



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 07:47 pm BST

PDB ID : 9I36 / pdb\_00009i36  
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with decanoyl-CoA  
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.  
Deposited on : 2025-01-22  
Resolution : 2.08 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

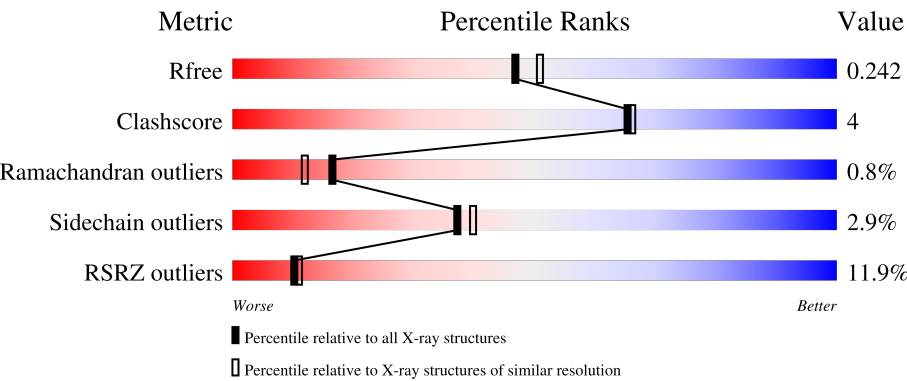
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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  $\geq 3$ , 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	364	<div><div>9%</div><div>87%</div><div>10%</div><div>...</div></div>
1	B	364	<div><div>11%</div><div>85%</div><div>12%</div><div>..</div></div>
1	C	364	<div><div>20%</div><div>88%</div><div>9%</div><div>..</div></div>
1	D	364	<div><div>7%</div><div>86%</div><div>10%</div><div>...</div></div>
1	E	364	<div><div>10%</div><div>88%</div><div>9%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	364	<div><div></div><div>15%</div><div>84%</div><div>12%</div><div>...</div></div>
1	G	364	<div><div></div><div>17%</div><div>86%</div><div>11%</div><div>..</div></div>
1	H	364	<div><div></div><div>11%</div><div>87%</div><div>9%</div><div>..</div></div>
1	I	364	<div><div></div><div>4%</div><div>88%</div><div>9%</div><div>...</div></div>
1	J	364	<div><div></div><div>11%</div><div>84%</div><div>12%</div><div>..</div></div>
1	K	364	<div><div></div><div>18%</div><div>84%</div><div>12%</div><div>...</div></div>
1	L	364	<div><div></div><div>7%</div><div>89%</div><div>8%</div><div>..</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34887 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 Alpha-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	2	0
			2706	1696	484	510	16			
1	B	357	Total	C	N	O	S	0	1	0
			2700	1694	484	506	16			
1	C	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	356	Total	C	N	O	S	0	2	0
			2699	1693	483	507	16			
1	F	358	Total	C	N	O	S	0	1	0
			2711	1701	485	509	16			
1	G	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	H	356	Total	C	N	O	S	0	1	0
			2696	1692	483	505	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	356	Total	C	N	O	S	0	1	0
			2696	1692	483	505	16			
1	K	357	Total	C	N	O	S	0	2	0
			2703	1695	484	508	16			
1	L	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLY	-	expression tag	UNP O06543
A	362	SER	-	expression tag	UNP O06543
A	363	GLY	-	expression tag	UNP O06543
A	364	CYS	-	expression tag	UNP O06543
B	361	GLY	-	expression tag	UNP O06543

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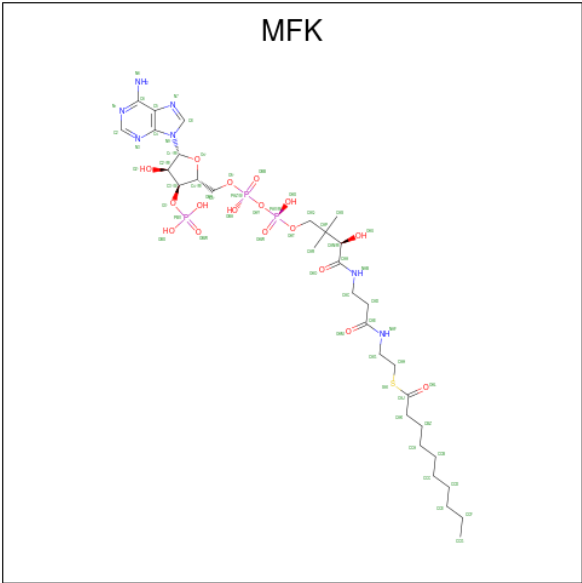
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	UNP O06543
D	361	GLY	-	expression tag	UNP O06543
D	362	SER	-	expression tag	UNP O06543
D	363	GLY	-	expression tag	UNP O06543
D	364	CYS	-	expression tag	UNP O06543
E	361	GLY	-	expression tag	UNP O06543
E	362	SER	-	expression tag	UNP O06543
E	363	GLY	-	expression tag	UNP O06543
E	364	CYS	-	expression tag	UNP O06543
F	361	GLY	-	expression tag	UNP O06543
F	362	SER	-	expression tag	UNP O06543
F	363	GLY	-	expression tag	UNP O06543
F	364	CYS	-	expression tag	UNP O06543
G	361	GLY	-	expression tag	UNP O06543
G	362	SER	-	expression tag	UNP O06543
G	363	GLY	-	expression tag	UNP O06543
G	364	CYS	-	expression tag	UNP O06543
H	361	GLY	-	expression tag	UNP O06543
H	362	SER	-	expression tag	UNP O06543
H	363	GLY	-	expression tag	UNP O06543
H	364	CYS	-	expression tag	UNP O06543
I	361	GLY	-	expression tag	UNP O06543
I	362	SER	-	expression tag	UNP O06543
I	363	GLY	-	expression tag	UNP O06543
I	364	CYS	-	expression tag	UNP O06543
J	361	GLY	-	expression tag	UNP O06543
J	362	SER	-	expression tag	UNP O06543
J	363	GLY	-	expression tag	UNP O06543
J	364	CYS	-	expression tag	UNP O06543
K	361	GLY	-	expression tag	UNP O06543
K	362	SER	-	expression tag	UNP O06543
K	363	GLY	-	expression tag	UNP O06543
K	364	CYS	-	expression tag	UNP O06543
L	361	GLY	-	expression tag	UNP O06543
L	362	SER	-	expression tag	UNP O06543
L	363	GLY	-	expression tag	UNP O06543

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Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is decanoyl-CoA (CCD ID: MFK) (formula: C<sub>31</sub>H<sub>54</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	B	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	C	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	D	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	E	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	F	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	G	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	H	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	I	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			
2	J	1	Total	C	N	O	P	S		0	0
			59	31	7	17	3	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			59	31	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			59	31	7	17	3	1		

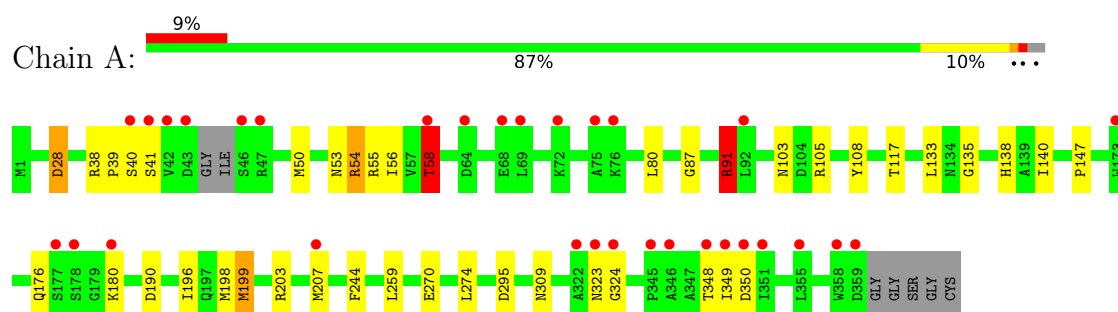
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	129	Total	O	0	0
			129	129		
3	C	137	Total	O	0	0
			137	137		
3	D	136	Total	O	0	0
			136	136		
3	E	135	Total	O	0	0
			135	135		
3	F	125	Total	O	0	0
			125	125		
3	G	114	Total	O	0	0
			114	114		
3	H	131	Total	O	0	0
			131	131		
3	I	161	Total	O	0	0
			161	161		
3	J	176	Total	O	0	0
			176	176		
3	K	155	Total	O	0	0
			155	155		
3	L	154	Total	O	0	0
			154	154		

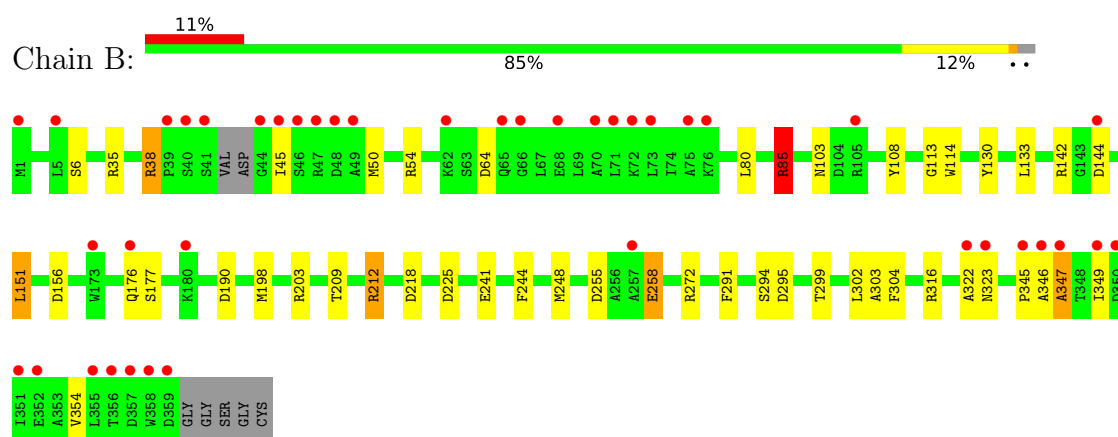
### 3 Residue-property plots [i](#)

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.

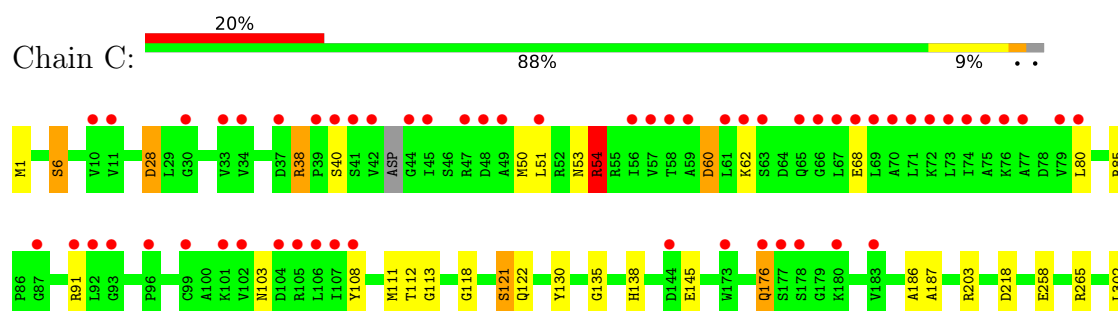
#### • Molecule 1: Alpha-methylacyl-CoA racemase

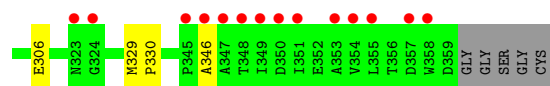


#### • Molecule 1: Alpha-methylacyl-CoA racemase

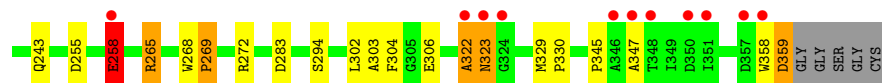
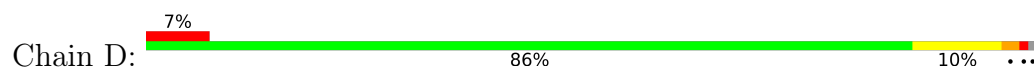


#### • Molecule 1: Alpha-methylacyl-CoA racemase

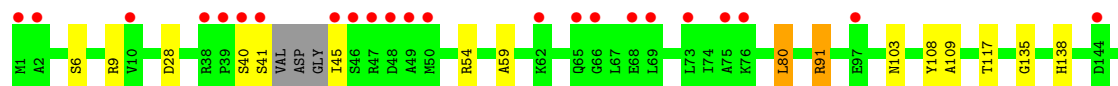
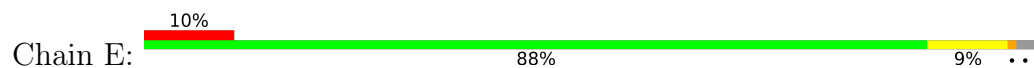




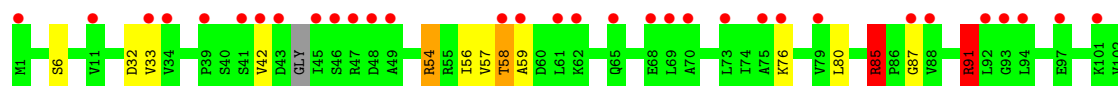
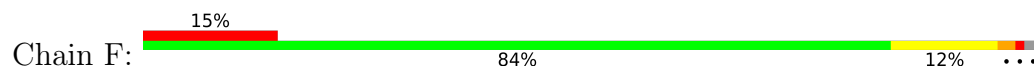
• Molecule 1: Alpha-methylacyl-CoA racemase



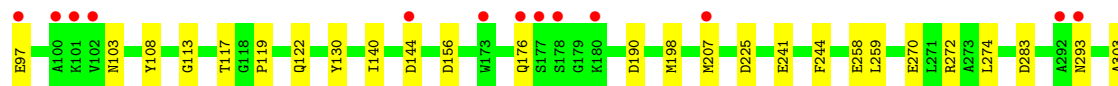
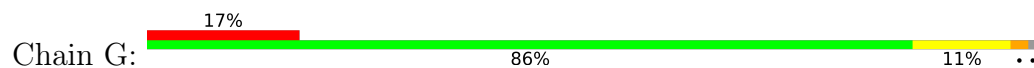
• Molecule 1: Alpha-methylacyl-CoA racemase

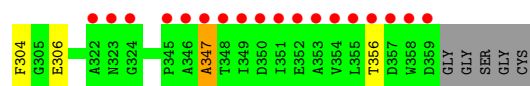


• Molecule 1: Alpha-methylacyl-CoA racemase

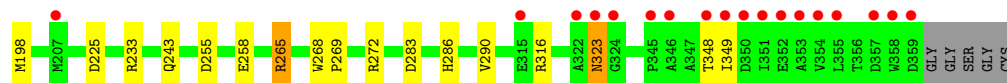
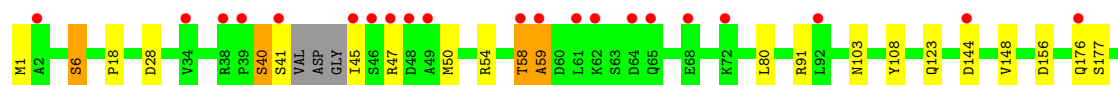
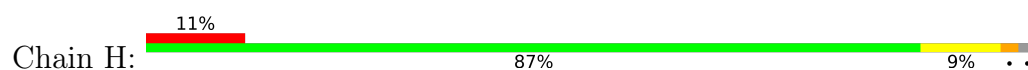


• Molecule 1: Alpha-methylacyl-CoA racemase

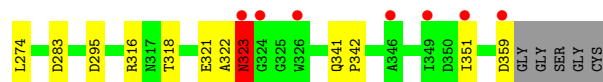
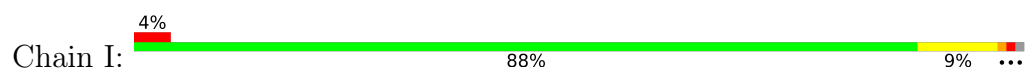




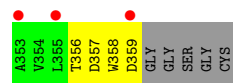
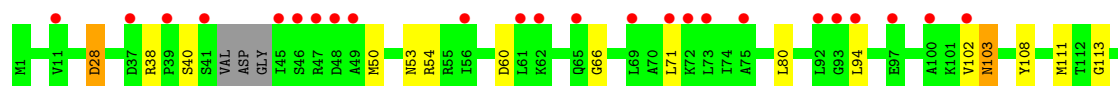
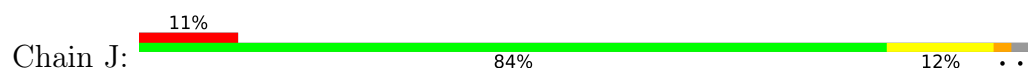
• Molecule 1: Alpha-methylacyl-CoA racemase



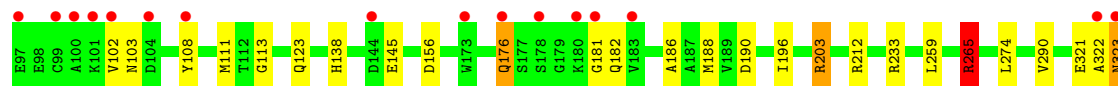
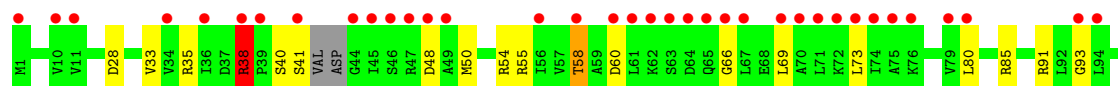
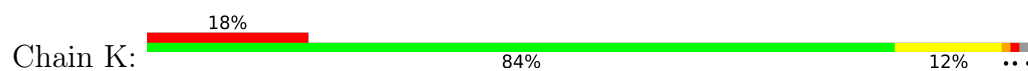
• Molecule 1: Alpha-methylacyl-CoA racemase

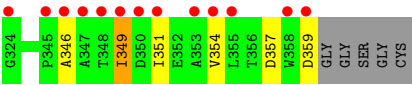


• Molecule 1: Alpha-methylacyl-CoA racemase

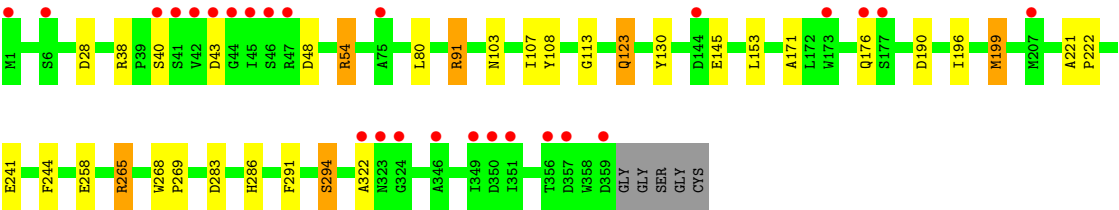
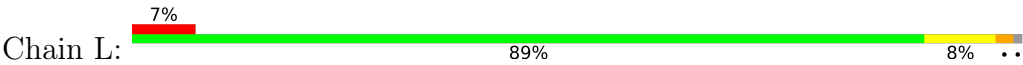


• Molecule 1: Alpha-methylacyl-CoA racemase





● Molecule 1: Alpha-methylacyl-CoA racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	276.31Å 276.31Å 390.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.59 – 2.08 225.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.59-2.08) 99.9 (225.59-2.08)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.202 , 0.234 0.213 , 0.242	Depositor DCC
$R_{free}$ test set	22342 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.008 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MFK

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	0.65	0/2778	1.22	15/3778 (0.4%)
1	B	0.67	0/2766	1.17	13/3761 (0.3%)
1	C	0.65	0/2782	1.19	11/3783 (0.3%)
1	D	0.65	0/2782	1.17	11/3785 (0.3%)
1	E	0.66	0/2771	1.14	8/3768 (0.2%)
1	F	0.66	0/2777	1.19	11/3777 (0.3%)
1	G	0.65	0/2791	1.19	9/3797 (0.2%)
1	H	0.66	0/2762	1.19	14/3756 (0.4%)
1	I	0.67	0/2791	1.17	16/3797 (0.4%)
1	J	0.66	0/2762	1.18	12/3756 (0.3%)
1	K	0.67	0/2775	1.18	11/3773 (0.3%)
1	L	0.66	0/2782	1.17	10/3785 (0.3%)
All	All	0.66	0/33319	1.18	141/45316 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	D	0	3
1	E	0	3
1	F	0	6
1	G	0	1
1	H	0	3
1	I	0	2
1	J	0	2
1	K	0	5
1	L	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	34

There are no bond length outliers.

