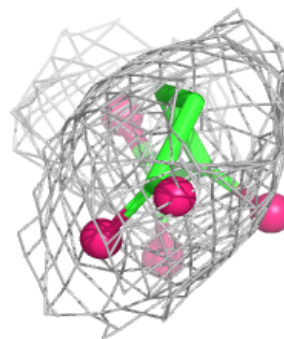
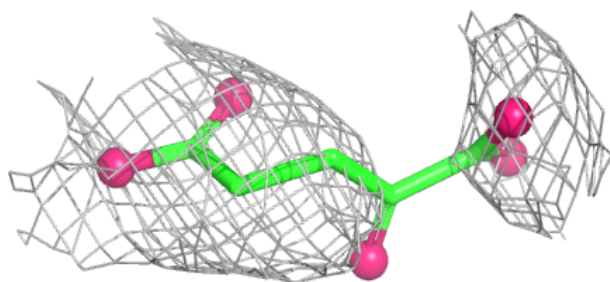
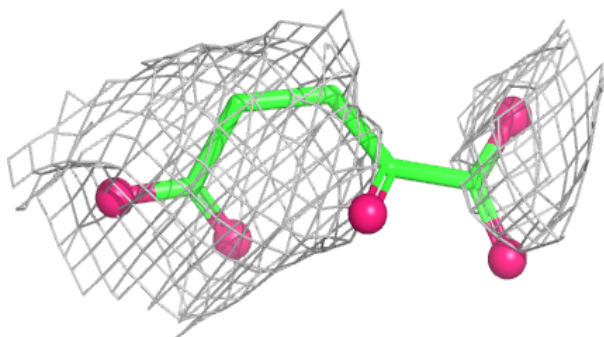


Electron density around AKG F 503:

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

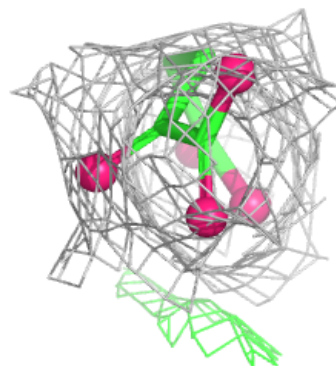
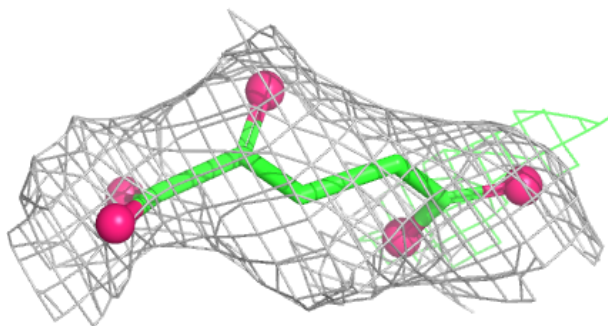
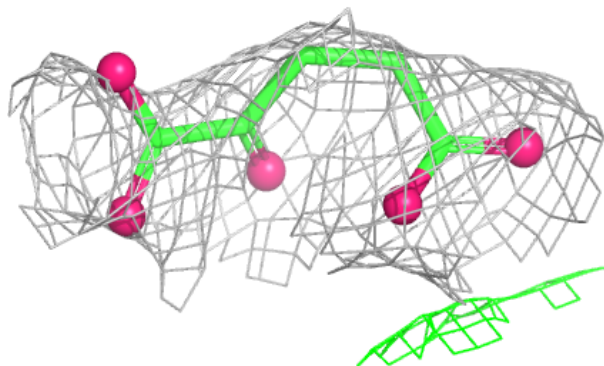
**Electron density around AKG G 502:**

