



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 07:52 pm BST

PDB ID : 9I2V / pdb\_00009i2v  
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with fenoprofenoyl-CoA  
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.  
Deposited on : 2025-01-22  
Resolution : 2.07 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

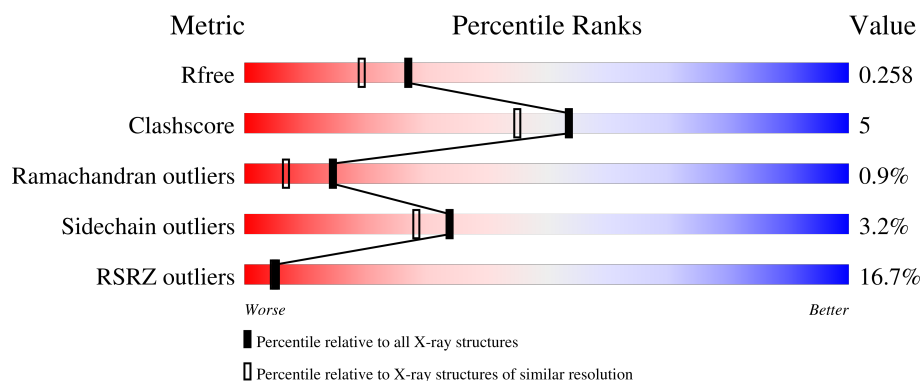
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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>17%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	364	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	364	<div> <div>19%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	364	<div> <div>16%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>...</div> </div> </div>
1	E	364	<div> <div>22%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	364	<div><div></div><div>23%79%16%<div><div></div><div></div><div></div></div></div></div>
1	G	364	<div><div></div><div>27%77%19%<div><div></div><div></div><div></div></div></div></div>
1	H	364	<div><div></div><div>20%84%12%<div><div></div><div></div><div></div></div></div></div>
1	I	364	<div><div></div><div>9%89%9%<div><div></div><div></div><div></div></div></div></div>
1	J	364	<div><div></div><div>7%88%10%<div><div></div><div></div><div></div></div></div></div>
1	K	364	<div><div></div><div>14%85%10%<div><div></div><div></div><div></div></div></div></div>
1	L	364	<div><div></div><div>15%85%12%<div><div></div><div></div><div></div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34666 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	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	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	3	0
			2705	1697	484	508	16			
1	F	357	Total	C	N	O	S	0	1	0
			2703	1695	484	508	16			
1	G	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	H	356	Total	C	N	O	S	0	1	0
			2694	1691	483	504	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	357	Total	C	N	O	S	0	1	0
			2700	1694	484	506	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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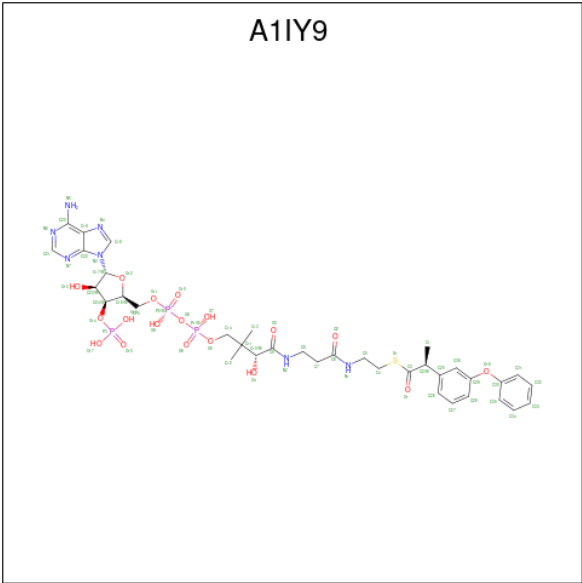
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	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 (S)-Fenoprofenoyl-CoA (CCD ID: A1IY9) (formula: C<sub>36</sub>H<sub>48</sub>N<sub>7</sub>O<sub>18</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
			65	36	7	18	3	1			
2	B	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	C	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	D	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	E	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	F	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	G	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	H	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	I	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			
2	J	1	Total	C	N	O	P	S		0	0
			65	36	7	18	3	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			65	36	7	18	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			65	36	7	18	3	1		