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	123	GLN	CB-CA-C	13.50	131.94	109.80
1	A	58	THR	CA-CB-OG1	-11.19	92.81	109.60
1	J	123	GLN	CB-CA-C	10.54	127.02	109.84
1	B	203	ARG	N-CA-CB	9.45	124.15	110.16
1	L	38	ARG	N-CA-CB	-9.36	96.94	110.14
1	C	203	ARG	N-CA-CB	8.80	123.18	110.16
1	A	203	ARG	CB-CA-C	-8.75	96.27	110.79
1	B	203	ARG	CB-CA-C	-8.68	96.10	110.85
1	C	203	ARG	CB-CA-C	-8.56	96.29	110.85
1	A	91	ARG	CB-CA-C	-8.51	93.96	110.46
1	J	123	GLN	N-CA-CB	-8.42	96.90	109.95
1	I	255	ASP	CB-CA-C	8.32	124.10	110.78
1	G	91	ARG	CB-CA-C	-8.20	93.03	110.32
1	A	203	ARG	N-CA-CB	8.10	122.03	110.12
1	L	123	GLN	N-CA-CB	-7.92	97.09	110.16
1	K	58	THR	CA-CB-OG1	-7.83	97.85	109.60
1	I	91	ARG	CB-CA-C	-7.78	95.74	110.67
1	H	123	GLN	CB-CA-C	7.70	122.39	109.84
1	C	38	ARG	CB-CA-C	-7.70	97.33	109.42
1	F	203	ARG	CB-CA-C	-7.69	98.02	110.79
1	D	58	THR	CA-CB-OG1	-7.55	98.27	109.60
1	H	265	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	L	190	ASP	CA-CB-CG	7.33	119.93	112.60
1	G	91	ARG	N-CA-CB	7.27	122.68	110.32
1	D	265	ARG	NE-CZ-NH2	7.25	125.73	119.20
1	A	91	ARG	N-CA-CB	7.10	121.36	110.14
1	L	91	ARG	CB-CA-C	-6.85	99.04	110.68
1	J	28	ASP	CA-CB-CG	6.80	119.40	112.60
1	E	176	GLN	N-CA-CB	6.76	120.63	110.22
1	J	265	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	D	283	ASP	CB-CA-C	6.67	123.11	110.51
1	F	203	ARG	N-CA-CB	6.64	119.89	110.12
1	B	190	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	255	ASP	CB-CA-C	6.61	121.25	110.22
1	A	190	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	265	ARG	CD-NE-CZ	6.57	133.60	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	91	ARG	N-CA-CB	6.56	120.45	110.28
1	L	283	ASP	CB-CA-C	6.53	122.76	109.76
1	H	283	ASP	CB-CA-C	-6.52	96.16	109.65
1	J	190	ASP	CA-CB-CG	6.50	119.10	112.60
1	E	28	ASP	CA-CB-CG	6.34	118.94	112.60
1	L	38	ARG	CB-CA-C	6.34	118.58	109.26
1	G	283	ASP	CA-CB-CG	6.34	118.94	112.60
1	K	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	54	ARG	N-CA-CB	-6.24	99.96	111.13
1	J	185	ASP	CA-CB-CG	6.20	118.80	112.60
1	D	85	ARG	CD-NE-CZ	6.18	133.05	124.40
1	E	290	VAL	N-CA-CB	-6.16	102.77	110.47
1	K	265	ARG	CD-NE-CZ	6.13	132.99	124.40
1	H	28	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	28	ASP	CA-CB-CG	6.12	118.72	112.60
1	H	148	VAL	CA-C-O	6.08	123.51	119.38
1	E	255	ASP	CA-CB-CG	6.07	118.67	112.60
1	L	28	ASP	CA-CB-CG	6.07	118.67	112.60
1	K	212	ARG	CB-CA-C	6.03	119.97	109.65
1	G	28	ASP	CA-CB-CG	6.03	118.63	112.60
1	H	123	GLN	N-CA-CB	-6.03	100.61	109.95
1	F	190	ASP	CA-CB-CG	6.02	118.62	112.60
1	F	91	ARG	CB-CA-C	-6.00	99.14	110.67
1	I	58	THR	CA-CB-OG1	-5.98	100.64	109.60
1	I	248	MET	CG-SD-CE	5.95	113.99	100.90
1	E	91	ARG	CB-CA-C	-5.95	100.73	110.85
1	G	91	ARG	CG-CD-NE	5.91	125.00	112.00
1	H	255	ASP	CB-CA-C	5.89	119.74	110.19
1	H	258	GLU	CB-CA-C	-5.84	99.51	110.01
1	C	60	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	38	ARG	CB-CA-C	5.82	117.81	109.26
1	F	211	THR	CA-CB-OG1	-5.82	100.88	109.60
1	D	258	GLU	CB-CA-C	-5.81	98.57	109.72
1	F	258	GLU	CB-CA-C	-5.80	98.40	109.95
1	G	144	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	258	GLU	CB-CA-C	-5.78	99.13	110.11
1	F	32	ASP	CA-CB-CG	5.74	118.34	112.60
1	J	285	ASP	CB-CA-C	5.72	121.65	110.67
1	K	321	GLU	CB-CA-C	-5.69	100.71	110.22
1	A	309	ASN	CB-CA-C	-5.69	100.58	110.09
1	F	350	ASP	CA-CB-CG	5.69	118.29	112.60
1	K	28	ASP	CA-CB-CG	5.68	118.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	38	ARG	N-CA-CB	5.65	117.67	110.04
1	D	190	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	299	THR	OG1-CB-CG2	-5.62	98.06	109.30
1	C	258	GLU	CB-CA-C	-5.60	101.09	110.56
1	D	28	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	248	MET	CG-SD-CE	5.57	113.14	100.90
1	A	207	MET	CG-SD-CE	5.54	113.09	100.90
1	D	265	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	I	91	ARG	CD-NE-CZ	-5.54	116.65	124.40
1	C	306	GLU	CB-CA-C	-5.53	100.03	109.65
1	D	38	ARG	CB-CA-C	5.52	116.81	108.86
1	B	38	ARG	CB-CA-C	5.51	117.05	108.61
1	J	265	ARG	CA-CB-CG	-5.50	103.11	114.10
1	B	156	ASP	CB-CA-C	-5.49	102.22	110.90
1	F	283	ASP	CA-CB-CG	5.48	118.08	112.60
1	J	265	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	F	306	GLU	CB-CA-C	-5.44	100.18	109.65
1	C	28	ASP	CA-CB-CG	5.44	118.04	112.60
1	I	176	GLN	N-CA-CB	5.44	118.71	110.28
1	B	218	ASP	CA-CB-CG	5.43	118.03	112.60
1	H	265	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	H	265	ARG	CD-NE-CZ	5.39	131.94	124.40
1	J	54	ARG	CB-CA-C	-5.39	98.22	110.07
1	J	283	ASP	CA-CB-CG	5.39	117.99	112.60
1	I	38	ARG	CB-CA-C	-5.35	100.65	109.27
1	C	218	ASP	CA-CB-CG	5.34	117.94	112.60
1	I	42	VAL	N-CA-CB	5.33	120.03	111.23
1	I	318	THR	CA-CB-OG1	-5.32	101.62	109.60
1	I	190	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	147	PRO	CA-C-N	-5.29	118.73	123.33
1	A	147	PRO	C-N-CA	-5.29	118.73	123.33
1	J	265	ARG	CD-NE-CZ	5.27	131.78	124.40
1	H	91	ARG	CB-CA-C	-5.26	100.56	110.67
1	K	33	VAL	N-CA-CB	5.25	118.47	111.64
1	G	306	GLU	CB-CA-C	-5.25	100.51	109.65
1	C	68	GLU	CB-CA-C	5.24	118.20	109.56
1	B	144	ASP	CA-CB-CG	5.23	117.83	112.60
1	L	54	ARG	CB-CA-C	-5.21	99.10	109.79
1	I	323	ASN	CB-CA-C	-5.20	100.06	110.42
1	K	203	ARG	CB-CA-C	-5.20	102.16	110.79
1	L	265	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	H	144	ASP	CA-CB-CG	5.19	117.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	283	ASP	CB-CA-C	5.18	120.30	110.51
1	E	91	ARG	N-CA-CB	5.17	117.81	110.16
1	H	323	ASN	CB-CA-C	-5.17	109.64	115.79
1	C	176	GLN	N-CA-CB	5.16	117.56	110.07
1	K	123	GLN	CB-CA-C	-5.16	101.63	109.89
1	G	190	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	255	ASP	CB-CA-C	5.15	118.54	110.19
1	G	97	GLU	CB-CA-C	-5.14	102.81	110.88
1	B	54	ARG	CB-CA-C	-5.13	98.17	109.56
1	A	55	ARG	CB-CA-C	5.11	118.18	109.75
1	I	58	THR	OG1-CB-CG2	5.11	119.52	109.30
1	E	265	ARG	CA-CB-CG	-5.10	103.89	114.10
1	I	144	ASP	CA-CB-CG	5.10	117.70	112.60
1	K	156	ASP	CB-CA-C	-5.08	102.87	110.90
1	F	33	VAL	N-CA-CB	5.08	118.42	111.41
1	H	348	THR	CA-CB-OG1	-5.07	101.99	109.60
1	I	207	MET	CG-SD-CE	5.05	112.02	100.90
1	B	209	THR	CA-CB-OG1	-5.02	102.07	109.60
1	D	306	GLU	CB-CA-C	-5.02	100.91	109.65
1	C	54	ARG	N-CA-CB	-5.02	102.20	111.53
1	A	58	THR	N-CA-CB	-5.01	102.11	110.23

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	322	ALA	Peptide
1	B	35	ARG	Sidechain
1	B	85	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	54	ARG	Peptide
1	D	85	ARG	Sidechain
1	E	348	THR	Peptide
1	E	350	ASP	Peptide
1	E	54	ARG	Peptide
1	F	110	ARG	Sidechain
1	F	233	ARG	Sidechain
1	F	322	ALA	Peptide
1	F	54	ARG	Peptide
1	F	85	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	91	ARG	Sidechain
1	G	91	ARG	Sidechain
1	H	233	ARG	Sidechain
1	H	323	ASN	Peptide
1	H	54	ARG	Peptide
1	I	233	ARG	Sidechain
1	I	54	ARG	Peptide
1	J	212	ARG	Sidechain
1	J	322	ALA	Peptide
1	K	233	ARG	Sidechain
1	K	265	ARG	Sidechain
1	K	35	ARG	Sidechain
1	K	38	ARG	Sidechain
1	K	54	ARG	Peptide
1	L	265	ARG	Sidechain
1	L	322	ALA	Peptide
1	L	54	ARG	Peptide
1	L	91	ARG	Sidechain

## 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	2706	0	2643	22	0
1	B	2700	0	2646	25	0
1	C	2710	0	2653	24	0
1	D	2715	0	2660	20	0
1	E	2699	0	2641	16	0
1	F	2711	0	2656	29	0
1	G	2718	0	2658	31	0
1	H	2696	0	2643	14	0
1	I	2718	0	2658	18	0
1	J	2696	0	2643	27	0
1	K	2703	0	2644	23	0
1	L	2715	0	2660	14	0
2	A	59	0	50	2	0
2	B	59	0	50	5	0
2	C	59	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	59	0	50	2	0
2	E	59	0	50	3	0
2	F	59	0	50	7	0
2	G	59	0	50	0	0
2	H	59	0	50	4	0
2	I	59	0	50	1	0
2	J	59	0	50	0	0
2	K	59	0	50	2	0
2	L	59	0	50	0	0
3	A	139	0	0	3	0
3	B	129	0	0	1	0
3	C	137	0	0	2	0
3	D	136	0	0	1	0
3	E	135	0	0	2	0
3	F	125	0	0	9	0
3	G	114	0	0	6	0
3	H	131	0	0	2	0
3	I	161	0	0	4	0
3	J	176	0	0	3	0
3	K	155	0	0	6	0
3	L	154	0	0	3	0
All	All	34887	0	32405	243	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 4.