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

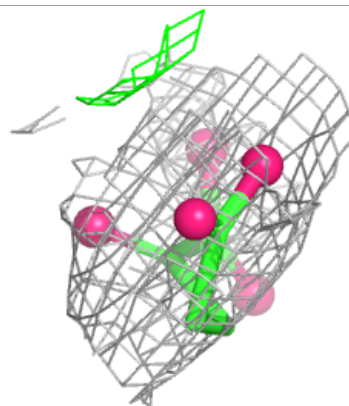
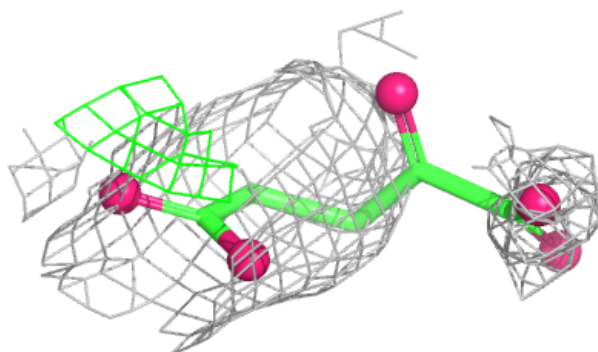
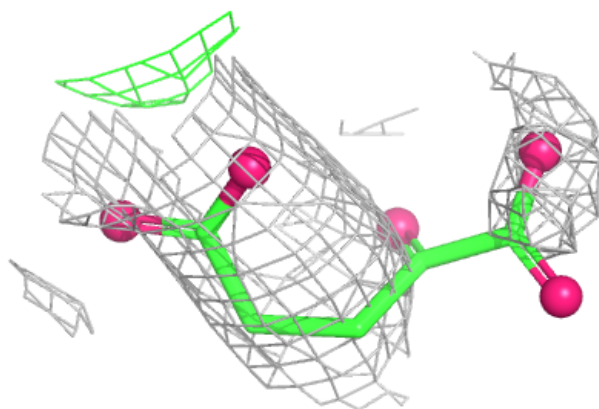


Electron density around AKG H 502:

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

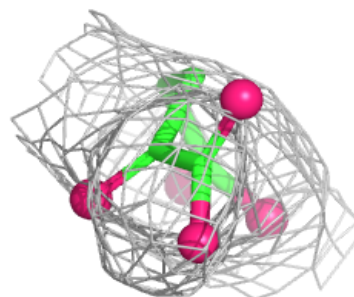
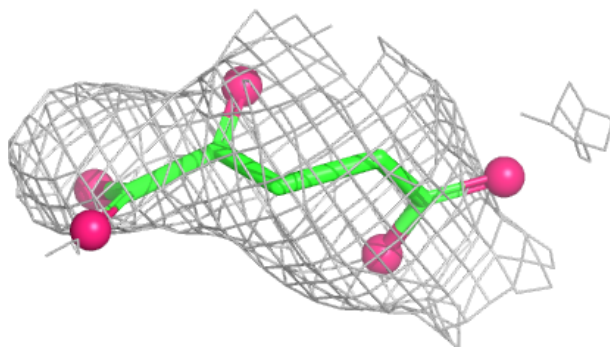
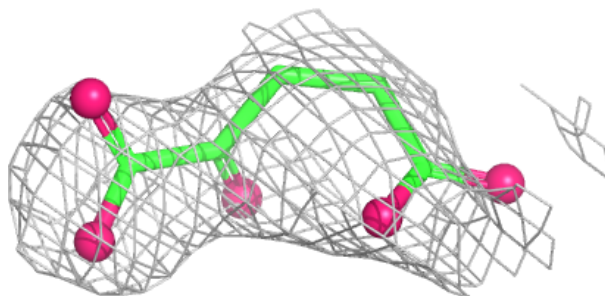
**Electron density around AKG I 501:**

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

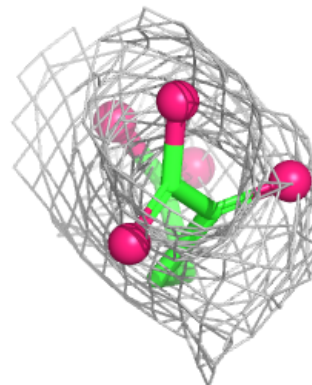
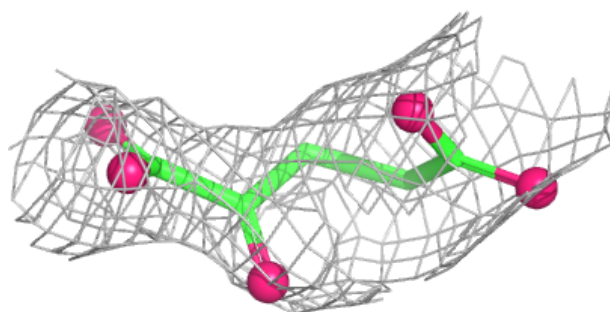
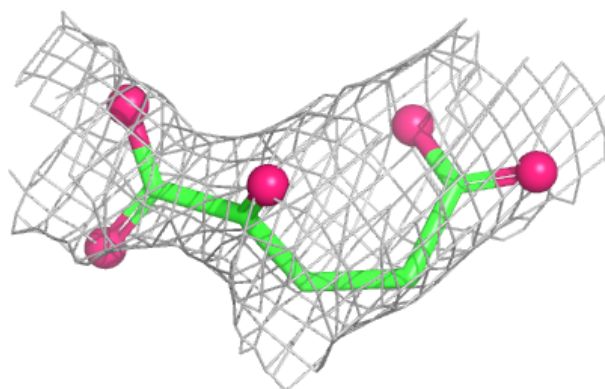