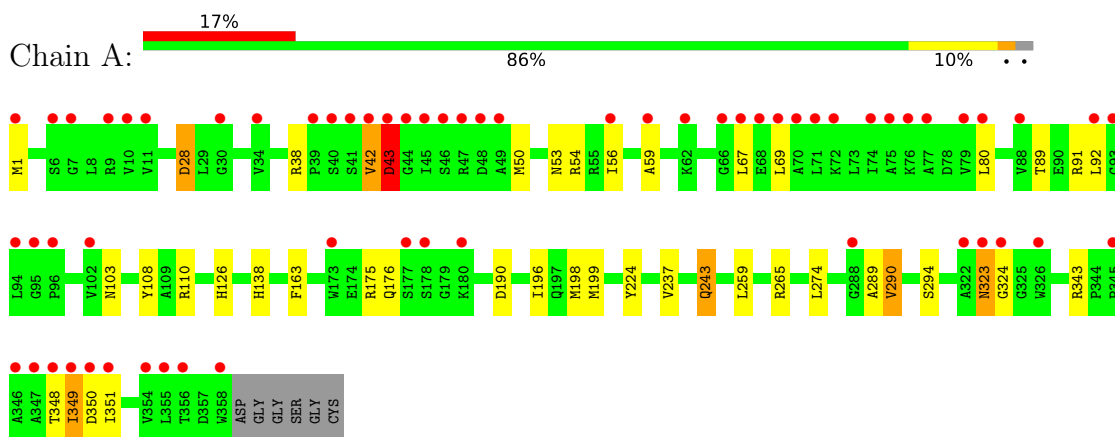
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	115	Total	O	0	0
			115	115		
3	C	128	Total	O	0	0
			128	128		
3	D	120	Total	O	0	0
			120	120		
3	E	112	Total	O	0	0
			112	112		
3	F	102	Total	O	0	0
			102	102		
3	G	104	Total	O	0	0
			104	104		
3	H	108	Total	O	0	0
			108	108		
3	I	127	Total	O	0	0
			127	127		
3	J	127	Total	O	0	0
			127	127		
3	K	121	Total	O	0	0
			121	121		
3	L	119	Total	O	0	0
			119	119		

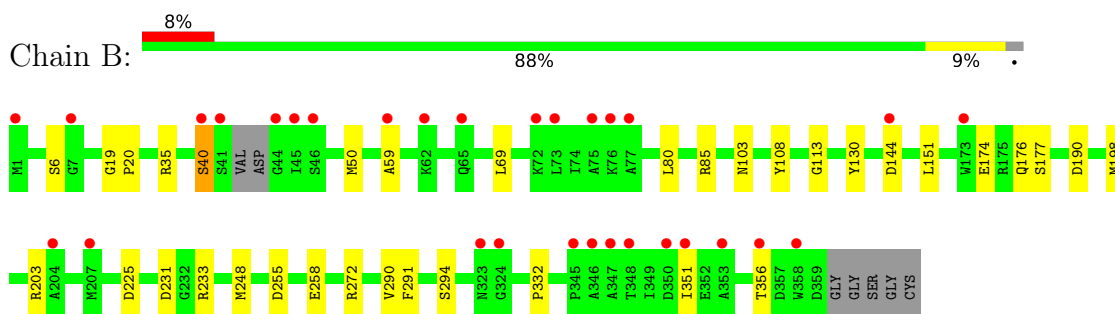
### 3 Residue-property plots

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

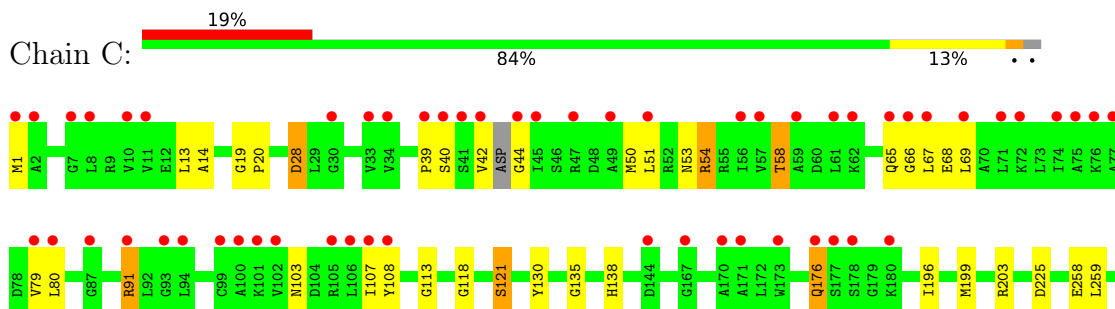
#### • Molecule 1: Alpha-methylacyl-CoA racemase