All (243) 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:F:85:ARG:HD3	2:F:401:MFK:OBB	1.56	1.05
1:F:243:GLN:HB2	3:F:604:HOH:O	1.63	0.97
1:C:118:GLY:O	1:C:121:SER:OG	1.97	0.80
1:D:85:ARG:HD3	2:D:401:MFK:OBB	1.84	0.77
1:F:80:LEU:HD23	1:F:108:TYR:CE2	2.19	0.77
1:L:48:ASP:HB2	3:L:617:HOH:O	1.84	0.76
2:F:401:MFK:H4	3:F:608:HOH:O	1.86	0.75
1:G:347:ALA:N	3:G:503:HOH:O	2.19	0.74
1:G:58:THR:O	1:G:59:ALA:HB2	1.88	0.72
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.74	0.70
1:H:243:GLN:HG3	3:H:620:HOH:O	1.89	0.70
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:MFK:H1	3:F:608:HOH:O	1.93	0.69
1:F:270:GLU:HG3	3:F:525:HOH:O	1.92	0.68
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.74	0.67
1:J:346:ALA:HB3	3:J:547:HOH:O	1.93	0.67
2:F:401:MFK:CCF	3:F:608:HOH:O	2.42	0.66
1:J:285:ASP:HB2	3:J:517:HOH:O	1.94	0.66
1:D:243:GLN:HG3	3:D:626:HOH:O	1.95	0.65
2:F:401:MFK:CCG	3:F:608:HOH:O	2.43	0.65
1:F:272:ARG:NH1	3:F:502:HOH:O	2.30	0.65
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.31	0.65
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.31	0.65
1:G:50:MET:HE1	1:H:198:MET:HB2	1.77	0.65
1:D:85:ARG:CD	2:D:401:MFK:OBB	2.47	0.62
1:G:39:PRO:HA	1:G:58:THR:HG23	1.83	0.61
1:K:138:HIS:HD2	3:K:546:HOH:O	1.84	0.61
1:C:138:HIS:HD2	3:C:557:HOH:O	1.83	0.60
1:J:358:TRP:O	1:J:359:ASP:C	2.44	0.60
1:I:351:ILE:HG23	3:I:577:HOH:O	2.00	0.60
1:J:356:THR:O	1:J:359:ASP:HA	2.02	0.60
1:G:176:GLN:CD	1:H:176:GLN:HG2	2.27	0.60
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.85	0.60
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.36	0.60
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.67	0.60
1:K:176:GLN:OE1	1:L:176:GLN:HG2	2.02	0.60
1:E:336:ARG:HG2	1:E:336:ARG:HH11	1.67	0.59
1:G:39:PRO:HB3	1:G:58:THR:CG2	2.31	0.59
1:B:346:ALA:O	1:B:347:ALA:O	2.21	0.59
1:H:1:MET:O	1:H:6:SER:OG	2.20	0.59
1:H:286:HIS:HE1	3:H:614:HOH:O	1.86	0.59
1:F:85:ARG:CD	2:F:401:MFK:OBB	2.42	0.59
1:B:291:PHE:O	1:B:294:SER:HB3	2.02	0.58
1:G:85:ARG:NH1	1:G:122:GLN:O	2.37	0.57
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.86	0.57
1:G:207:MET:HE1	2:H:401:MFK:H4	1.87	0.57
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.40	0.57
1:G:119:PRO:O	3:G:502:HOH:O	2.17	0.56
1:G:58:THR:O	1:G:59:ALA:CB	2.55	0.55
1:F:118:GLY:O	1:F:121:SER:OG	2.24	0.55
1:G:80:LEU:HD23	1:G:108:TYR:CE2	2.42	0.55
1:G:270:GLU:HG3	3:G:553:HOH:O	2.07	0.54
1:B:85:ARG:HD3	2:B:401:MFK:OBA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:ASP:OD2	3:K:501:HOH:O	2.18	0.54
1:G:272:ARG:NH1	3:G:506:HOH:O	2.40	0.54
1:G:38:ARG:NH2	3:G:501:HOH:O	2.13	0.54
1:A:198:MET:HB2	1:B:50:MET:HE1	1.88	0.54
1:E:80:LEU:CD2	1:E:108:TYR:CE2	2.91	0.54
1:C:80:LEU:HD22	1:C:108:TYR:CE2	2.43	0.54
1:K:93:GLY:C	3:K:536:HOH:O	2.51	0.54
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.42	0.54
1:F:80:LEU:HD23	1:F:108:TYR:CD2	2.44	0.53
1:C:38:ARG:NH2	2:C:401:MFK:O4'	2.42	0.52
1:K:80:LEU:HD23	1:K:108:TYR:CE1	2.44	0.52
1:I:61:LEU:HD22	1:I:94:LEU:HD11	1.90	0.52
1:F:323:ASN:CG	1:F:324:GLY:N	2.68	0.52
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.93	0.52
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.45	0.52
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.43	0.52
1:I:270:GLU:HG3	3:I:585:HOH:O	2.10	0.52
1:A:105:ARG:NH1	3:A:509:HOH:O	2.42	0.51
1:A:50:MET:HE1	1:B:198:MET:HB2	1.92	0.51
1:A:176:GLN:HG3	1:B:176:GLN:HE21	1.75	0.51
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.93	0.51
1:B:85:ARG:CD	2:B:401:MFK:OBA	2.59	0.51
1:A:138:HIS:HD2	3:A:534:HOH:O	1.94	0.51
1:G:80:LEU:CD2	1:G:108:TYR:CE2	2.94	0.50
1:J:285:ASP:CB	3:J:517:HOH:O	2.54	0.50
1:A:87:GLY:O	1:A:91:ARG:HG3	2.11	0.50
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.35	0.50
1:E:138:HIS:HD2	3:E:576:HOH:O	1.94	0.50
1:E:259:LEU:HD22	1:E:274:LEU:HD13	1.93	0.50
1:C:50:MET:HE1	1:D:198:MET:HB2	1.92	0.50
1:K:322:ALA:O	1:K:323:ASN:C	2.54	0.50
1:E:196:ILE:HG12	1:E:199:MET:HB2	1.93	0.50
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.94	0.50
1:F:323:ASN:CG	1:F:324:GLY:H	2.20	0.49
1:J:111:MET:HE3	1:J:186:ALA:O	2.12	0.49
1:I:176:GLN:HG3	1:J:176:GLN:NE2	2.28	0.49
1:G:18:PRO:HB3	1:G:156:ASP:O	2.13	0.49
2:H:401:MFK:H36	2:H:401:MFK:OAO	2.11	0.49
1:G:241:GLU:HB2	1:G:244:PHE:CD2	2.48	0.49
1:I:138:HIS:HD2	3:I:524:HOH:O	1.96	0.49
1:E:91:ARG:NH2	2:E:401:MFK:OBX	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD23	1:C:108:TYR:CE2	2.47	0.48
1:B:345:PRO:HA	3:B:543:HOH:O	2.13	0.48
1:G:176:GLN:HE21	1:G:176:GLN:HA	1.77	0.48
1:F:346:ALA:HB3	3:F:545:HOH:O	2.13	0.48
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.48	0.48
1:C:176:GLN:CD	1:D:176:GLN:HG2	2.39	0.48
1:B:244:PHE:HB3	1:B:295:ASP:O	2.14	0.48
1:C:1:MET:O	1:C:6:SER:OG	2.24	0.48
1:D:45:ILE:HG23	1:D:345:PRO:O	2.14	0.48
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.46	0.47
1:L:286:HIS:HD2	3:L:646:HOH:O	1.96	0.47
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.29	0.47
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.95	0.47
1:C:111:MET:HE3	1:C:186:ALA:O	2.14	0.47
1:I:198:MET:HB2	1:J:50:MET:HE1	1.96	0.47
1:A:270:GLU:HG3	3:A:548:HOH:O	2.13	0.47
1:G:39:PRO:HB3	1:G:58:THR:HG22	1.95	0.47
1:K:196:ILE:HG13	1:L:153:LEU:HD21	1.96	0.47
1:J:196:ILE:HG12	1:J:199:MET:HB2	1.96	0.47
1:C:91:ARG:NH2	2:C:401:MFK:OBX	2.48	0.47
1:L:291:PHE:O	1:L:294:SER:HB3	2.15	0.47
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.97	0.47
1:J:102:VAL:O	1:J:103:ASN:HB2	2.14	0.47
1:K:69:LEU:HD13	1:K:351:ILE:HG21	1.95	0.47
1:K:111:MET:HE3	1:K:186:ALA:O	2.15	0.46
1:A:295:ASP:CG	1:B:85:ARG:HH22	2.23	0.46
1:E:40:SER:O	1:E:41:SER:C	2.58	0.46
1:F:105:ARG:NH1	3:F:505:HOH:O	2.36	0.46
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.48	0.46
1:I:196:ILE:HG12	1:I:199:MET:HB2	1.98	0.46
1:H:58:THR:O	1:H:59:ALA:HB2	2.16	0.46
1:J:322:ALA:O	1:J:324:GLY:N	2.49	0.46
1:A:244:PHE:HB3	1:A:295:ASP:O	2.16	0.46
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.33	0.46
1:F:76:LYS:HB2	1:F:358:TRP:HE3	1.80	0.46
1:G:38:ARG:NE	3:G:501:HOH:O	2.47	0.46
1:K:73:LEU:HD21	1:K:354:VAL:HG12	1.98	0.46
1:C:85:ARG:NH1	1:C:122:GLN:O	2.43	0.45
1:E:302:LEU:O	1:F:135:GLY:HA2	2.16	0.45
1:L:107:ILE:HD12	1:L:171:ALA:HB1	1.97	0.45
1:K:60:ASP:O	1:K:66:GLY:HA3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ARG:NH1	2:I:401:MFK:O4'	2.49	0.45
1:A:140:ILE:CD1	1:B:151:LEU:HG	2.46	0.45
1:F:291:PHE:O	1:F:292:ALA:C	2.60	0.45
1:I:135:GLY:HA2	1:J:302:LEU:O	2.15	0.45
1:B:349:ILE:HD11	1:B:354:VAL:HG22	1.98	0.45
1:D:10:VAL:HG22	1:D:79:VAL:HB	1.99	0.45
1:L:268:TRP:N	1:L:269:PRO:CD	2.80	0.45
1:K:346:ALA:HB3	3:K:562:HOH:O	2.17	0.45
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.32	0.45
3:I:579:HOH:O	1:J:50:MET:HE1	2.15	0.45
1:J:28:ASP:HA	1:J:53:ASN:ND2	2.32	0.45
2:E:401:MFK:H5	1:F:202:MET:HE3	1.98	0.44
1:E:117:THR:O	1:F:316:ARG:HD2	2.16	0.44
1:K:113:GLY:CA	1:K:188:MET:HE3	2.47	0.44
1:K:91:ARG:NH2	2:K:401:MFK:OBW	2.50	0.44
1:A:135:GLY:HA2	1:B:302:LEU:O	2.18	0.44
1:B:142:ARG:O	1:B:212:ARG:HD2	2.18	0.44
1:D:255:ASP:HB3	1:D:258:GLU:HG2	2.00	0.44
2:B:401:MFK:H19	2:B:401:MFK:H20	1.92	0.44
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.53	0.44
1:E:109:ALA:HB1	1:E:164:LEU:HD11	2.00	0.44
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.99	0.43
1:E:9:ARG:NH2	1:E:358:TRP:HA	2.33	0.43
1:F:85:ARG:HD3	2:F:401:MFK:PAZ	2.55	0.43
1:I:322:ALA:O	1:I:323:ASN:C	2.59	0.43
1:G:113:GLY:HA3	1:G:130:TYR:CE1	2.54	0.43
1:A:39:PRO:HB3	1:A:58:THR:HG23	1.99	0.43
1:E:135:GLY:HA2	1:F:302:LEU:O	2.18	0.43
1:F:106:LEU:O	1:F:181:GLY:HA3	2.19	0.43
1:G:198:MET:HB2	1:H:50:MET:HE1	2.01	0.43
1:C:135:GLY:HA2	1:D:302:LEU:O	2.18	0.43
1:H:18:PRO:HB3	1:H:156:ASP:O	2.19	0.43
1:A:28:ASP:HA	1:A:53:ASN:ND2	2.34	0.43
1:I:316:ARG:HD2	1:J:117:THR:O	2.19	0.43
2:A:401:MFK:H34	2:A:401:MFK:H23	2.00	0.43
1:L:196:ILE:HG12	1:L:199:MET:HB2	2.00	0.43
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.52	0.43
1:F:255:ASP:HB3	1:F:258:GLU:HG2	2.01	0.42
1:B:38:ARG:NH2	2:B:401:MFK:O4'	2.52	0.42
1:D:170:ALA:O	1:D:173:TRP:HB3	2.20	0.42
1:D:329:MET:HE3	1:D:330:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH2	2:A:401:MFK:OBW	2.52	0.42
1:J:142:ARG:O	1:J:212:ARG:HD2	2.19	0.42
1:C:60:ASP:OD1	1:C:62:LYS:HB2	2.20	0.42
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.45	0.42
1:J:94:LEU:HD23	1:J:94:LEU:HA	1.81	0.42
1:A:323:ASN:O	1:A:324:GLY:C	2.62	0.42
1:C:176:GLN:HA	1:C:176:GLN:NE2	2.32	0.42
1:J:252:LEU:HD21	1:J:279:PHE:CE1	2.55	0.42
1:C:346:ALA:HB3	3:C:522:HOH:O	2.20	0.42
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.54	0.42
1:F:322:ALA:O	1:F:323:ASN:C	2.62	0.42
1:J:244:PHE:HB3	1:J:295:ASP:O	2.20	0.42
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.55	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.83	0.42
1:D:322:ALA:O	1:D:323:ASN:C	2.62	0.42
1:F:57:VAL:HG12	1:F:349:ILE:O	2.20	0.42
1:G:50:MET:HE3	1:G:50:MET:HB2	1.95	0.42
1:G:176:GLN:HA	1:G:176:GLN:NE2	2.35	0.42
1:F:87:GLY:O	1:F:91:ARG:HG3	2.20	0.41
1:K:359:ASP:HA	3:K:615:HOH:O	2.20	0.41
1:B:114:TRP:CZ3	1:B:133:LEU:HD22	2.55	0.41
1:B:241:GLU:HB2	1:B:244:PHE:CD2	2.56	0.41
1:C:112:THR:O	1:C:187:ALA:HA	2.20	0.41
1:C:302:LEU:O	1:D:135:GLY:HA2	2.20	0.41
1:G:303:ALA:O	1:G:304:PHE:C	2.63	0.41
1:H:268:TRP:N	1:H:269:PRO:CD	2.83	0.41
1:A:80:LEU:CD2	1:A:108:TYR:CE2	3.01	0.41
1:A:117:THR:O	1:B:316:ARG:HD2	2.20	0.41
1:F:196:ILE:HG12	1:F:199:MET:HB2	2.01	0.41
1:K:38:ARG:HH11	1:K:38:ARG:HG3	1.85	0.41
1:K:80:LEU:CD2	1:K:108:TYR:CE1	3.03	0.41
1:K:145:GLU:OE1	1:L:145:GLU:OE1	2.38	0.41
1:F:58:THR:O	1:F:59:ALA:HB2	2.21	0.41
1:G:117:THR:O	1:H:316:ARG:HD2	2.21	0.41
1:G:225:ASP:OD2	1:G:272:ARG:NH1	2.53	0.41
1:J:322:ALA:O	1:J:323:ASN:C	2.63	0.41
1:D:225:ASP:OD2	1:D:272:ARG:NH1	2.54	0.41
1:G:42:VAL:O	1:G:43:ASP:HB2	2.21	0.41
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.55	0.41
1:E:336:ARG:HG2	1:E:336:ARG:NH1	2.35	0.41
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ASP:O	1:J:66:GLY:HA3	2.20	0.41
1:L:221:ALA:HA	1:L:222:PRO:HD3	1.96	0.41
1:B:45:ILE:H	1:B:45:ILE:HD12	1.86	0.41
1:D:358:TRP:O	1:D:359:ASP:C	2.63	0.41
1:E:272:ARG:NH1	3:E:515:HOH:O	2.50	0.41
1:K:50:MET:HB3	3:K:501:HOH:O	2.21	0.41
1:K:55:ARG:HG2	1:K:349:ILE:HD12	2.02	0.41
1:K:85:ARG:NH2	2:K:401:MFK:OAW	2.29	0.41
1:L:113:GLY:HA3	1:L:130:TYR:CE1	2.56	0.41
1:G:207:MET:CE	2:H:401:MFK:H4	2.50	0.41
2:B:401:MFK:H34	2:B:401:MFK:H23	2.02	0.40
1:D:303:ALA:O	1:D:304:PHE:C	2.65	0.40
2:E:401:MFK:OAO	2:E:401:MFK:H36	2.21	0.40
1:I:244:PHE:CD1	1:I:295:ASP:HB3	2.56	0.40
1:J:316:ARG:O	1:J:317:ASN:C	2.64	0.40
1:F:54:ARG:HG2	1:F:54:ARG:HH11	1.86	0.40
2:H:401:MFK:OAO	2:H:401:MFK:CAS	2.68	0.40
1:B:303:ALA:O	1:B:304:PHE:C	2.65	0.40
1:C:51:LEU:HA	1:C:54:ARG:NH1	2.35	0.40
1:H:265:ARG:HG2	1:H:268:TRP:CZ3	2.57	0.40
1:L:43:ASP:HB2	3:L:634:HOH:O	2.21	0.40
1:L:241:GLU:HB2	1:L:244:PHE:CD2	2.56	0.40
1:I:75:ALA:HA	1:I:103:ASN:HB2	2.04	0.40
1:I:341:GLN:HA	1:I:342:PRO:HD3	1.97	0.40
1:J:71:LEU:HD23	1:J:71:LEU:HA	2.02	0.40
1:K:181:GLY:O	1:K:182:GLN:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	355/364 (98%)	336 (95%)	18 (5%)	1 (0%)	37	36
1	B	354/364 (97%)	340 (96%)	10 (3%)	4 (1%)	12	7
1	C	356/364 (98%)	336 (94%)	19 (5%)	1 (0%)	37	36
1	D	358/364 (98%)	335 (94%)	19 (5%)	4 (1%)	12	7
1	E	354/364 (97%)	338 (96%)	12 (3%)	4 (1%)	12	7
1	F	355/364 (98%)	336 (95%)	17 (5%)	2 (1%)	22	18
1	G	359/364 (99%)	338 (94%)	16 (4%)	5 (1%)	9	5
1	H	353/364 (97%)	334 (95%)	16 (4%)	3 (1%)	16	12
1	I	359/364 (99%)	345 (96%)	12 (3%)	2 (1%)	22	18
1	J	353/364 (97%)	337 (96%)	13 (4%)	3 (1%)	16	12
1	K	355/364 (98%)	337 (95%)	16 (4%)	2 (1%)	22	18
1	L	358/364 (98%)	341 (95%)	16 (4%)	1 (0%)	37	36
All	All	4269/4368 (98%)	4053 (95%)	184 (4%)	32 (1%)	16	15

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	347	ALA
1	G	347	ALA
1	H	40	SER
1	A	103	ASN
1	B	323	ASN
1	D	347	ALA
1	G	42	VAL
1	G	59	ALA
1	J	103	ASN
1	K	103	ASN
1	B	103	ASN
1	C	103	ASN
1	E	348	THR
1	G	43	ASP
1	H	59	ALA
1	J	40	SER
1	K	323	ASN
1	D	103	ASN
1	F	103	ASN
1	G	103	ASN
1	H	103	ASN
1	I	103	ASN

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Mol	Chain	Res	Type
1	B	151	LEU
1	D	40	SER
1	D	151	LEU
1	E	59	ALA
1	E	103	ASN
1	E	151	LEU
1	F	42	VAL
1	I	42	VAL
1	J	323	ASN
1	L	103	ASN

### 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	276/277 (100%)	265 (96%)	11 (4%)	27	27
1	B	274/277 (99%)	269 (98%)	5 (2%)	54	59
1	C	276/277 (100%)	271 (98%)	5 (2%)	54	59
1	D	276/277 (100%)	266 (96%)	10 (4%)	30	31
1	E	275/277 (99%)	269 (98%)	6 (2%)	47	51
1	F	276/277 (100%)	265 (96%)	11 (4%)	27	27
1	G	277/277 (100%)	269 (97%)	8 (3%)	37	40
1	H	274/277 (99%)	265 (97%)	9 (3%)	33	34
1	I	277/277 (100%)	270 (98%)	7 (2%)	42	46
1	J	274/277 (99%)	268 (98%)	6 (2%)	47	51
1	K	275/277 (99%)	264 (96%)	11 (4%)	27	27
1	L	276/277 (100%)	271 (98%)	5 (2%)	54	59
All	All	3306/3324 (100%)	3212 (97%)	94 (3%)	37	41

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	41	SER
1	A	54	ARG
1	A	56	ILE
1	A	58	THR
1	A	133	LEU
1	A	180	LYS
1	A	199	MET
1	A	348	THR
1	A	349	ILE
1	A	350	ASP
1	B	6	SER
1	B	64	ASP
1	B	85	ARG
1	B	177	SER
1	B	258	GLU
1	C	6	SER
1	C	40	SER
1	C	54	ARG
1	C	121	SER
1	C	265	ARG
1	D	6	SER
1	D	40	SER
1	D	85	ARG
1	D	199	MET
1	D	258	GLU
1	D	265	ARG
1	D	269	PRO
1	D	294	SER
1	D	323	ASN
1	D	359	ASP
1	E	6	SER
1	E	45	ILE
1	E	80	LEU
1	E	290	VAL
1	E	351	ILE
1	E	352	GLU
1	F	6	SER
1	F	56	ILE
1	F	58	THR
1	F	85	ARG
1	F	121	SER
1	F	176	GLN

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Mol	Chain	Res	Type
1	F	199	MET
1	F	293	ASN
1	F	323	ASN
1	F	350	ASP
1	F	352	GLU
1	G	6	SER
1	G	40	SER
1	G	47	ARG
1	G	68	GLU
1	G	140	ILE
1	G	258	GLU
1	G	293	ASN
1	G	356	THR
1	H	6	SER
1	H	40	SER
1	H	41	SER
1	H	45	ILE
1	H	47	ARG
1	H	58	THR
1	H	177	SER
1	H	290	VAL
1	H	349	ILE
1	I	42	VAL
1	I	58	THR
1	I	76	LYS
1	I	199	MET
1	I	321	GLU
1	I	323	ASN
1	I	359	ASP
1	J	38	ARG
1	J	176	GLN
1	J	177	SER
1	J	243	GLN
1	J	348	THR
1	J	357	ASP
1	K	38	ARG
1	K	40	SER
1	K	41	SER
1	K	58	THR
1	K	102	VAL
1	K	176	GLN
1	K	203	ARG

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Mol	Chain	Res	Type
1	K	265	ARG
1	K	290	VAL
1	K	349	ILE
1	K	357	ASP
1	L	40	SER
1	L	123	GLN
1	L	199	MET
1	L	258	GLU
1	L	294	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	138	HIS
1	A	263	ASN
1	A	327	GLN
1	B	176	GLN
1	B	282	HIS
1	B	286	HIS
1	B	323	ASN
1	C	116	GLN
1	C	138	HIS
1	C	176	GLN
1	C	243	GLN
1	C	263	ASN
1	C	327	GLN
1	D	282	HIS
1	D	308	HIS
1	D	323	ASN
1	E	116	GLN
1	E	122	GLN
1	E	138	HIS
1	E	263	ASN
1	E	293	ASN
1	E	327	GLN
1	F	122	GLN
1	F	282	HIS
1	G	122	GLN
1	G	138	HIS
1	G	176	GLN
1	G	263	ASN

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Mol	Chain	Res	Type
1	G	282	HIS
1	G	286	HIS
1	G	327	GLN
1	H	116	GLN
1	H	122	GLN
1	H	282	HIS
1	H	286	HIS
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	282	HIS
1	I	308	HIS
1	I	323	ASN
1	I	327	GLN
1	J	123	GLN
1	J	134	ASN
1	J	176	GLN
1	J	243	GLN
1	J	282	HIS
1	J	286	HIS
1	K	138	HIS
1	K	327	GLN
1	L	282	HIS
1	L	323	ASN
1	L	341	GLN

### 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

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MFK	H	401	-	53,61,61	1.60	3 (5%)	64,87,87	1.90	8 (12%)
2	MFK	I	401	-	53,61,61	1.41	2 (3%)	64,87,87	1.55	6 (9%)
2	MFK	A	401	-	53,61,61	1.55	3 (5%)	64,87,87	1.92	8 (12%)
2	MFK	F	401	-	53,61,61	1.57	3 (5%)	64,87,87	1.54	8 (12%)
2	MFK	J	401	-	53,61,61	0.98	2 (3%)	64,87,87	1.95	11 (17%)
2	MFK	C	401	-	53,61,61	1.33	2 (3%)	64,87,87	1.69	8 (12%)
2	MFK	K	401	-	53,61,61	1.59	3 (5%)	64,87,87	1.74	11 (17%)
2	MFK	E	401	-	53,61,61	0.87	2 (3%)	64,87,87	1.66	9 (14%)
2	MFK	B	401	-	53,61,61	1.62	3 (5%)	64,87,87	1.97	12 (18%)
2	MFK	G	401	-	53,61,61	0.98	2 (3%)	64,87,87	1.95	8 (12%)
2	MFK	L	401	-	53,61,61	1.24	5 (9%)	64,87,87	1.80	12 (18%)
2	MFK	D	401	-	53,61,61	1.57	4 (7%)	64,87,87	1.44	5 (7%)

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	MFK	H	401	-	-	17/56/76/76	0/3/3/3
2	MFK	I	401	-	-	8/56/76/76	0/3/3/3
2	MFK	A	401	-	-	12/56/76/76	0/3/3/3
2	MFK	F	401	-	-	10/56/76/76	0/3/3/3
2	MFK	J	401	-	-	15/56/76/76	0/3/3/3
2	MFK	C	401	-	-	14/56/76/76	0/3/3/3
2	MFK	K	401	-	-	10/56/76/76	0/3/3/3
2	MFK	E	401	-	-	7/56/76/76	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MFK	B	401	-	-	14/56/76/76	0/3/3/3
2	MFK	G	401	-	-	15/56/76/76	0/3/3/3
2	MFK	L	401	-	-	10/56/76/76	0/3/3/3
2	MFK	D	401	-	-	7/56/76/76	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	MFK	CAJ-SAI	8.95	1.97	1.76
2	K	401	MFK	CAJ-SAI	8.89	1.97	1.76
2	D	401	MFK	CAJ-SAI	8.78	1.97	1.76
2	B	401	MFK	CAJ-SAI	8.62	1.97	1.76
2	A	401	MFK	CAJ-SAI	8.51	1.96	1.76
2	F	401	MFK	CAJ-SAI	8.38	1.96	1.76
2	I	401	MFK	CAJ-SAI	8.13	1.95	1.76
2	C	401	MFK	CAJ-SAI	7.07	1.93	1.76
2	B	401	MFK	OAL-CAJ	5.59	1.30	1.21
2	L	401	MFK	CAJ-SAI	5.45	1.89	1.76
2	F	401	MFK	OAL-CAJ	5.11	1.29	1.21
2	A	401	MFK	OAL-CAJ	4.89	1.29	1.21
2	K	401	MFK	OAL-CAJ	4.79	1.28	1.21
2	H	401	MFK	OAL-CAJ	4.66	1.28	1.21
2	D	401	MFK	OAL-CAJ	4.59	1.28	1.21
2	I	401	MFK	OAL-CAJ	4.41	1.28	1.21
2	C	401	MFK	OAL-CAJ	4.12	1.27	1.21
2	G	401	MFK	CAJ-SAI	3.77	1.85	1.76
2	J	401	MFK	CAJ-SAI	3.65	1.85	1.76
2	L	401	MFK	OAL-CAJ	3.59	1.26	1.21
2	E	401	MFK	CAJ-SAI	3.40	1.84	1.76
2	J	401	MFK	CAK-CAJ	2.89	1.53	1.50
2	F	401	MFK	CAK-CAJ	2.86	1.53	1.50
2	H	401	MFK	CAK-CAJ	2.76	1.53	1.50
2	L	401	MFK	CAK-CAJ	2.38	1.53	1.50
2	K	401	MFK	CAK-CAJ	2.38	1.53	1.50
2	E	401	MFK	OAL-CAJ	2.34	1.24	1.21
2	B	401	MFK	CAK-CAJ	2.34	1.53	1.50
2	G	401	MFK	CAH-CAG	2.33	1.60	1.51
2	L	401	MFK	CAC-CAD	2.24	1.58	1.51
2	A	401	MFK	CAK-CAJ	2.22	1.53	1.50
2	D	401	MFK	CAK-CAJ	2.17	1.53	1.50
2	D	401	MFK	PBV-O3'	2.13	1.63	1.59
2	L	401	MFK	C8-N7	-2.00	1.31	1.34