Electron density around AKG J 502:

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

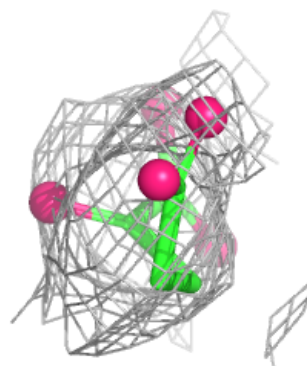
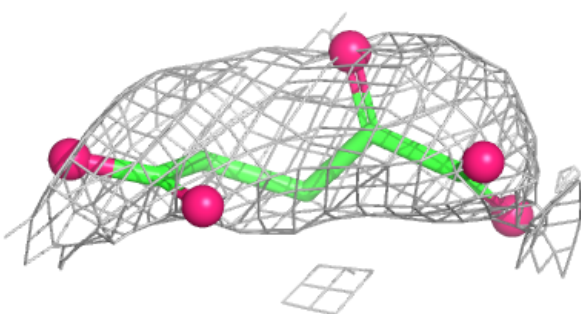
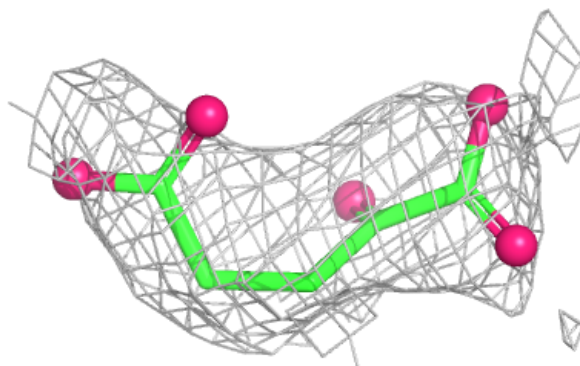
**Electron density around AKG K 503:**

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

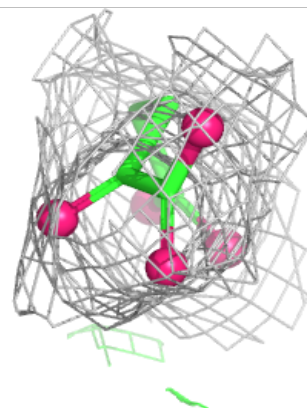
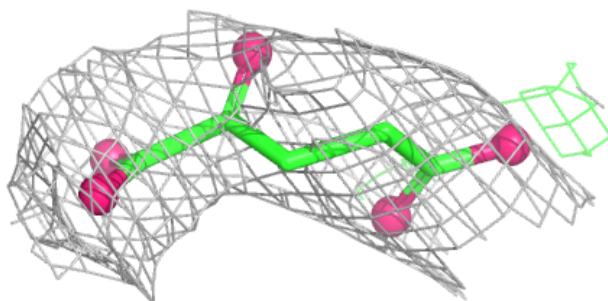
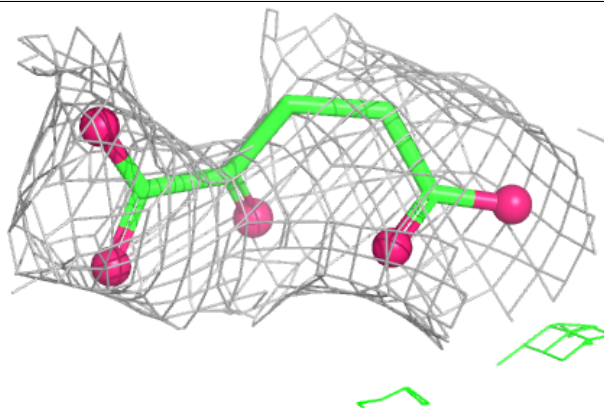