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	MFK	CAH-SAI-CAJ	10.15	133.46	101.87
2	G	401	MFK	CAH-SAI-CAJ	9.40	131.12	101.87
2	E	401	MFK	CAH-SAI-CAJ	8.68	128.90	101.87
2	B	401	MFK	OAL-CAJ-SAI	8.30	133.39	122.61
2	A	401	MFK	CAG-NAF-CAE	-7.83	108.30	122.84
2	C	401	MFK	OAL-CAJ-SAI	7.49	132.34	122.61
2	L	401	MFK	CAH-SAI-CAJ	7.23	124.39	101.87
2	I	401	MFK	OAL-CAJ-CAK	-6.66	116.12	123.99
2	H	401	MFK	CAS-CAP-CAQ	-6.64	97.40	108.23
2	G	401	MFK	CAR-CAP-CAQ	-6.52	97.60	108.23
2	K	401	MFK	OAL-CAJ-SAI	6.50	131.05	122.61
2	A	401	MFK	OAL-CAJ-SAI	6.50	131.05	122.61
2	D	401	MFK	OAL-CAJ-SAI	6.39	130.91	122.61
2	A	401	MFK	OAL-CAJ-CAK	-6.22	116.64	123.99
2	D	401	MFK	OAL-CAJ-CAK	-6.09	116.80	123.99
2	I	401	MFK	OAL-CAJ-SAI	6.08	130.52	122.61
2	H	401	MFK	OAL-CAJ-SAI	6.03	130.44	122.61
2	L	401	MFK	CAD-CAE-NAF	5.98	126.49	116.42
2	C	401	MFK	OAL-CAJ-CAK	-5.83	117.11	123.99
2	H	401	MFK	CAR-CAP-CAQ	5.80	117.69	108.23
2	H	401	MFK	OAL-CAJ-CAK	-5.77	117.17	123.99
2	B	401	MFK	CAG-NAF-CAE	-5.76	112.15	122.84
2	K	401	MFK	OAL-CAJ-CAK	-5.70	117.25	123.99
2	J	401	MFK	CAK-CAJ-SAI	5.64	120.03	113.46
2	F	401	MFK	OAL-CAJ-SAI	5.38	129.60	122.61
2	B	401	MFK	OAL-CAJ-CAK	-5.24	117.80	123.99
2	C	401	MFK	OAX-PAV-OAW	5.07	137.31	112.24
2	H	401	MFK	OAX-PAV-OAW	4.85	136.23	112.24
2	A	401	MFK	OAX-PAV-OAW	4.84	136.15	112.24
2	G	401	MFK	OAX-PAV-OAW	4.82	136.06	112.24
2	F	401	MFK	OAL-CAJ-CAK	-4.74	118.40	123.99
2	F	401	MFK	OAX-PAV-OAW	4.65	135.24	112.24
2	L	401	MFK	OAL-CAJ-SAI	4.64	128.64	122.61
2	K	401	MFK	OAX-PAV-OAW	4.63	135.12	112.24
2	J	401	MFK	OAX-PAV-OAW	4.50	134.49	112.24
2	B	401	MFK	CAK-CAJ-SAI	-4.03	108.77	113.46
2	B	401	MFK	OAX-PAV-OAW	3.96	131.83	112.24
2	G	401	MFK	OAL-CAJ-CAK	-3.94	119.33	123.99
2	E	401	MFK	OAX-PAV-OAW	3.82	131.14	112.24
2	E	401	MFK	OAL-CAJ-SAI	3.72	127.44	122.61
2	K	401	MFK	OAT-CAQ-CAP	-3.71	104.59	110.55
2	L	401	MFK	OAX-PAV-OAW	3.46	129.35	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	MFK	CAH-SAI-CAJ	-3.41	91.24	101.87
2	I	401	MFK	OAX-PAV-OAW	3.34	128.73	112.24
2	J	401	MFK	OAL-CAJ-CAK	-3.26	120.14	123.99
2	L	401	MFK	OAM-CAE-CAD	-3.23	116.10	122.02
2	H	401	MFK	OAX-PAV-OAT	-3.23	92.75	107.75
2	K	401	MFK	OBX-PBV-OBV	3.19	119.81	107.64
2	G	401	MFK	OAT-PAV-OAW	-3.08	97.02	109.07
2	A	401	MFK	OAT-CAQ-CAP	-3.07	105.61	110.55
2	G	401	MFK	OBX-PBV-OBV	3.07	119.35	107.64
2	D	401	MFK	OAX-PAV-OAW	3.06	127.35	112.24
2	J	401	MFK	OAT-CAQ-CAP	-3.04	105.66	110.55
2	F	401	MFK	OAT-CAQ-CAP	-3.04	105.67	110.55
2	G	401	MFK	CAS-CAP-CAQ	3.03	113.17	108.23
2	K	401	MFK	C5-C6-N6	3.00	124.91	120.35
2	L	401	MFK	OAM-CAE-NAF	-2.99	117.37	123.01
2	K	401	MFK	OAT-PAV-OAW	-2.97	97.45	109.07
2	B	401	MFK	OAT-PAV-OAW	-2.96	97.51	109.07
2	L	401	MFK	OAL-CAJ-CAK	-2.95	120.50	123.99
2	E	401	MFK	C5-C6-N6	2.89	124.74	120.35
2	I	401	MFK	OBX-PBV-OBV	2.86	118.56	107.64
2	C	401	MFK	OAT-CAQ-CAP	-2.85	105.96	110.55
2	F	401	MFK	CAR-CAP-CAQ	2.82	112.83	108.23
2	F	401	MFK	OAT-PAV-OAW	-2.79	98.16	109.07
2	J	401	MFK	C5-C6-N6	2.79	124.59	120.35
2	E	401	MFK	OAT-PAV-OAW	-2.74	98.38	109.07
2	F	401	MFK	C5-C6-N6	2.68	124.43	120.35
2	C	401	MFK	C5-C6-N6	2.67	124.41	120.35
2	F	401	MFK	OAU-CAN-CAP	-2.65	104.02	110.25
2	B	401	MFK	OBX-PBV-OBV	2.63	117.68	107.64
2	B	401	MFK	OBV-PBV-OBW	-2.55	100.70	110.68
2	J	401	MFK	OAU-CAN-CAP	-2.53	104.28	110.25
2	L	401	MFK	OBX-PBV-OBW	2.52	120.53	110.68
2	B	401	MFK	O2'-C2'-C1'	-2.52	101.57	110.85
2	J	401	MFK	CAS-CAP-CAQ	2.51	112.33	108.23
2	C	401	MFK	CAK-CAJ-SAI	-2.49	110.55	113.46
2	D	401	MFK	CAG-NAF-CAE	-2.49	118.22	122.84
2	E	401	MFK	OAT-CAQ-CAP	-2.44	106.62	110.55
2	K	401	MFK	OBV-PBV-OBW	-2.42	101.19	110.68
2	A	401	MFK	CAR-CAP-CAQ	-2.42	104.28	108.23
2	J	401	MFK	CBZ-CAK-CAJ	2.39	117.63	112.33
2	K	401	MFK	OBX-PBV-O3'	-2.39	95.29	105.99
2	L	401	MFK	OAT-PAV-OAW	-2.34	99.92	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	MFK	OBX-PBV-OBW	2.30	119.67	110.68
2	I	401	MFK	C5-C6-N6	2.29	123.83	120.35
2	H	401	MFK	C5-C6-N6	2.29	123.83	120.35
2	L	401	MFK	O3'-PBV-OBW	-2.26	100.66	109.39
2	L	401	MFK	CAK-CAJ-SAI	-2.26	110.83	113.46
2	A	401	MFK	CAH-SAI-CAJ	-2.25	94.86	101.87
2	A	401	MFK	OAU-CAN-CAP	-2.23	105.00	110.25
2	L	401	MFK	OAU-CAN-CAP	-2.23	105.00	110.25
2	I	401	MFK	OAT-CAQ-CAP	-2.21	107.00	110.55
2	J	401	MFK	OAL-CAJ-SAI	-2.17	119.79	122.61
2	K	401	MFK	CAR-CAP-CAQ	2.15	111.75	108.23
2	E	401	MFK	OAL-CAJ-CAK	-2.13	121.47	123.99
2	B	401	MFK	OBX-PBV-OBW	2.12	118.99	110.68
2	H	401	MFK	OAT-PAV-OAW	2.10	117.29	109.07
2	J	401	MFK	O3'-PBV-OBW	-2.10	101.28	109.39
2	G	401	MFK	C5-C6-N6	2.09	123.53	120.35
2	E	401	MFK	C1'-N9-C4	-2.09	122.97	126.64
2	E	401	MFK	CAK-CAJ-SAI	-2.07	111.05	113.46
2	D	401	MFK	O4'-C1'-C2'	-2.07	103.91	106.93
2	B	401	MFK	C5-C6-N6	2.05	123.47	120.35
2	C	401	MFK	OBX-PBV-OBW	2.03	115.40	107.64
2	C	401	MFK	O2'-C2'-C3'	-2.03	105.40	111.17

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	MFK	CAK-CAJ-SAI-CAH
2	A	401	MFK	OAL-CAJ-SAI-CAH
2	A	401	MFK	CAG-CAH-SAI-CAJ
2	B	401	MFK	CAJ-CAK-CBZ-CCA
2	B	401	MFK	CAK-CAJ-SAI-CAH
2	B	401	MFK	OAL-CAJ-SAI-CAH
2	B	401	MFK	CAG-CAH-SAI-CAJ
2	B	401	MFK	NAB-CAC-CAD-CAE
2	B	401	MFK	C5'-O5'-PAZ-OAY
2	B	401	MFK	C5'-O5'-PAZ-OBW
2	C	401	MFK	CAJ-CAK-CBZ-CCA
2	C	401	MFK	CAK-CAJ-SAI-CAH
2	C	401	MFK	OAL-CAJ-SAI-CAH
2	D	401	MFK	CAJ-CAK-CBZ-CCA
2	D	401	MFK	CAK-CAJ-SAI-CAH

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Mol	Chain	Res	Type	Atoms
2	D	401	MFK	OAL-CAJ-SAI-CAH
2	E	401	MFK	CAJ-CAK-CBZ-CCA
2	E	401	MFK	CAG-CAH-SAI-CAJ
2	F	401	MFK	CAJ-CAK-CBZ-CCA
2	F	401	MFK	CAK-CAJ-SAI-CAH
2	F	401	MFK	OAL-CAJ-SAI-CAH
2	F	401	MFK	NAB-CAC-CAD-CAE
2	F	401	MFK	C5'-O5'-PAZ-OAY
2	G	401	MFK	CAJ-CAK-CBZ-CCA
2	G	401	MFK	CAA-CAN-CAP-CAQ
2	G	401	MFK	CAN-CAP-CAQ-OAT
2	H	401	MFK	CAJ-CAK-CBZ-CCA
2	H	401	MFK	CAK-CAJ-SAI-CAH
2	H	401	MFK	OAL-CAJ-SAI-CAH
2	H	401	MFK	CAA-CAN-CAP-CAQ
2	H	401	MFK	CAQ-OAT-PAV-OAW
2	H	401	MFK	C3'-O3'-PBV-OBW
2	I	401	MFK	CAK-CAJ-SAI-CAH
2	I	401	MFK	OAL-CAJ-SAI-CAH
2	I	401	MFK	CAQ-OAT-PAV-OAW
2	J	401	MFK	CAJ-CAK-CBZ-CCA
2	K	401	MFK	CAK-CAJ-SAI-CAH
2	K	401	MFK	OAL-CAJ-SAI-CAH
2	L	401	MFK	CAJ-CAK-CBZ-CCA
2	L	401	MFK	OAM-CAE-NAF-CAG
2	L	401	MFK	CAD-CAE-NAF-CAG
2	L	401	MFK	CAQ-OAT-PAV-OAX
2	C	401	MFK	CCC-CCD-CCE-CCF
2	C	401	MFK	CCA-CCB-CCC-CCD
2	F	401	MFK	CAK-CBZ-CCA-CCB
2	G	401	MFK	CAS-CAP-CAQ-OAT
2	K	401	MFK	CCC-CCD-CCE-CCF
2	L	401	MFK	CCC-CCD-CCE-CCF
2	F	401	MFK	CCB-CCC-CCD-CCE
2	L	401	MFK	CCA-CCB-CCC-CCD
2	H	401	MFK	CAK-CBZ-CCA-CCB
2	B	401	MFK	CCC-CCD-CCE-CCF
2	J	401	MFK	CCC-CCD-CCE-CCF
2	J	401	MFK	CCB-CCC-CCD-CCE
2	A	401	MFK	CCC-CCD-CCE-CCF
2	G	401	MFK	CCC-CCD-CCE-CCF
2	H	401	MFK	CCC-CCD-CCE-CCF

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Mol	Chain	Res	Type	Atoms
2	J	401	MFK	CCA-CCB-CCC-CCD
2	H	401	MFK	CCB-CCC-CCD-CCE
2	K	401	MFK	CAK-CBZ-CCA-CCB
2	C	401	MFK	CAK-CBZ-CCA-CCB
2	B	401	MFK	CCA-CCB-CCC-CCD
2	D	401	MFK	CAK-CBZ-CCA-CCB
2	H	401	MFK	CCA-CCB-CCC-CCD
2	J	401	MFK	CAK-CBZ-CCA-CCB
2	G	401	MFK	CCA-CCB-CCC-CCD
2	I	401	MFK	CCD-CCE-CCF-CCG
2	K	401	MFK	CCA-CCB-CCC-CCD
2	B	401	MFK	CCB-CCC-CCD-CCE
2	A	401	MFK	NAB-CAC-CAD-CAE
2	C	401	MFK	NAB-CAC-CAD-CAE
2	D	401	MFK	NAB-CAC-CAD-CAE
2	A	401	MFK	CAK-CBZ-CCA-CCB
2	E	401	MFK	CCD-CCE-CCF-CCG
2	F	401	MFK	O4'-C4'-C5'-O5'
2	I	401	MFK	CCC-CCD-CCE-CCF
2	G	401	MFK	CAR-CAP-CAQ-OAT
2	L	401	MFK	CAK-CBZ-CCA-CCB
2	G	401	MFK	CCD-CCE-CCF-CCG
2	C	401	MFK	CBZ-CCA-CCB-CCC
2	H	401	MFK	CBZ-CCA-CCB-CCC
2	F	401	MFK	CBZ-CCA-CCB-CCC
2	B	401	MFK	CCD-CCE-CCF-CCG
2	E	401	MFK	CCA-CCB-CCC-CCD
2	F	401	MFK	CCC-CCD-CCE-CCF
2	B	401	MFK	CAK-CBZ-CCA-CCB
2	J	401	MFK	OAL-CAJ-SAI-CAH
2	G	401	MFK	OAL-CAJ-CAK-CBZ
2	G	401	MFK	SAI-CAJ-CAK-CBZ
2	J	401	MFK	OAL-CAJ-CAK-CBZ
2	J	401	MFK	SAI-CAJ-CAK-CBZ
2	E	401	MFK	C3'-O3'-PBV-OBW
2	K	401	MFK	C3'-O3'-PBV-OBW
2	J	401	MFK	CAK-CAJ-SAI-CAH
2	A	401	MFK	C5'-O5'-PAZ-OAY
2	H	401	MFK	C3'-O3'-PBV-OBW
2	J	401	MFK	C5'-O5'-PAZ-OAY
2	G	401	MFK	OAM-CAE-NAF-CAG
2	D	401	MFK	CBZ-CCA-CCB-CCC

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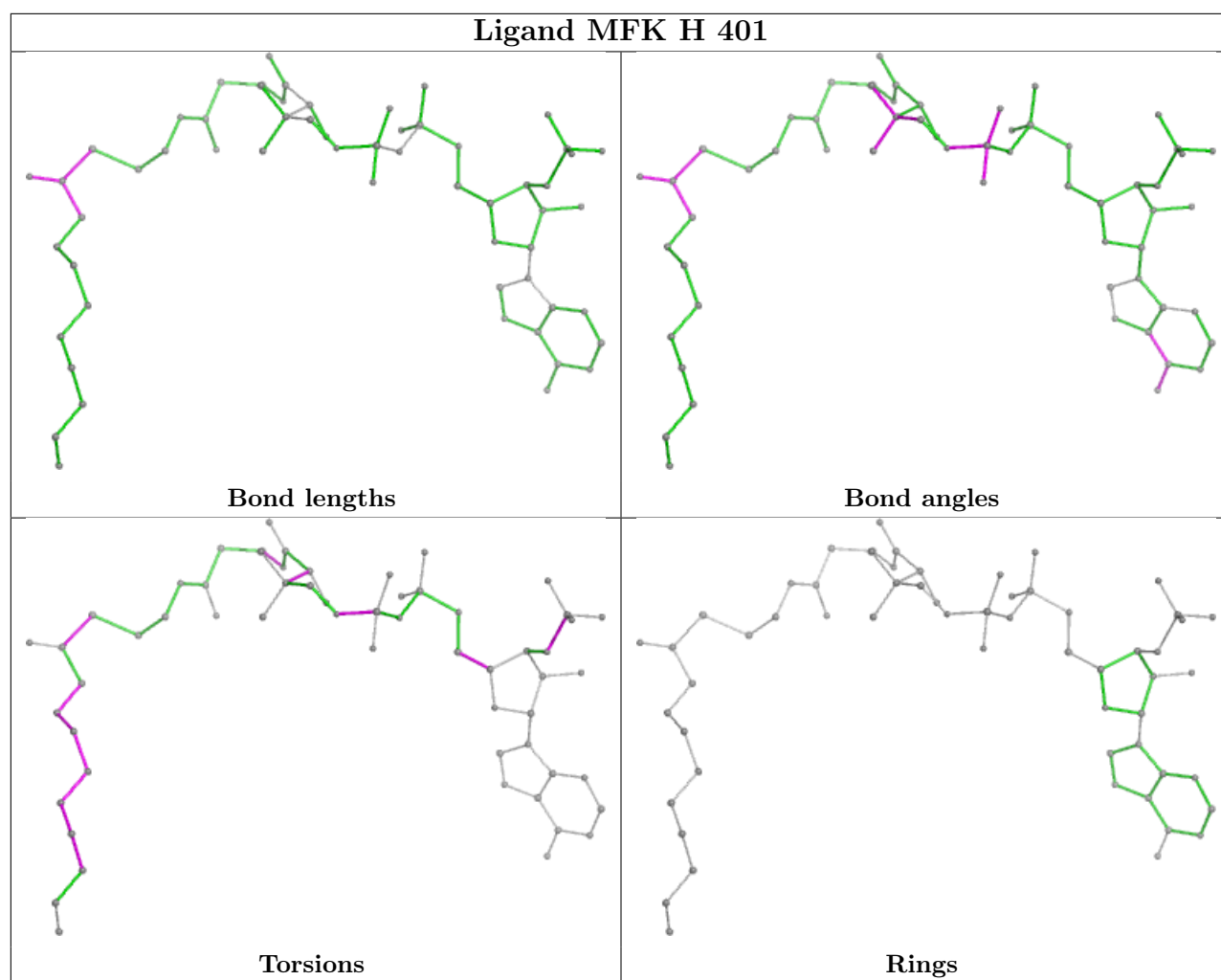
Mol	Chain	Res	Type	Atoms
2	G	401	MFK	CAQ-OAT-PAV-OAW
2	H	401	MFK	CAQ-OAT-PAV-OAX
2	H	401	MFK	OAU-CAN-CAP-CAQ
2	A	401	MFK	CBZ-CCA-CCB-CCC
2	A	401	MFK	CCD-CCE-CCF-CCG
2	K	401	MFK	NAB-CAC-CAD-CAE
2	A	401	MFK	O4'-C4'-C5'-O5'
2	B	401	MFK	O4'-C4'-C5'-O5'
2	J	401	MFK	O4'-C4'-C5'-O5'
2	J	401	MFK	CBZ-CCA-CCB-CCC
2	G	401	MFK	O4'-C4'-C5'-O5'
2	G	401	MFK	CAG-CAH-SAI-CAJ
2	J	401	MFK	CAG-CAH-SAI-CAJ
2	L	401	MFK	CAG-CAH-SAI-CAJ
2	B	401	MFK	PAV-OAY-PAZ-OBA
2	L	401	MFK	CCD-CCE-CCF-CCG
2	D	401	MFK	O4'-C4'-C5'-O5'
2	J	401	MFK	C3'-O3'-PBV-OBW
2	C	401	MFK	CCD-CCE-CCF-CCG
2	C	401	MFK	C3'-O3'-PBV-OBX
2	C	401	MFK	C3'-O3'-PBV-OBX
2	E	401	MFK	C3'-O3'-PBV-OBX
2	G	401	MFK	CAQ-OAT-PAV-OAY
2	H	401	MFK	CAQ-OAT-PAV-OAY
2	J	401	MFK	C3'-O3'-PBV-OBX
2	K	401	MFK	CCB-CCC-CCD-CCE
2	E	401	MFK	O4'-C4'-C5'-O5'
2	K	401	MFK	O4'-C4'-C5'-O5'
2	L	401	MFK	O4'-C4'-C5'-O5'
2	A	401	MFK	PAV-OAY-PAZ-OBA
2	C	401	MFK	PAV-OAY-PAZ-OBX
2	K	401	MFK	PAV-OAY-PAZ-OBA
2	A	401	MFK	CCA-CCB-CCC-CCD
2	C	401	MFK	O4'-C4'-C5'-O5'
2	H	401	MFK	O4'-C4'-C5'-O5'
2	I	401	MFK	O4'-C4'-C5'-O5'
2	C	401	MFK	CCB-CCC-CCD-CCE
2	I	401	MFK	CAD-CAC-NAB-CAA
2	I	401	MFK	CBZ-CCA-CCB-CCC
2	H	401	MFK	CAD-CAC-NAB-CAA

There are no ring outliers.

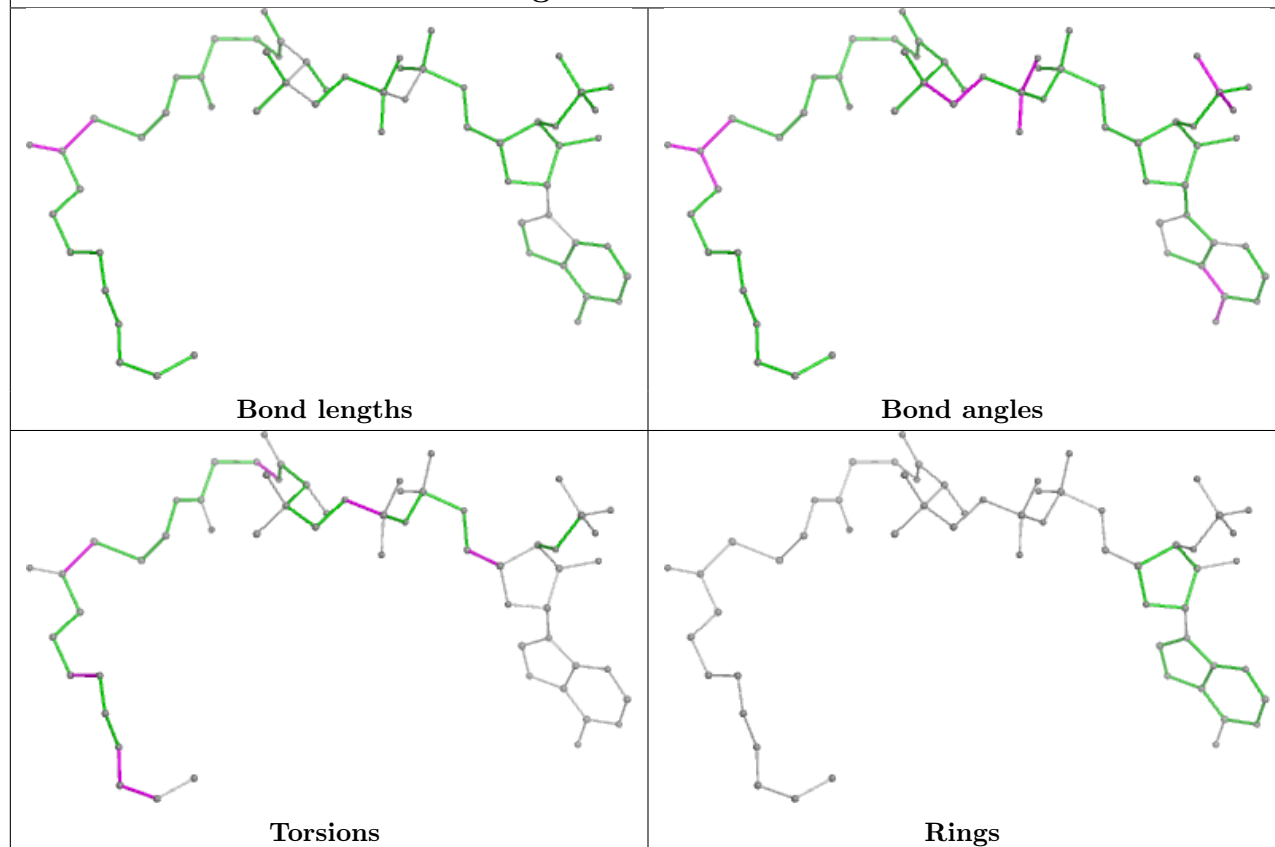
9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	MFK	4	0
2	I	401	MFK	1	0
2	A	401	MFK	2	0
2	F	401	MFK	7	0
2	C	401	MFK	2	0
2	K	401	MFK	2	0
2	E	401	MFK	3	0
2	B	401	MFK	5	0
2	D	401	MFK	2	0

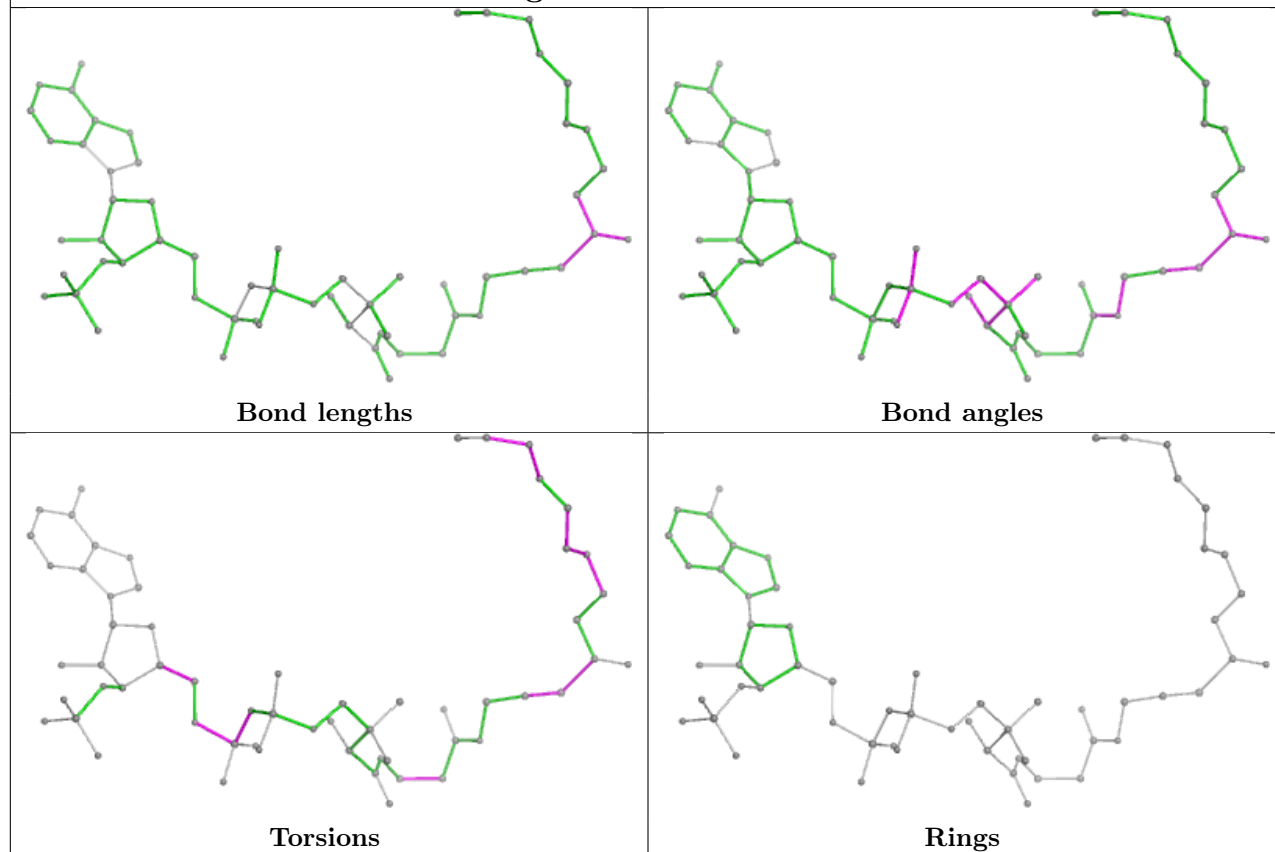
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