Electron density around AKG L 501:

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

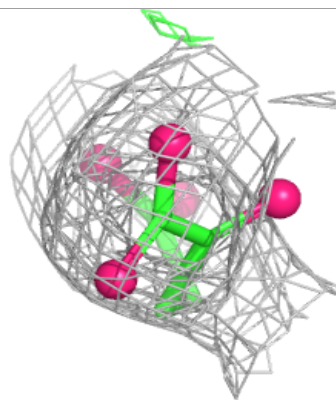
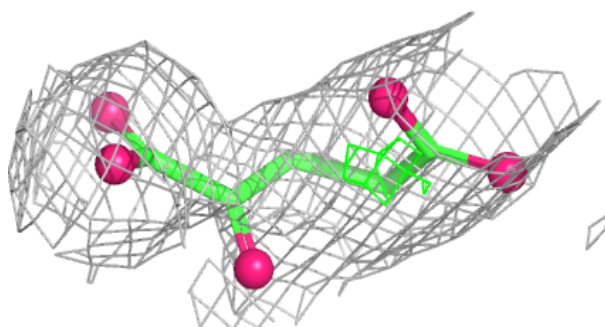
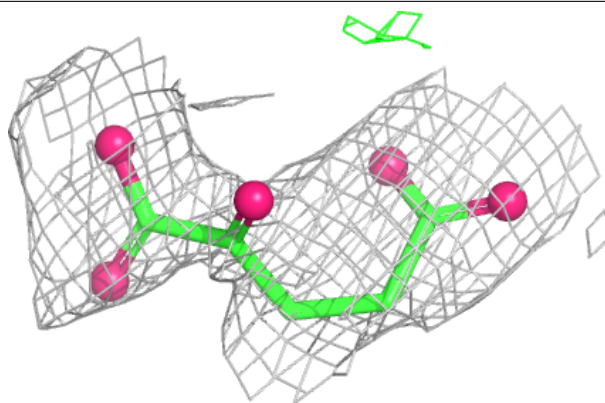
**Electron density around AKG P 505:**

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

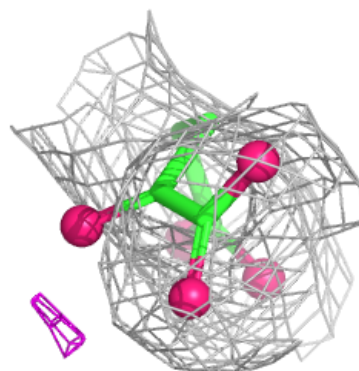
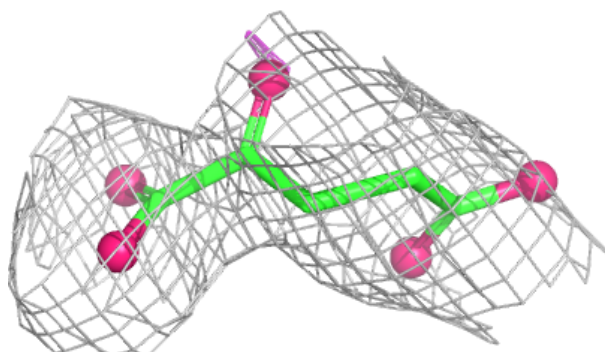
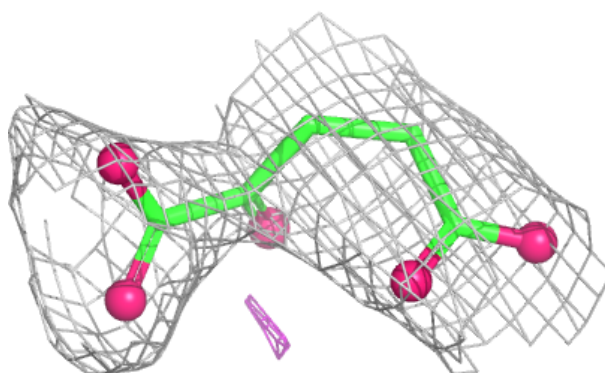


Electron density around AKG Q 503:

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

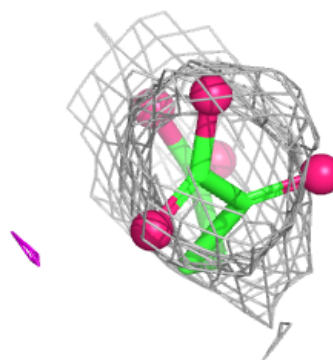
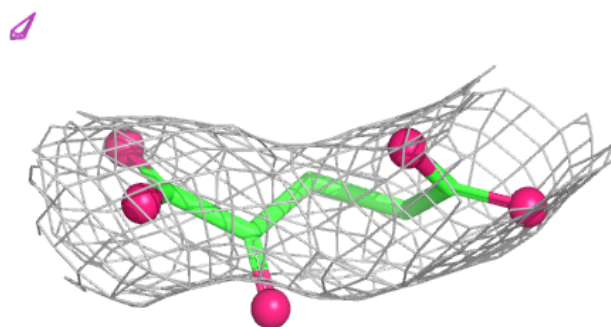
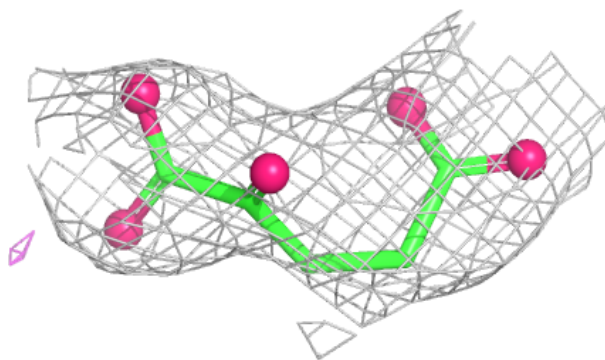
**Electron density around AKG S 603:**

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

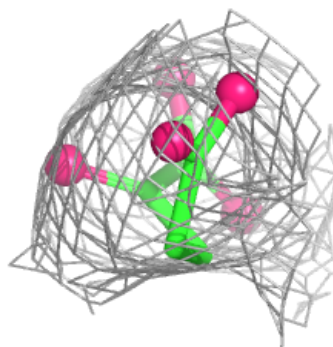
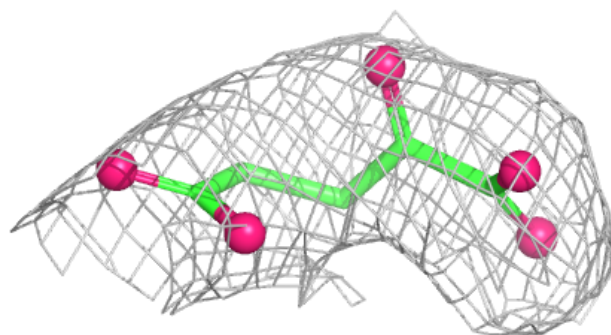
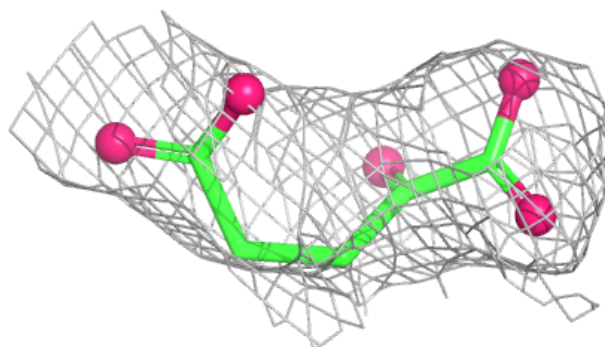


Electron density around AKG T 504:

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

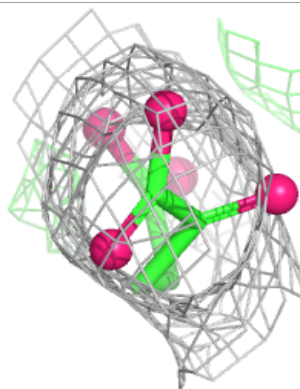
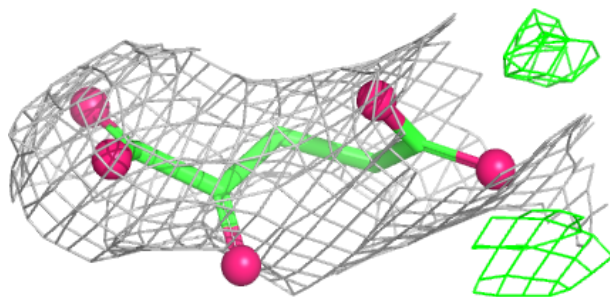
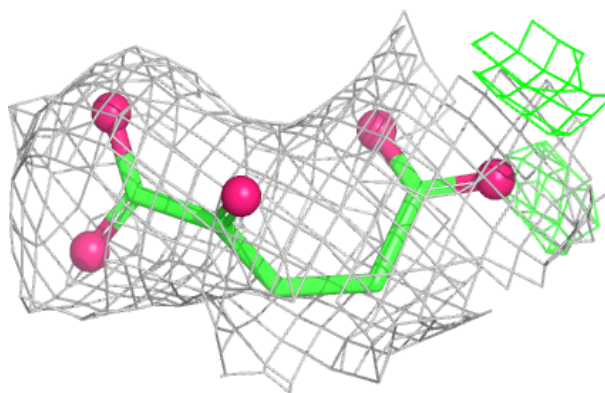
**Electron density around AKG U 503:**