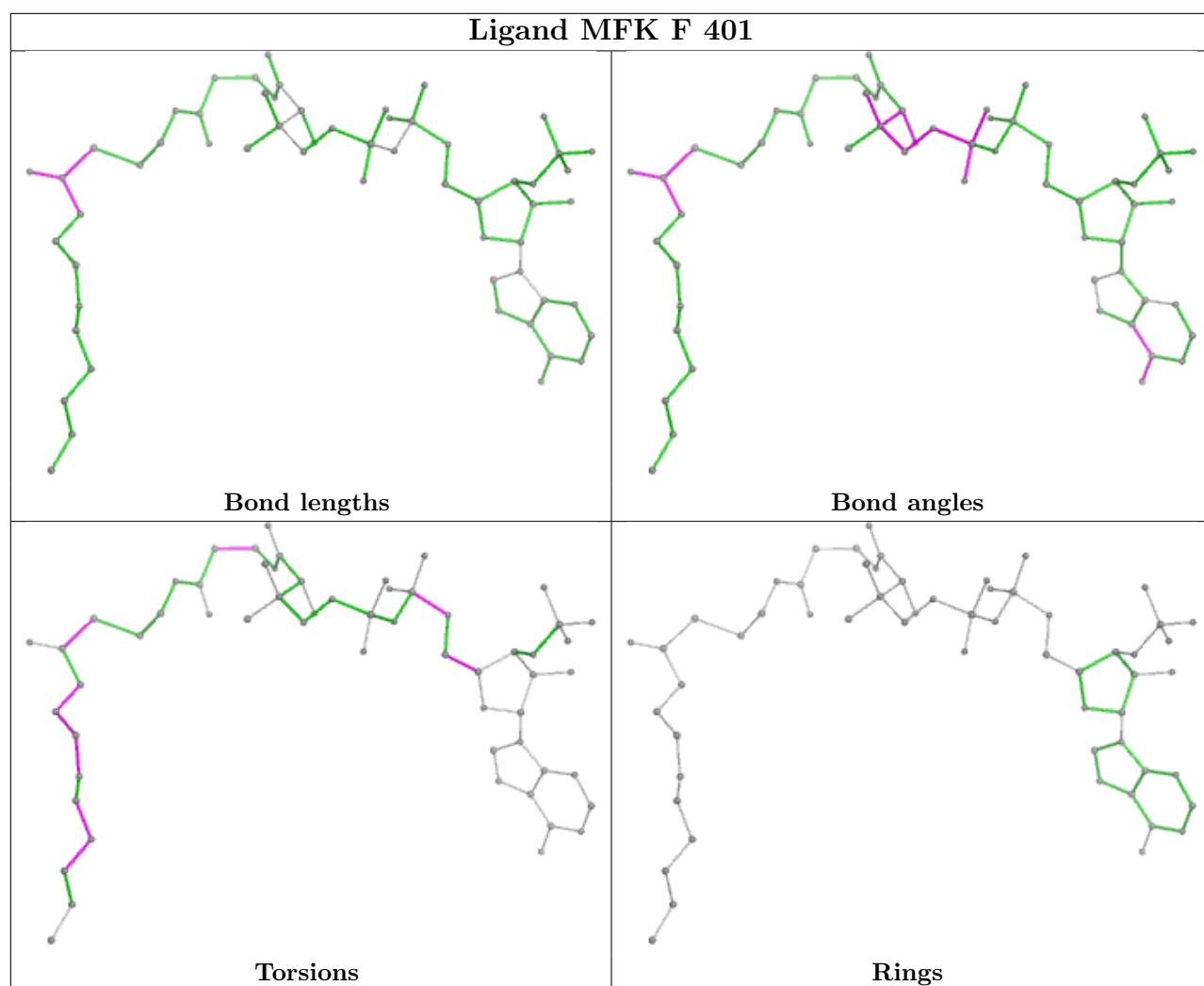


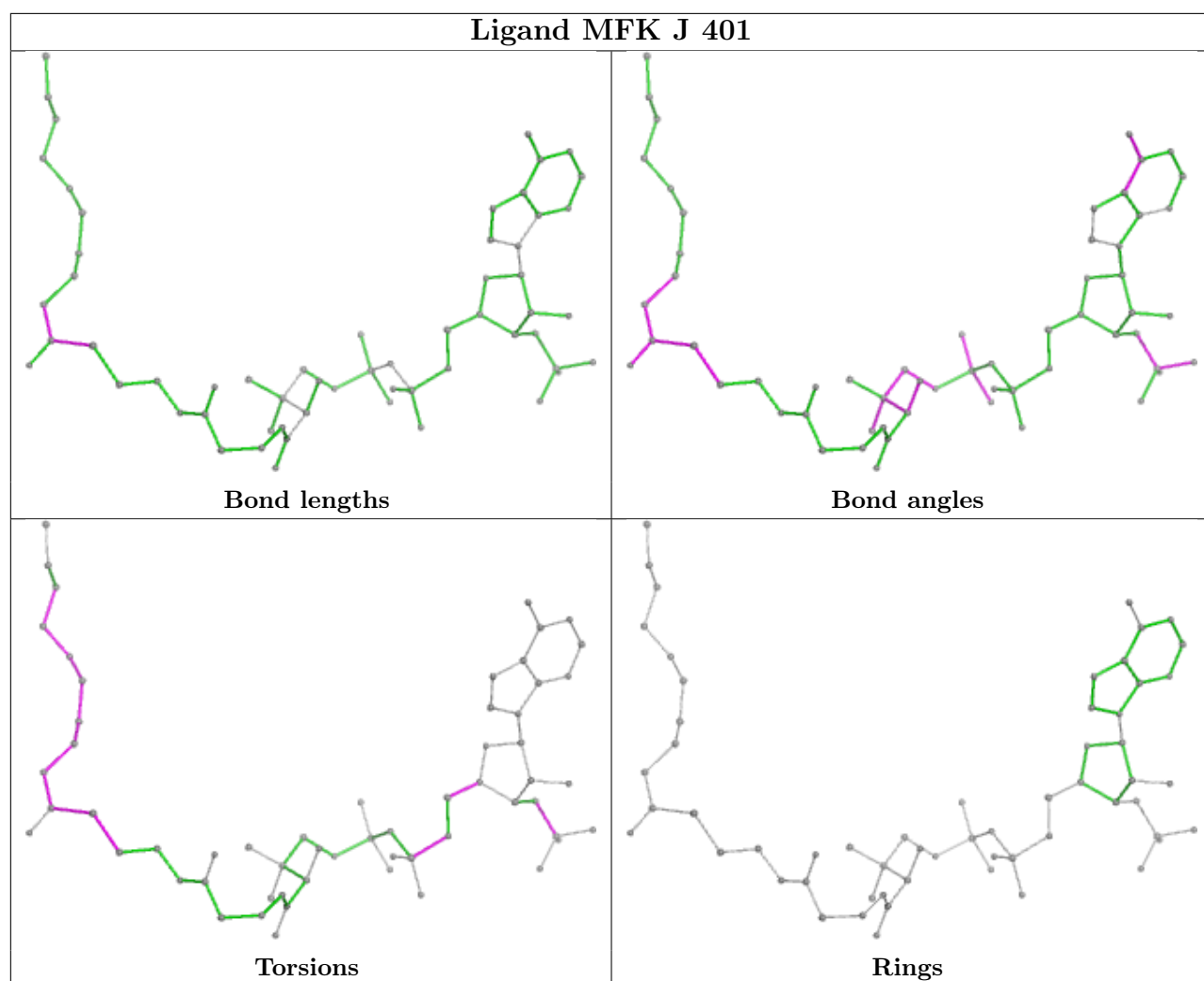
## Ligand MFK I 401

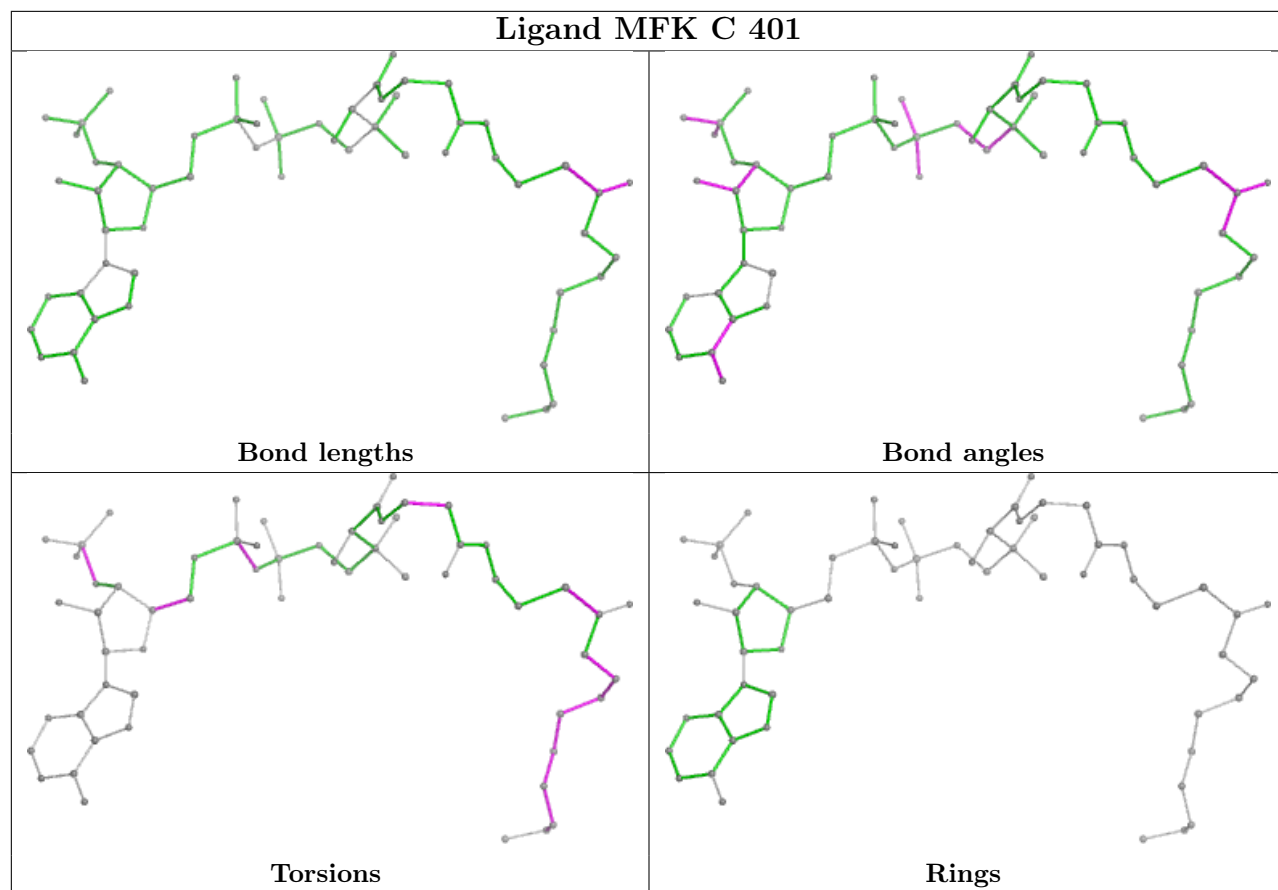


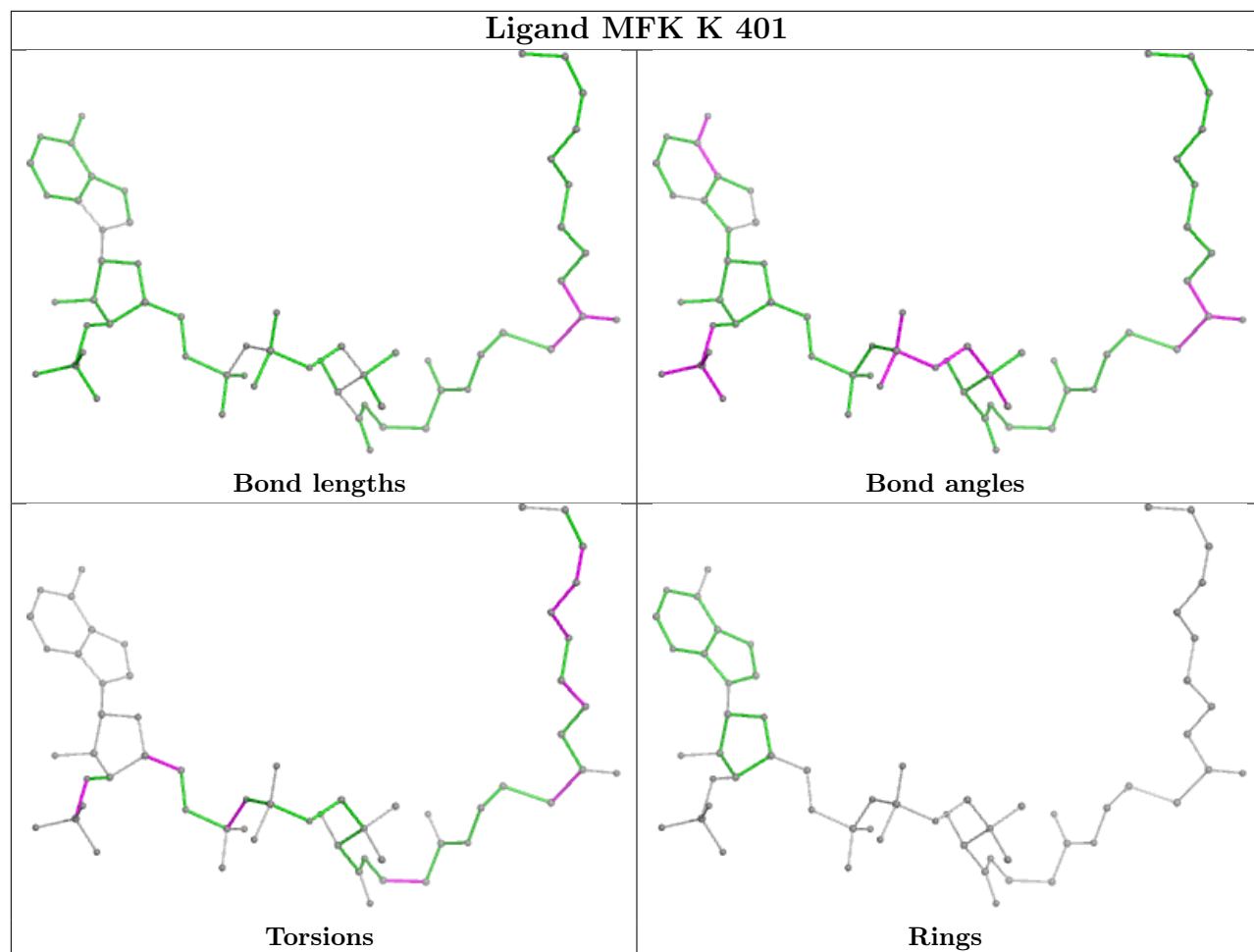
## Ligand MFK A 401

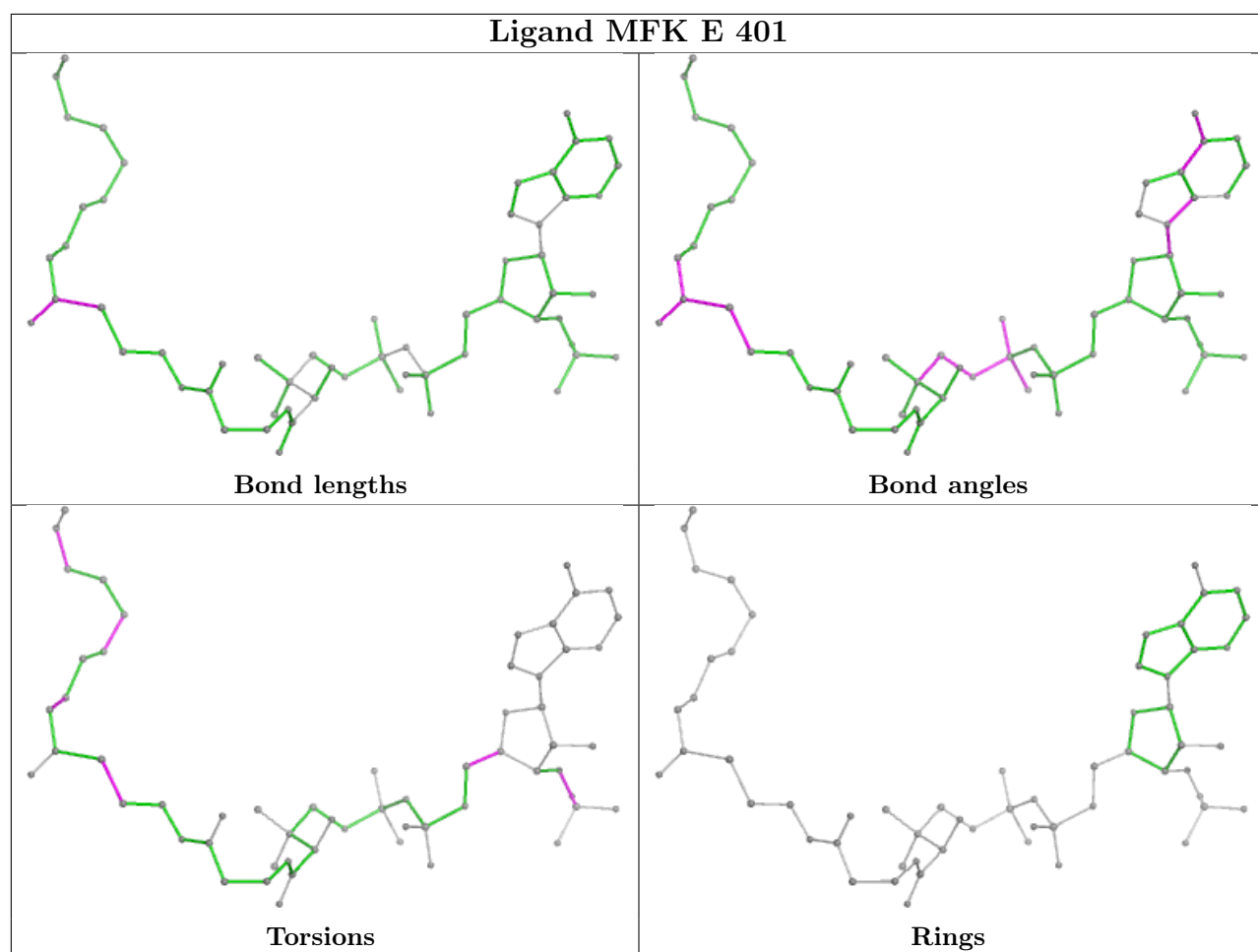


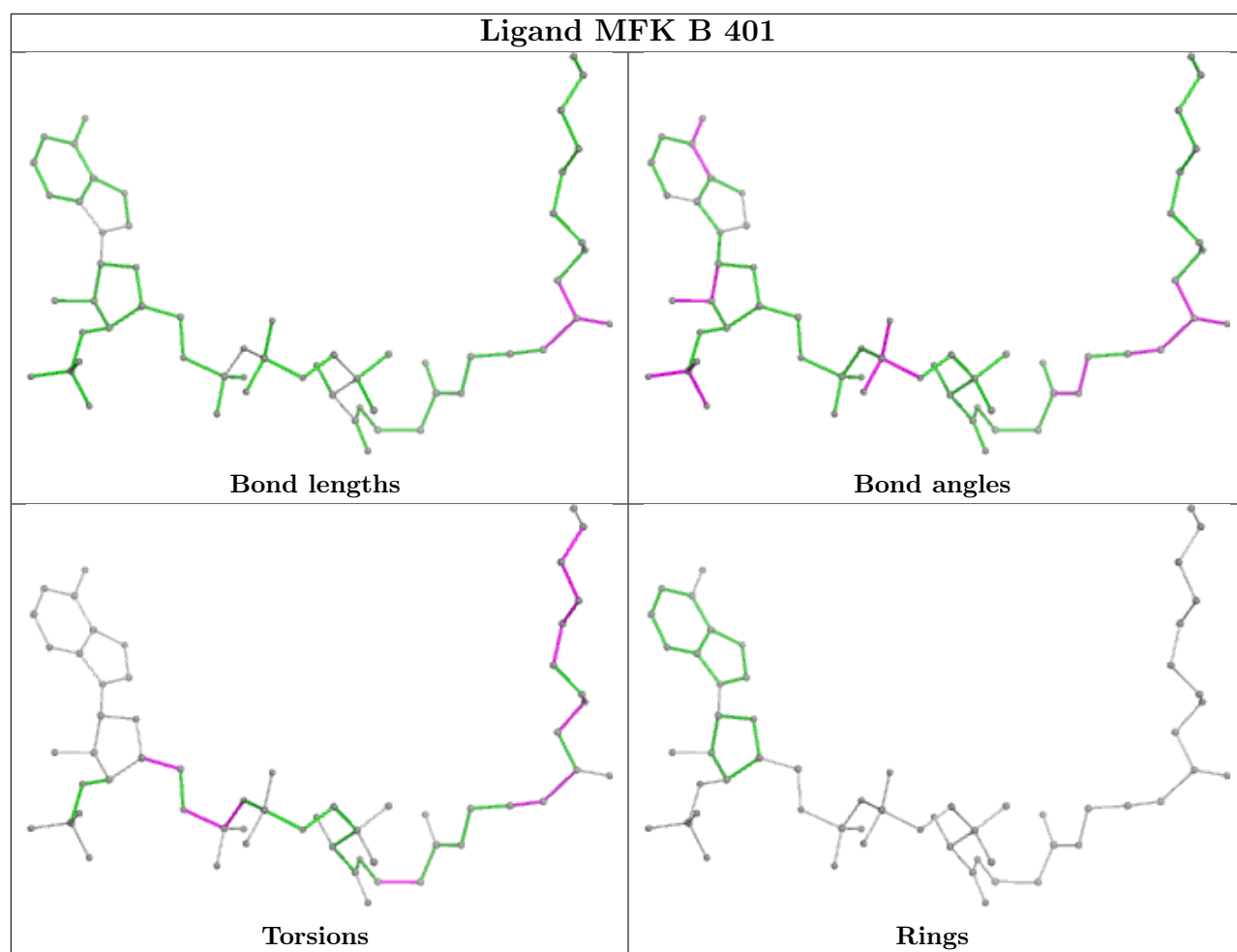


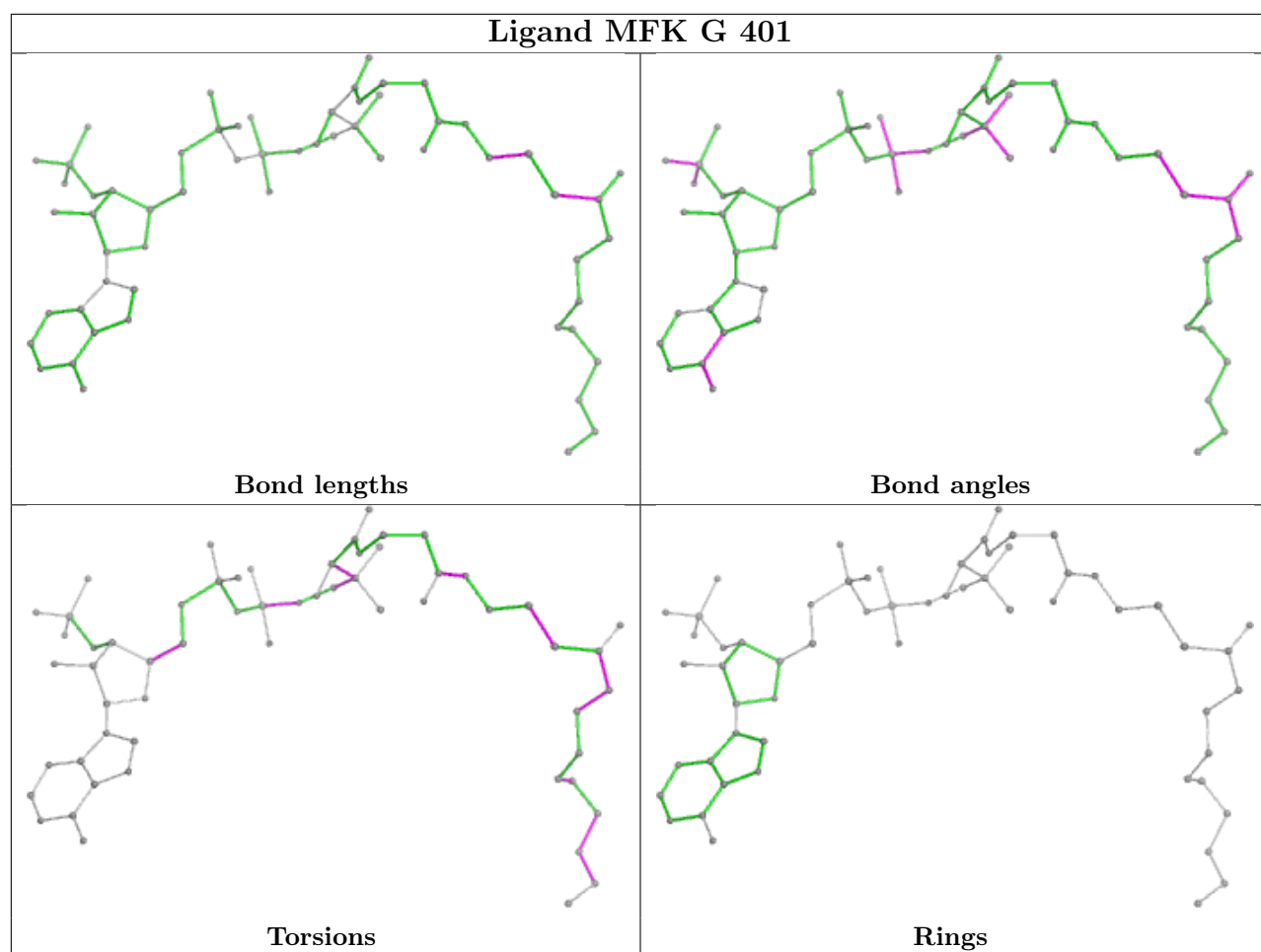


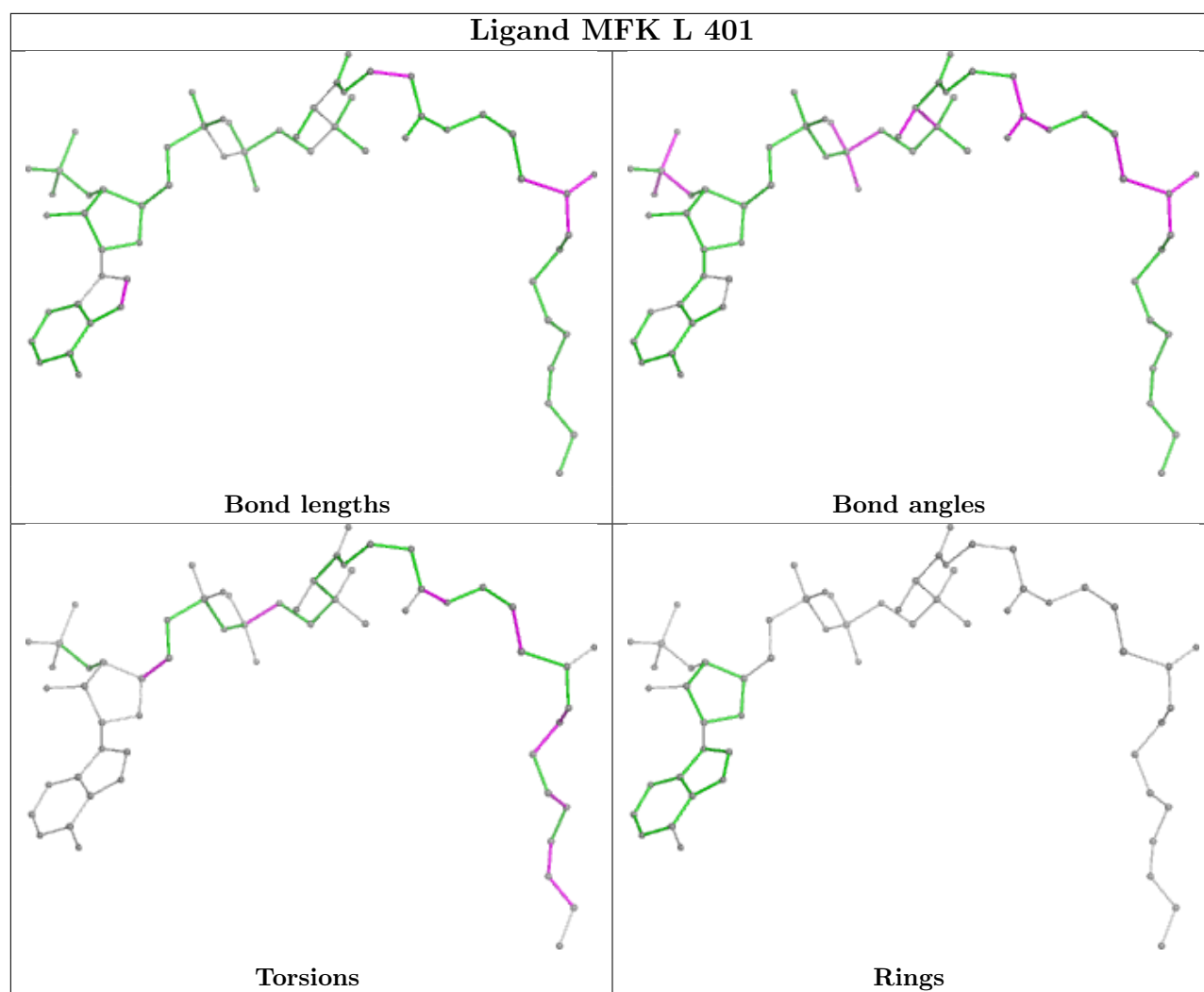


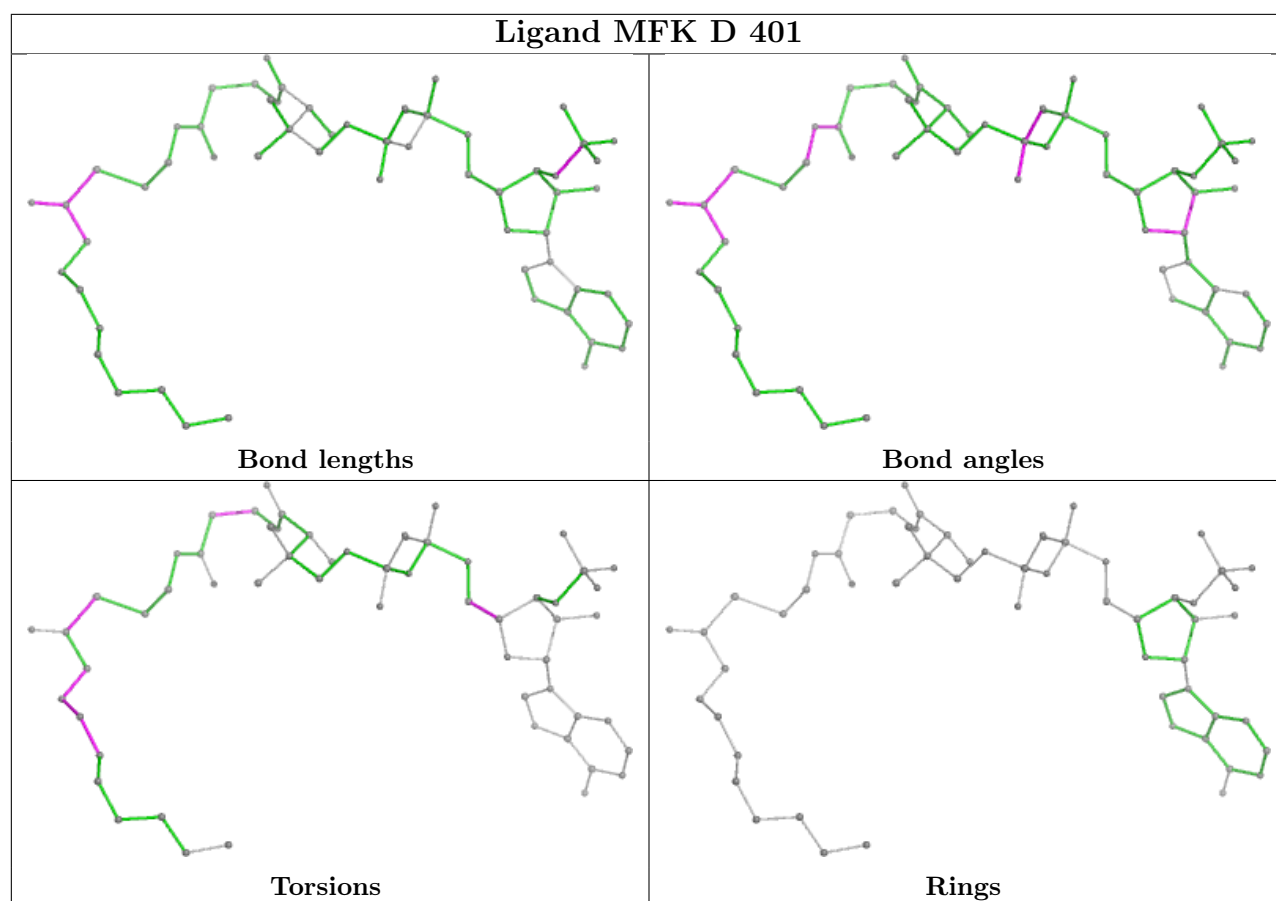












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	357/364 (98%)	0.46	31 (8%)	17 19	21, 35, 69, 106	2 (0%)
1	B	357/364 (98%)	0.53	41 (11%)	11 12	21, 36, 74, 111	1 (0%)
1	C	358/364 (98%)	0.71	72 (20%)	3 4	21, 35, 75, 113	2 (0%)
1	D	359/364 (98%)	0.37	24 (6%)	25 27	21, 34, 67, 110	1 (0%)
1	E	356/364 (97%)	0.46	38 (10%)	12 13	21, 35, 71, 103	2 (0%)
1	F	358/364 (98%)	0.64	55 (15%)	6 7	20, 37, 73, 105	1 (0%)
1	G	359/364 (98%)	0.71	63 (17%)	5 5	21, 38, 76, 124	2 (0%)
1	H	356/364 (97%)	0.48	39 (10%)	12 13	21, 36, 74, 110	1 (0%)
1	I	359/364 (98%)	0.20	16 (4%)	39 41	19, 33, 63, 99	2 (0%)
1	J	356/364 (97%)	0.41	39 (10%)	12 13	21, 34, 70, 104	1 (0%)
1	K	357/364 (98%)	0.67	65 (18%)	4 5	21, 34, 74, 102	2 (0%)
1	L	359/364 (98%)	0.30	26 (7%)	23 25	20, 34, 64, 106	1 (0%)
All	All	4291/4368 (98%)	0.49	509 (11%)	10 11	19, 35, 72, 124	18 (0%)