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

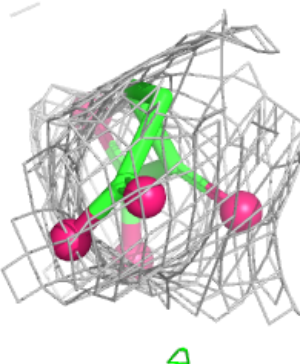
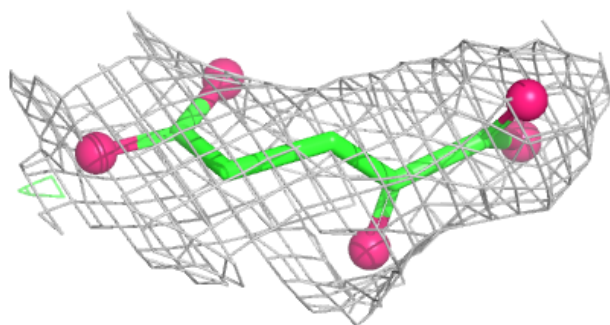
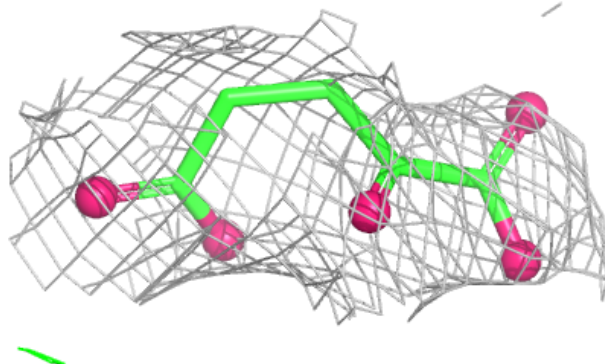


Electron density around AKG V 503:

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

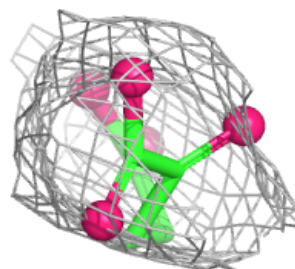
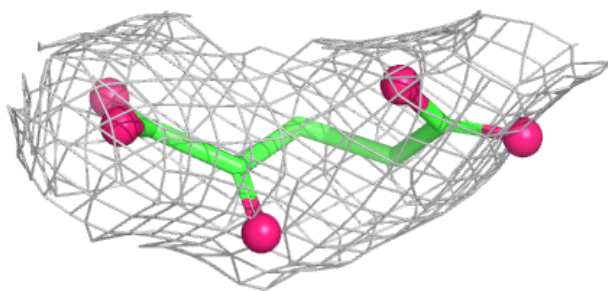
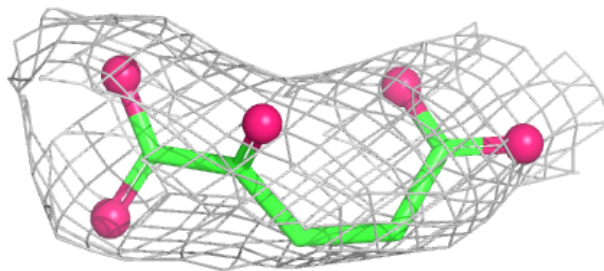
**Electron density around AKG X 603:**