All (509) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	346	ALA	7.4
1	B	346	ALA	7.0
1	K	346	ALA	6.6
1	D	42	VAL	6.5
1	B	45	ILE	6.3
1	A	42	VAL	6.2
1	F	42	VAL	6.1
1	C	42	VAL	6.0
1	H	45	ILE	6.0
1	G	42	VAL	5.7
1	J	45	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	346	ALA	5.4
1	E	39	PRO	5.4
1	K	45	ILE	5.3
1	F	346	ALA	5.0
1	H	39	PRO	5.0
1	C	346	ALA	4.9
1	E	349	ILE	4.9
1	I	47	ARG	4.8
1	E	45	ILE	4.8
1	C	45	ILE	4.7
1	B	46	SER	4.7
1	D	45	ILE	4.7
1	C	93	GLY	4.7
1	F	292	ALA	4.6
1	K	345	PRO	4.5
1	K	176	GLN	4.5
1	L	323	ASN	4.5
1	E	345	PRO	4.4
1	H	323	ASN	4.4
1	J	346	ALA	4.4
1	H	47	ARG	4.4
1	F	41	SER	4.4
1	G	45	ILE	4.4
1	H	49	ALA	4.4
1	F	176	GLN	4.4
1	A	68	GLU	4.4
1	H	346	ALA	4.4
1	G	44	GLY	4.3
1	K	72	LYS	4.3
1	L	45	ILE	4.3
1	E	346	ALA	4.2
1	D	323	ASN	4.2
1	G	177	SER	4.2
1	K	47	ARG	4.2
1	A	324	GLY	4.2
1	L	41	SER	4.1
1	C	68	GLU	4.1
1	A	349	ILE	4.1
1	D	40	SER	4.0
1	E	351	ILE	4.0
1	K	349	ILE	4.0
1	C	176	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	69	LEU	4.0
1	K	44	GLY	4.0
1	C	47	ARG	3.9
1	G	43	ASP	3.9
1	I	42	VAL	3.9
1	A	40	SER	3.9
1	J	49	ALA	3.9
1	F	47	ARG	3.9
1	D	43	ASP	3.9
1	I	41	SER	3.9
1	K	75	ALA	3.9
1	H	349	ILE	3.9
1	A	43	ASP	3.9
1	K	73	LEU	3.9
1	A	177	SER	3.9
1	B	347	ALA	3.9
1	G	355	LEU	3.8
1	C	349	ILE	3.8
1	F	45	ILE	3.8
1	K	49	ALA	3.8
1	F	49	ALA	3.8
1	A	180	LYS	3.8
1	G	351	ILE	3.7
1	J	351	ILE	3.7
1	C	180	LYS	3.7
1	G	176	GLN	3.7
1	J	48	ASP	3.7
1	K	46	SER	3.7
1	G	61	LEU	3.7
1	K	324	GLY	3.6
1	C	324	GLY	3.6
1	A	346	ALA	3.6
1	H	207	MET	3.6
1	C	66	GLY	3.5
1	C	49	ALA	3.5
1	L	346	ALA	3.5
1	F	324	GLY	3.5
1	H	351	ILE	3.5
1	E	355	LEU	3.5
1	C	75	ALA	3.4
1	C	353	ALA	3.4
1	A	351	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	46	SER	3.4
1	B	44	GLY	3.4
1	H	48	ASP	3.4
1	B	47	ARG	3.4
1	G	47	ARG	3.4
1	B	351	ILE	3.4
1	G	349	ILE	3.4
1	K	348	THR	3.4
1	D	347	ALA	3.4
1	K	180	LYS	3.4
1	G	324	GLY	3.4
1	L	42	VAL	3.4
1	F	349	ILE	3.4
1	C	59	ALA	3.4
1	J	75	ALA	3.4
1	G	93	GLY	3.4
1	G	354	VAL	3.3
1	I	45	ILE	3.3
1	K	350	ASP	3.3
1	F	293	ASN	3.3
1	D	348	THR	3.3
1	F	92	LEU	3.3
1	G	94	LEU	3.3
1	G	59	ALA	3.3
1	G	75	ALA	3.3
1	J	144	ASP	3.3
1	K	66	GLY	3.3
1	L	44	GLY	3.3
1	K	69	LEU	3.3
1	C	70	ALA	3.3
1	C	48	ASP	3.3
1	B	345	PRO	3.2
1	C	347	ALA	3.2
1	G	62	LYS	3.2
1	G	101	LYS	3.2
1	H	352	GLU	3.2
1	K	347	ALA	3.2
1	G	178	SER	3.2
1	F	61	LEU	3.2
1	B	75	ALA	3.2
1	I	44	GLY	3.2
1	K	93	GLY	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	354	VAL	3.2
1	H	144	ASP	3.2
1	E	47	ARG	3.2
1	G	348	THR	3.1
1	C	44	GLY	3.1
1	F	180	LYS	3.1
1	D	351	ILE	3.1
1	F	39	PRO	3.1
1	K	323	ASN	3.1
1	C	348	THR	3.1
1	F	48	ASP	3.1
1	J	41	SER	3.1
1	H	72	LYS	3.1
1	F	207	MET	3.1
1	B	73	LEU	3.1
1	C	71	LEU	3.1
1	D	322	ALA	3.1
1	G	292	ALA	3.1
1	H	348	THR	3.1
1	J	47	ARG	3.1
1	C	76	LYS	3.1
1	K	39	PRO	3.0
1	E	324	GLY	3.0
1	G	100	ALA	3.0
1	F	43	ASP	3.0
1	E	40	SER	3.0
1	G	58	THR	3.0
1	K	102	VAL	3.0
1	L	324	GLY	3.0
1	K	355	LEU	3.0
1	G	347	ALA	3.0
1	K	74	ILE	3.0
1	L	351	ILE	3.0
1	B	359	ASP	3.0
1	J	46	SER	3.0
1	A	58	THR	3.0
1	F	93	GLY	3.0
1	G	92	LEU	3.0
1	C	351	ILE	3.0
1	K	64	ASP	3.0
1	L	40	SER	3.0
1	A	348	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	354	VAL	3.0
1	H	176	GLN	3.0
1	L	47	ARG	3.0
1	G	353	ALA	3.0
1	I	43	ASP	2.9
1	D	44	GLY	2.9
1	J	69	LEU	2.9
1	E	352	GLU	2.9
1	C	177	SER	2.9
1	F	345	PRO	2.9
1	A	69	LEU	2.9
1	B	49	ALA	2.9
1	E	144	ASP	2.9
1	F	351	ILE	2.9
1	L	46	SER	2.9
1	B	65	GLN	2.9
1	G	293	ASN	2.9
1	J	345	PRO	2.8
1	C	40	SER	2.8
1	K	63	SER	2.8
1	B	323	ASN	2.8
1	J	323	ASN	2.8
1	K	351	ILE	2.8
1	F	352	GLU	2.8
1	J	61	LEU	2.8
1	C	354	VAL	2.8
1	G	49	ALA	2.8
1	A	47	ARG	2.8
1	B	62	LYS	2.8
1	J	349	ILE	2.8
1	J	324	GLY	2.8
1	C	39	PRO	2.8
1	B	358	TRP	2.8
1	F	355	LEU	2.8
1	F	358	TRP	2.8
1	H	358	TRP	2.8
1	C	79	VAL	2.8
1	K	101	LYS	2.8
1	B	66	GLY	2.8
1	B	350	ASP	2.8
1	C	80	LEU	2.8
1	C	173	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	46	SER	2.8
1	G	207	MET	2.7
1	B	39	PRO	2.7
1	G	345	PRO	2.7
1	J	350	ASP	2.7
1	G	68	GLU	2.7
1	J	73	LEU	2.7
1	D	41	SER	2.7
1	I	323	ASN	2.7
1	J	347	ALA	2.7
1	L	75	ALA	2.7
1	L	173	TRP	2.7
1	I	324	GLY	2.7
1	F	58	THR	2.7
1	L	349	ILE	2.7
1	F	68	GLU	2.7
1	F	46	SER	2.7
1	K	178	SER	2.7
1	C	10	VAL	2.7
1	H	353	ALA	2.7
1	C	107	ILE	2.7
1	G	144	ASP	2.7
1	G	359	ASP	2.7
1	L	43	ASP	2.7
1	C	345	PRO	2.7
1	J	39	PRO	2.7
1	B	352	GLU	2.7
1	K	62	LYS	2.7
1	F	323	ASN	2.7
1	J	355	LEU	2.7
1	A	345	PRO	2.6
1	D	180	LYS	2.6
1	F	62	LYS	2.6
1	F	69	LEU	2.6
1	C	102	VAL	2.6
1	D	49	ALA	2.6
1	J	100	ALA	2.6
1	J	353	ALA	2.6
1	K	65	GLN	2.6
1	D	258	GLU	2.6
1	D	48	ASP	2.6
1	C	41	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	41	SER	2.6
1	B	355	LEU	2.6
1	J	94	LEU	2.6
1	B	322	ALA	2.6
1	C	108	TYR	2.6
1	C	33	VAL	2.6
1	E	66	GLY	2.6
1	F	70	ALA	2.6
1	G	322	ALA	2.6
1	K	10	VAL	2.6
1	E	68	GLU	2.6
1	E	97	GLU	2.6
1	F	144	ASP	2.6
1	A	173	TRP	2.6
1	C	74	ILE	2.6
1	K	36	ILE	2.6
1	F	1	MET	2.6
1	C	63	SER	2.6
1	E	176	GLN	2.6
1	C	61	LEU	2.6
1	J	92	LEU	2.6
1	K	71	LEU	2.6
1	K	80	LEU	2.6
1	B	357	ASP	2.6
1	C	96	PRO	2.6
1	C	323	ASN	2.6
1	A	92	LEU	2.6
1	F	97	GLU	2.6
1	G	69	LEU	2.6
1	H	355	LEU	2.6
1	J	352	GLU	2.6
1	D	324	GLY	2.5
1	F	75	ALA	2.5
1	F	347	ALA	2.5
1	H	359	ASP	2.5
1	K	58	THR	2.5
1	A	207	MET	2.5
1	G	1	MET	2.5
1	B	176	GLN	2.5
1	K	56	ILE	2.5
1	G	41	SER	2.5
1	D	358	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	358	TRP	2.5
1	C	67	LEU	2.5
1	J	72	LYS	2.5
1	K	99	CYS	2.5
1	C	350	ASP	2.5
1	J	359	ASP	2.5
1	K	144	ASP	2.5
1	C	34	VAL	2.5
1	K	1	MET	2.5
1	E	348	THR	2.5
1	J	348	THR	2.5
1	C	91	ARG	2.5
1	F	65	GLN	2.5
1	J	176	GLN	2.5
1	E	62	LYS	2.5
1	E	322	ALA	2.5
1	K	322	ALA	2.5
1	B	356	THR	2.5
1	H	58	THR	2.5
1	J	65	GLN	2.5
1	F	101	LYS	2.5
1	C	355	LEU	2.5
1	B	173	TRP	2.5
1	D	173	TRP	2.5
1	K	359	ASP	2.5
1	B	257	ALA	2.5
1	F	59	ALA	2.5
1	H	2	ALA	2.5
1	C	58	THR	2.5
1	C	183	VAL	2.5
1	G	79	VAL	2.5
1	G	180	LYS	2.4
1	K	76	LYS	2.4
1	K	181	GLY	2.4
1	C	51	LEU	2.4
1	C	106	LEU	2.4
1	G	48	ASP	2.4
1	G	350	ASP	2.4
1	I	144	ASP	2.4
1	G	173	TRP	2.4
1	F	356	THR	2.4
1	B	72	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	1	MET	2.4
1	F	87	GLY	2.4
1	J	93	GLY	2.4
1	I	359	ASP	2.4
1	B	5	LEU	2.4
1	H	92	LEU	2.4
1	E	258	GLU	2.4
1	G	70	ALA	2.4
1	I	346	ALA	2.4
1	B	180	LYS	2.4
1	C	87	GLY	2.4
1	G	352	GLU	2.4
1	C	358	TRP	2.4
1	H	345	PRO	2.4
1	H	46	SER	2.4
1	A	359	ASP	2.4
1	D	350	ASP	2.4
1	F	359	ASP	2.4
1	I	176	GLN	2.4
1	I	349	ILE	2.4
1	J	56	ILE	2.4
1	G	97	GLU	2.3
1	C	73	LEU	2.3
1	G	356	THR	2.3
1	C	11	VAL	2.3
1	D	207	MET	2.3
1	E	10	VAL	2.3
1	F	34	VAL	2.3
1	G	102	VAL	2.3
1	K	183	VAL	2.3
1	K	173	TRP	2.3
1	K	48	ASP	2.3
1	H	61	LEU	2.3
1	A	322	ALA	2.3
1	K	100	ALA	2.3
1	L	1	MET	2.3
1	A	41	SER	2.3
1	E	41	SER	2.3
1	L	177	SER	2.3
1	C	65	GLN	2.3
1	F	79	VAL	2.3
1	K	79	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	358	TRP	2.3
1	H	324	GLY	2.3
1	A	76	LYS	2.3
1	C	101	LYS	2.3
1	G	323	ASN	2.3
1	K	94	LEU	2.3
1	C	105	ARG	2.3
1	G	57	VAL	2.3
1	G	88	VAL	2.3
1	C	104	ASP	2.3
1	D	357	ASP	2.3
1	H	68	GLU	2.3
1	K	104	ASP	2.3
1	K	358	TRP	2.3
1	C	72	LYS	2.3
1	F	76	LYS	2.3
1	J	62	LYS	2.3
1	D	47	ARG	2.3
1	E	38	ARG	2.3
1	K	38	ARG	2.3
1	G	71	LEU	2.3
1	G	46	SER	2.3
1	J	37	ASP	2.2
1	K	60	ASP	2.2
1	C	57	VAL	2.2
1	F	11	VAL	2.2
1	J	102	VAL	2.2
1	K	11	VAL	2.2
1	G	76	LYS	2.2
1	F	173	TRP	2.2
1	I	351	ILE	2.2
1	E	69	LEU	2.2
1	E	207	MET	2.2
1	H	322	ALA	2.2
1	K	353	ALA	2.2
1	B	76	LYS	2.2
1	B	349	ILE	2.2
1	B	68	GLU	2.2
1	C	77	ALA	2.2
1	A	350	ASP	2.2
1	B	144	ASP	2.2
1	C	144	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	357	ASP	2.2
1	H	38	ARG	2.2
1	F	88	VAL	2.2
1	H	34	VAL	2.2
1	B	1	MET	2.2
1	A	355	LEU	2.2
1	B	40	SER	2.2
1	B	70	ALA	2.2
1	C	178	SER	2.2
1	F	353	ALA	2.2
1	H	41	SER	2.2
1	C	62	LYS	2.2
1	E	48	ASP	2.2
1	H	350	ASP	2.2
1	L	144	ASP	2.2
1	C	30	GLY	2.2
1	D	1	MET	2.2
1	H	315	GLU	2.1
1	E	73	LEU	2.1
1	K	67	LEU	2.1
1	A	178	SER	2.1
1	H	62	LYS	2.1
1	A	75	ALA	2.1
1	E	49	ALA	2.1
1	K	70	ALA	2.1
1	K	108	TYR	2.1
1	C	99	CYS	2.1
1	F	33	VAL	2.1
1	A	72	LYS	2.1
1	C	92	LEU	2.1
1	F	73	LEU	2.1
1	F	94	LEU	2.1
1	G	73	LEU	2.1
1	B	41	SER	2.1
1	B	105	ARG	2.1
1	F	348	THR	2.1
1	E	75	ALA	2.1
1	E	347	ALA	2.1
1	H	59	ALA	2.1
1	G	10	VAL	2.1
1	G	72	LYS	2.1
1	A	64	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	71	LEU	2.1
1	C	56	ILE	2.1
1	C	357	ASP	2.1
1	G	357	ASP	2.1
1	K	61	LEU	2.1
1	E	178	SER	2.1
1	L	350	ASP	2.1
1	L	357	ASP	2.1
1	A	323	ASN	2.1
1	E	65	GLN	2.1
1	H	65	GLN	2.1
1	I	1	MET	2.1
1	F	183	VAL	2.1
1	H	354	VAL	2.1
1	E	76	LYS	2.1
1	B	48	ASP	2.1
1	H	64	ASP	2.1
1	J	71	LEU	2.1
1	L	6	SER	2.1
1	G	36	ILE	2.1
1	L	356	THR	2.1
1	L	176	GLN	2.1
1	G	96	PRO	2.0
1	K	97	GLU	2.0
1	J	97	GLU	2.0
1	E	2	ALA	2.0
1	L	322	ALA	2.0
1	I	326	TRP	2.0
1	J	11	VAL	2.0
1	K	34	VAL	2.0
1	C	37	ASP	2.0
1	E	359	ASP	2.0
1	G	64	ASP	2.0
1	L	359	ASP	2.0
1	E	50	MET	2.0
1	L	207	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

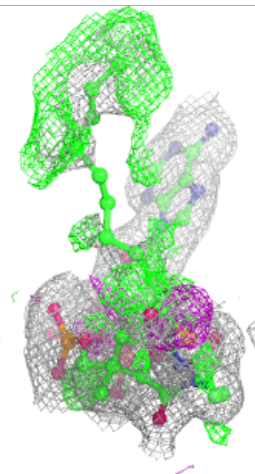
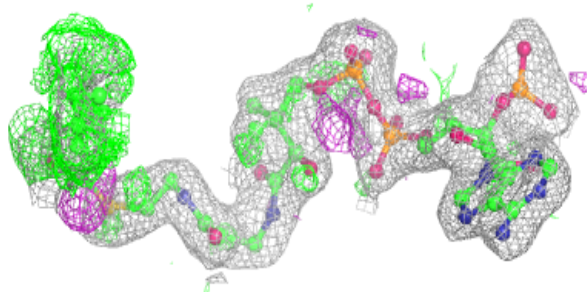
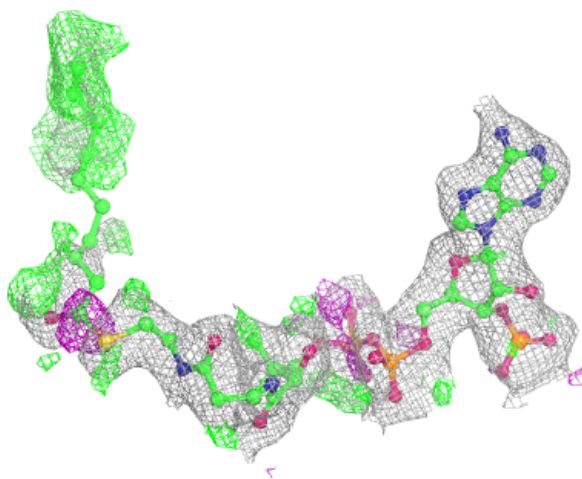
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MFK	H	401	59/59	0.90	0.17	32,46,106,117	0
2	MFK	J	401	59/59	0.91	0.16	26,44,86,94	0
2	MFK	E	401	59/59	0.92	0.16	28,45,113,115	0
2	MFK	F	401	59/59	0.93	0.14	24,44,97,102	0
2	MFK	G	401	59/59	0.93	0.14	25,41,88,94	0
2	MFK	C	401	59/59	0.93	0.14	27,44,83,90	0
2	MFK	A	401	59/59	0.93	0.14	26,41,89,96	0
2	MFK	K	401	59/59	0.93	0.14	25,45,91,100	0
2	MFK	B	401	59/59	0.94	0.14	25,45,88,95	0
2	MFK	L	401	59/59	0.94	0.14	21,31,96,98	0
2	MFK	I	401	59/59	0.96	0.11	22,32,88,96	0
2	MFK	D	401	59/59	0.96	0.11	21,32,90,96	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.