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

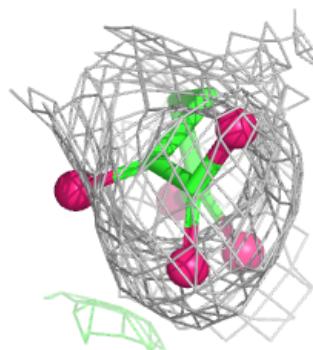
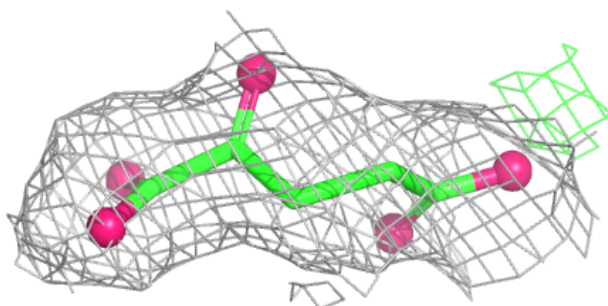
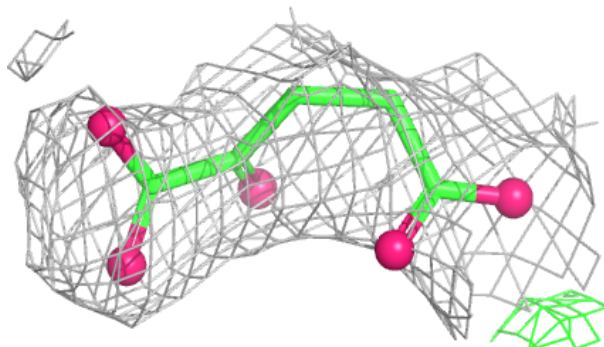


Electron density around AKG Y 604:

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

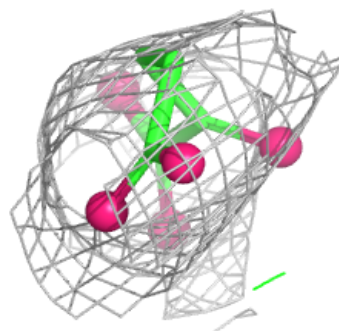
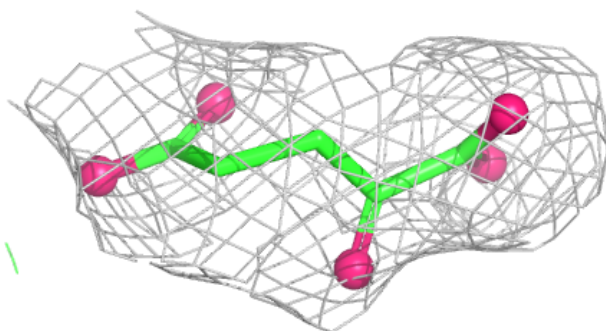
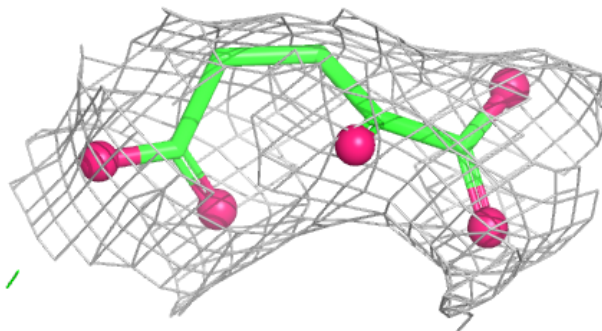
**Electron density around AKG Z 503:**

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

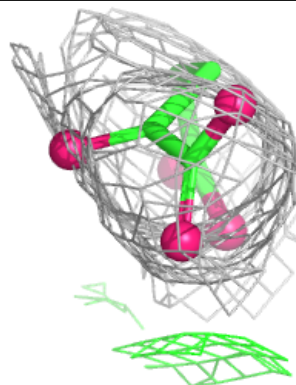
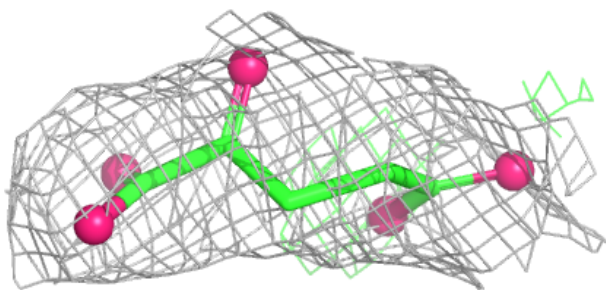
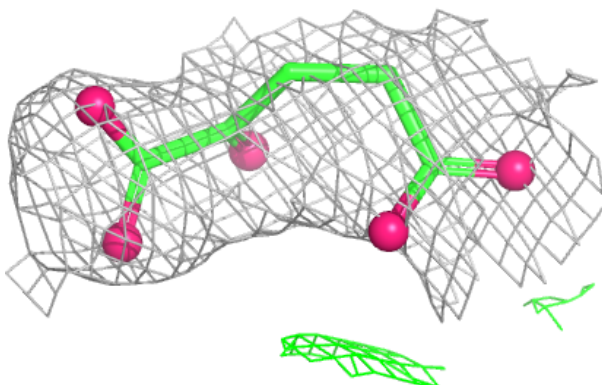