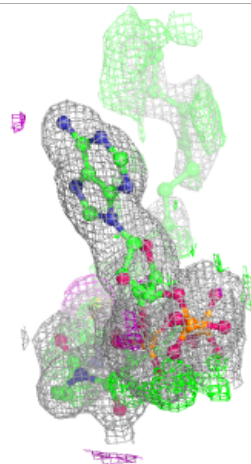
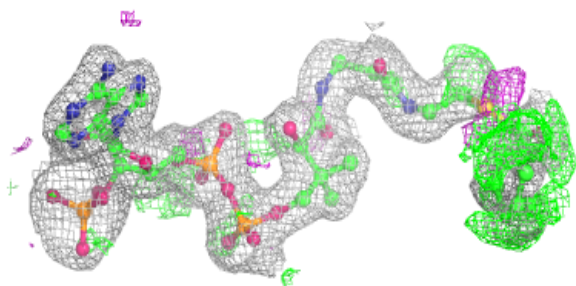
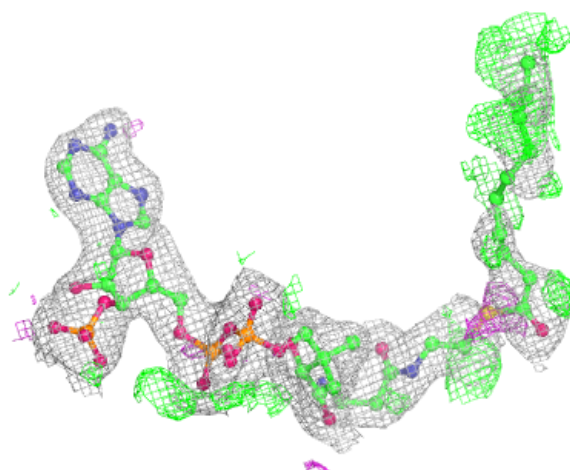
**Electron density around MFK H 401:**

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



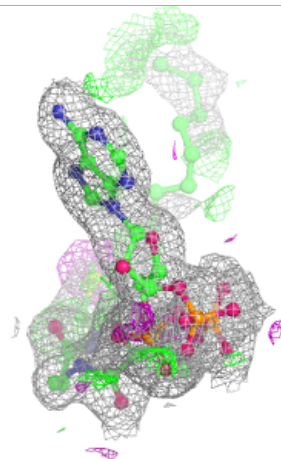
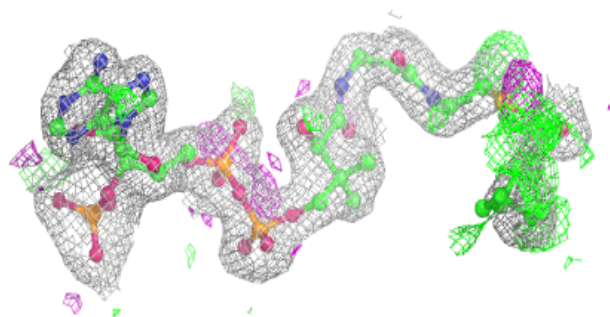
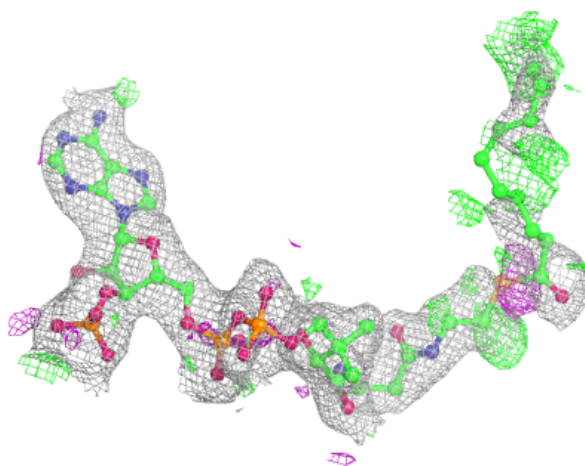
**Electron density around MFK J 401:**

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



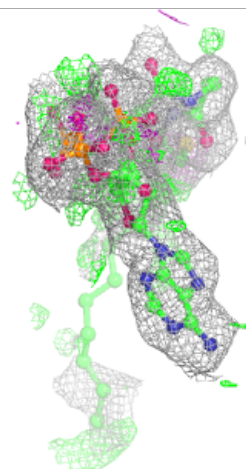
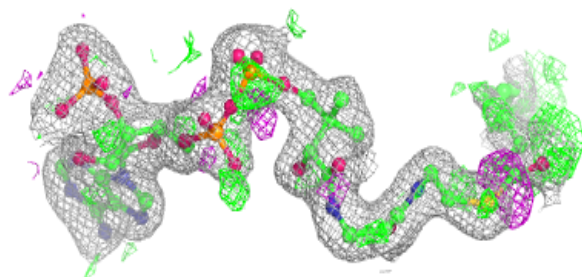
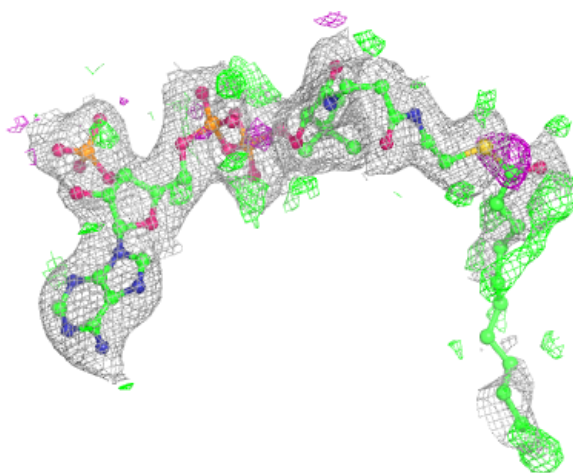
**Electron density around MFK E 401:**

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



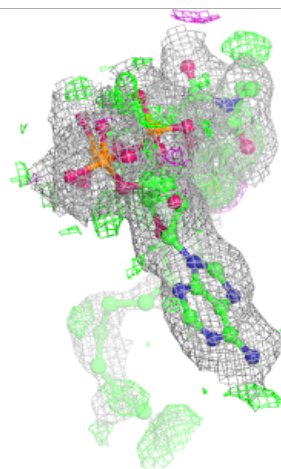
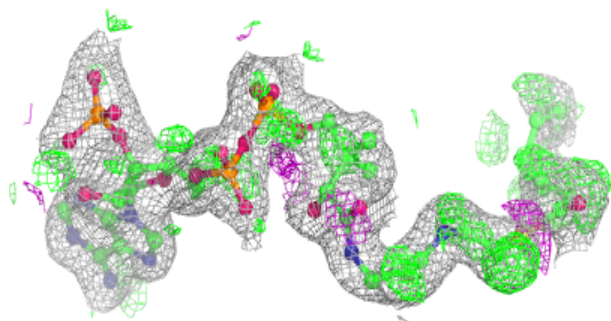
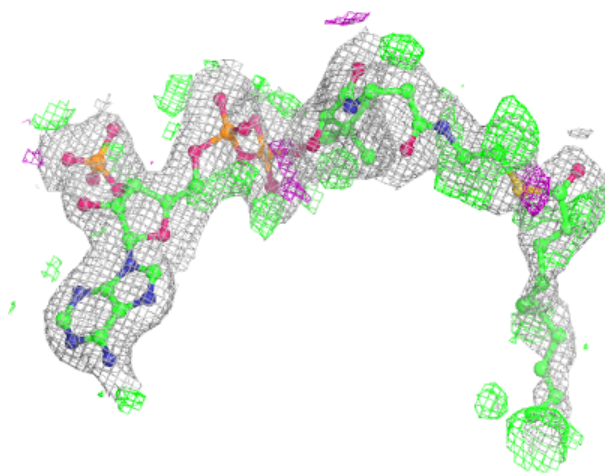
**Electron density around MFK F 401:**

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



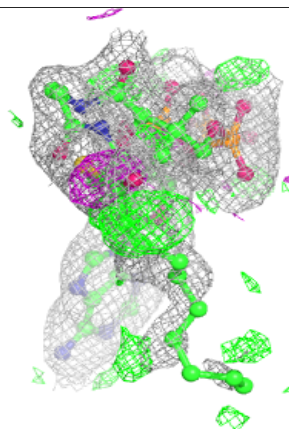
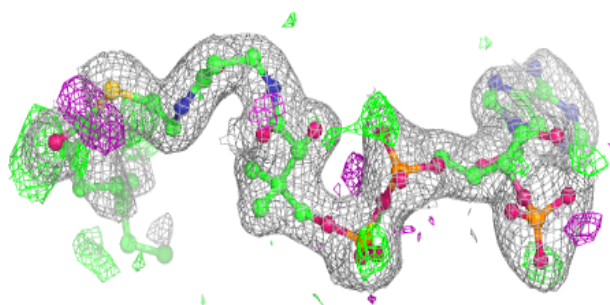
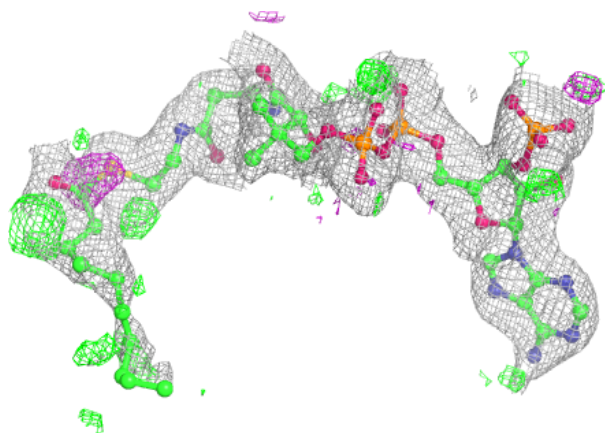
**Electron density around MFK G 401:**

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



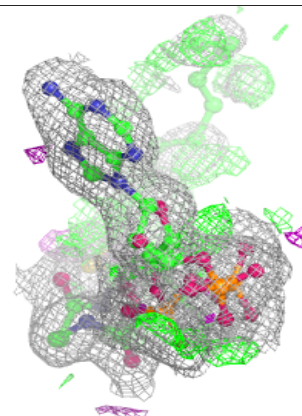
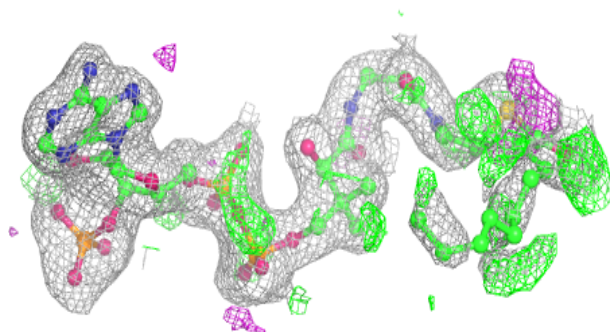
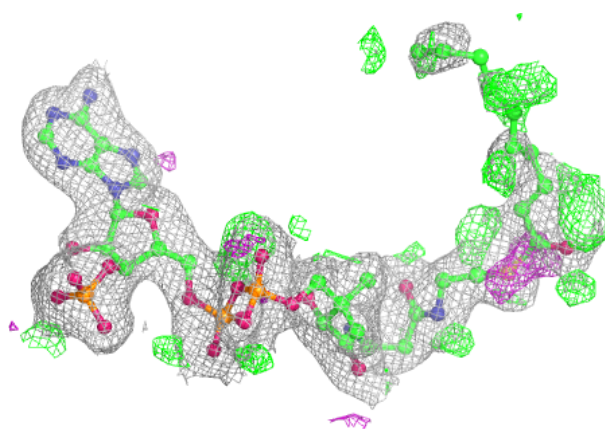
**Electron density around MFK C 401:**

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



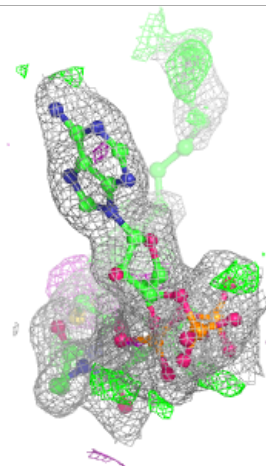
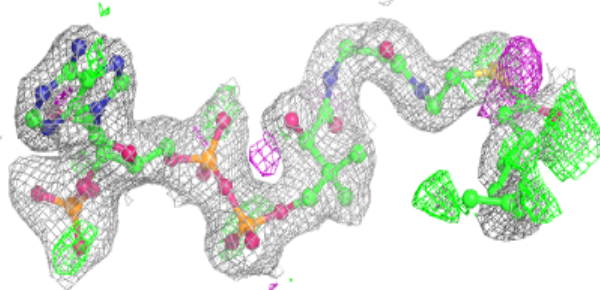
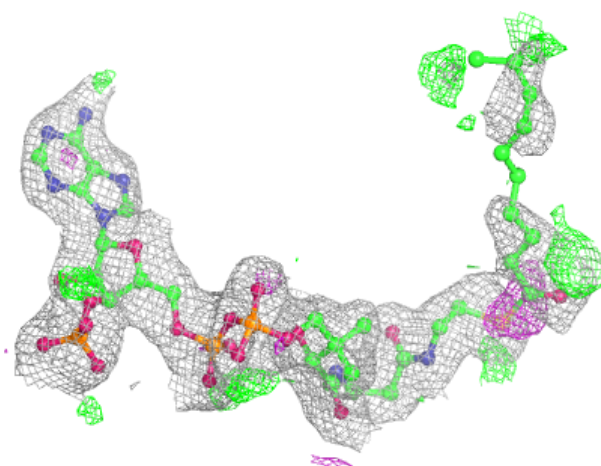
**Electron density around MFK A 401:**

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



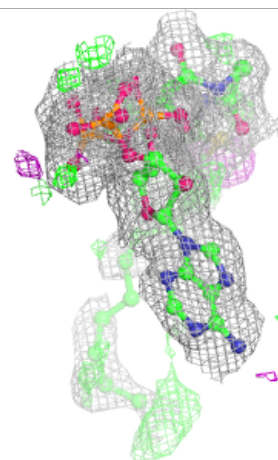
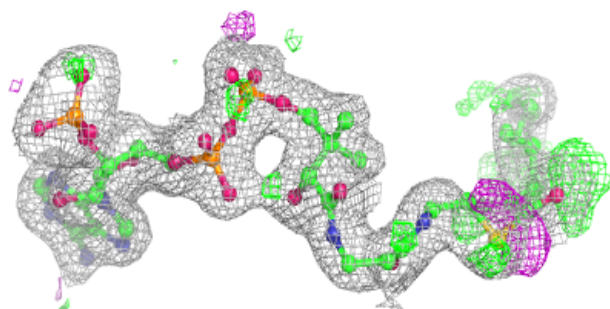
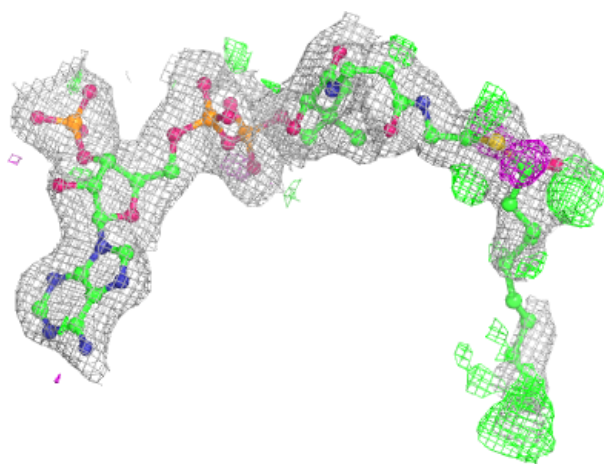
**Electron density around MFK K 401:**

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



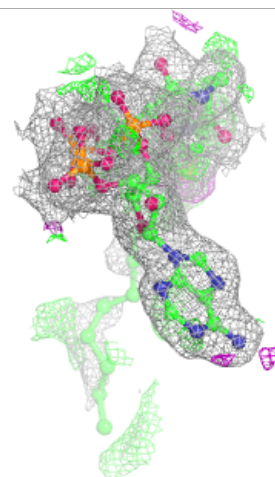
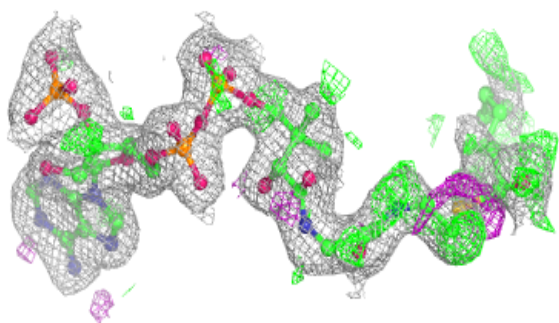
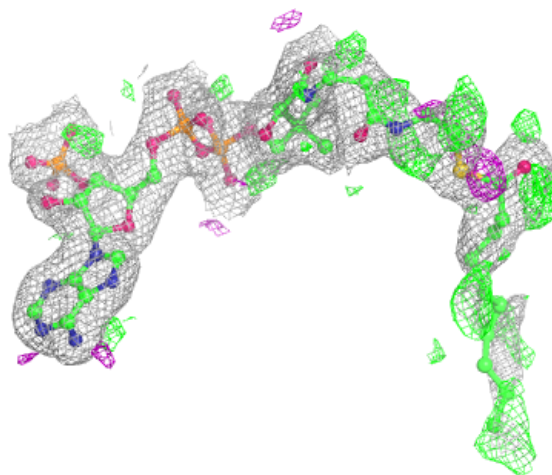
**Electron density around MFK B 401:**

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



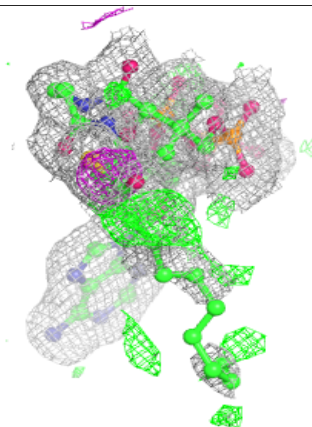
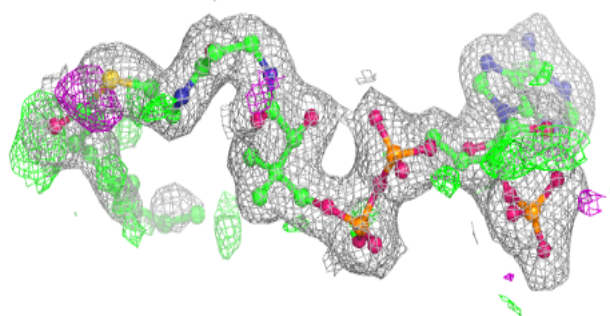
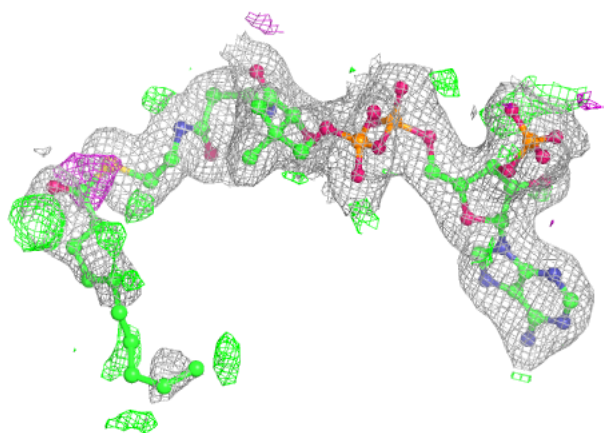
**Electron density around MFK L 401:**

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



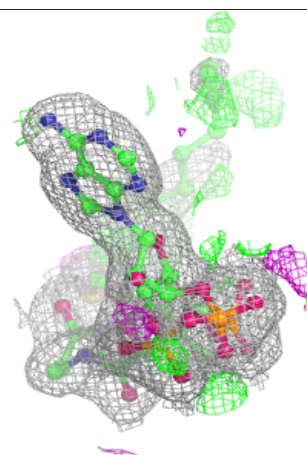
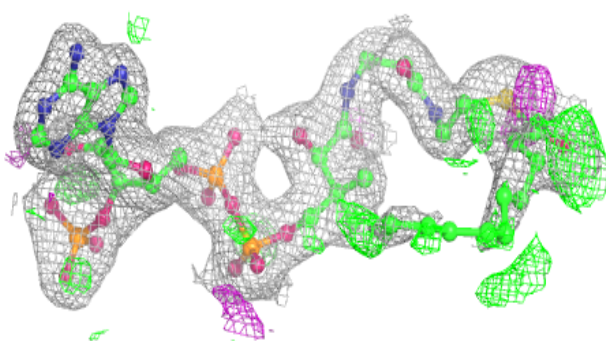
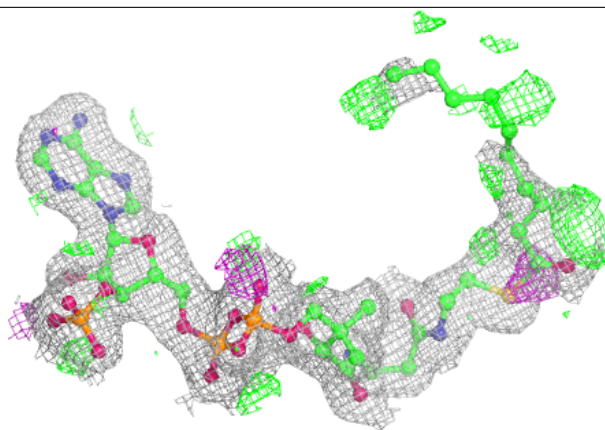
**Electron density around MFK I 401:**

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



**Electron density around MFK D 401:**

$2mF_o-DF_c$  (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.