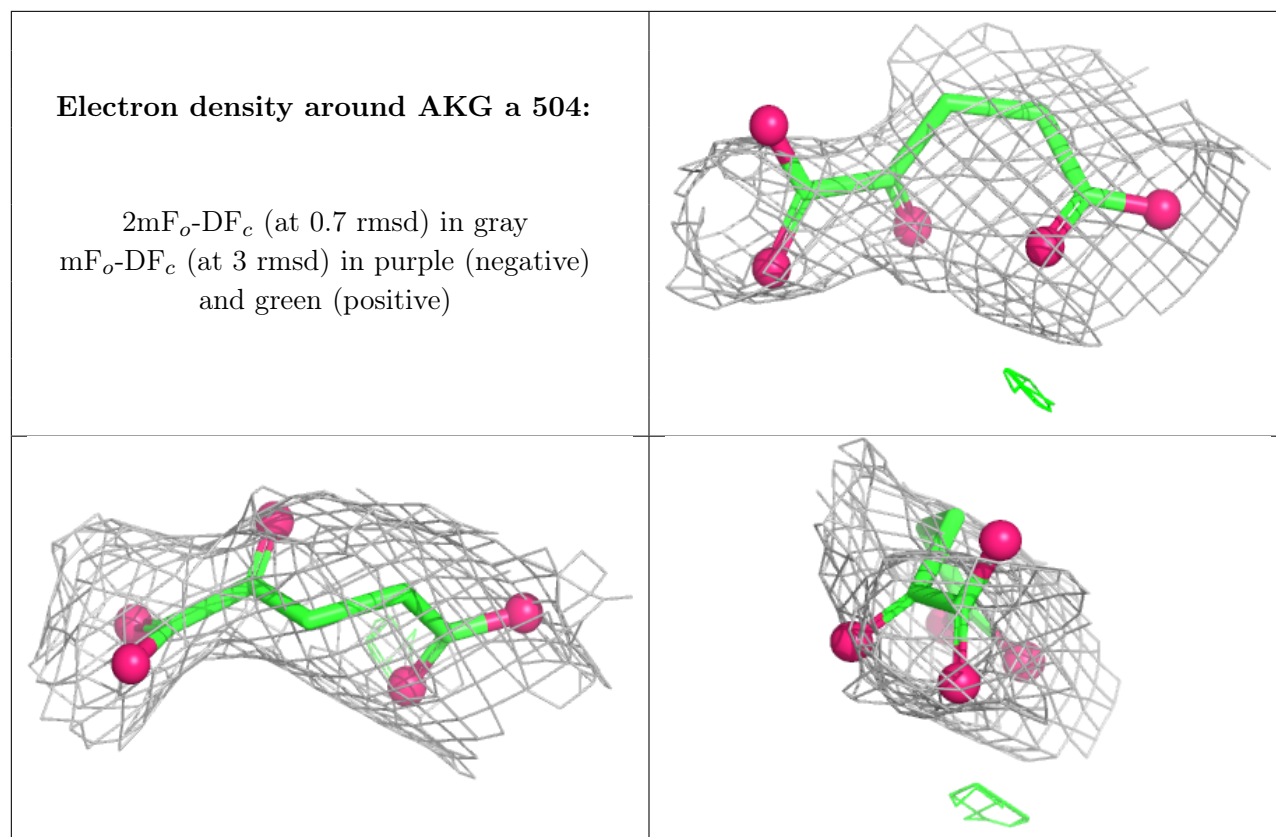
Electron density around AKG b 505:

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

**Electron density around AKG c 504:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.