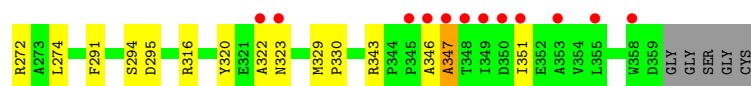
#### • Molecule 1: Alpha-methylacyl-CoA racemase



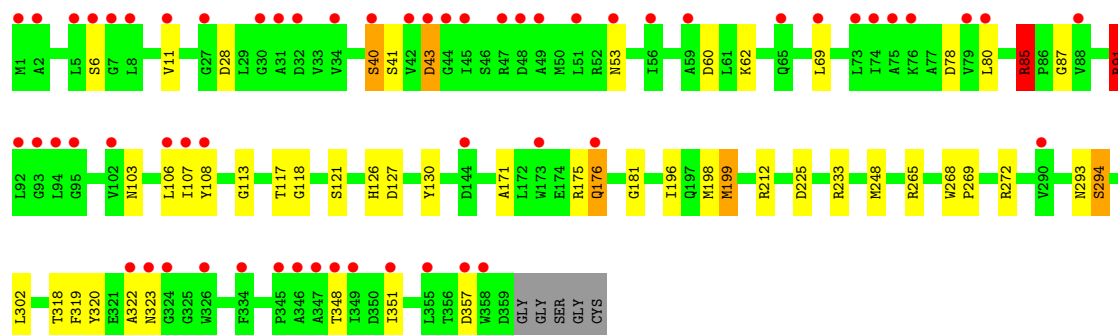
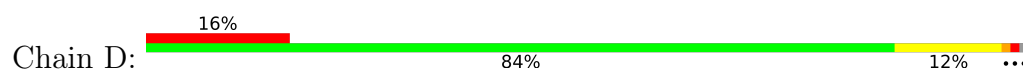
#### • Molecule 1: Alpha-methylacyl-CoA racemase



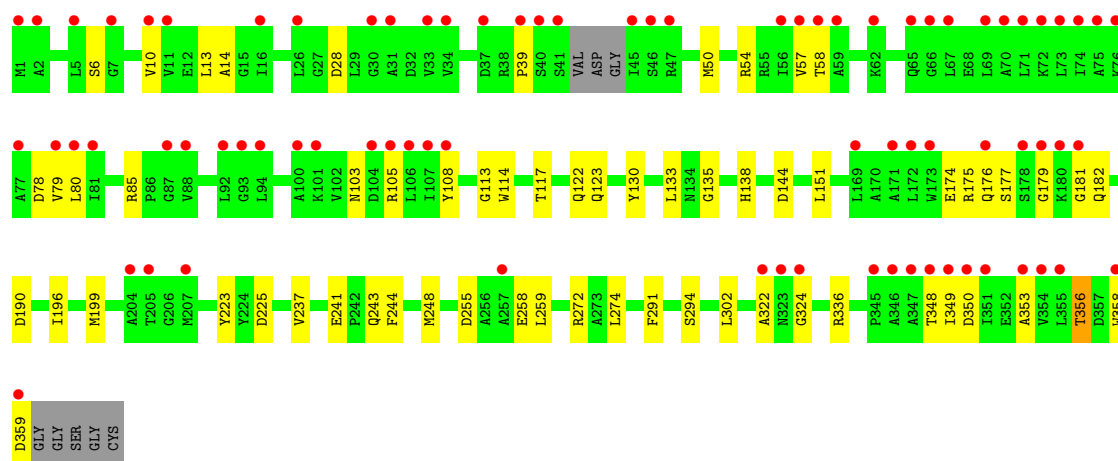
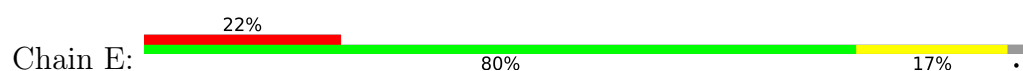




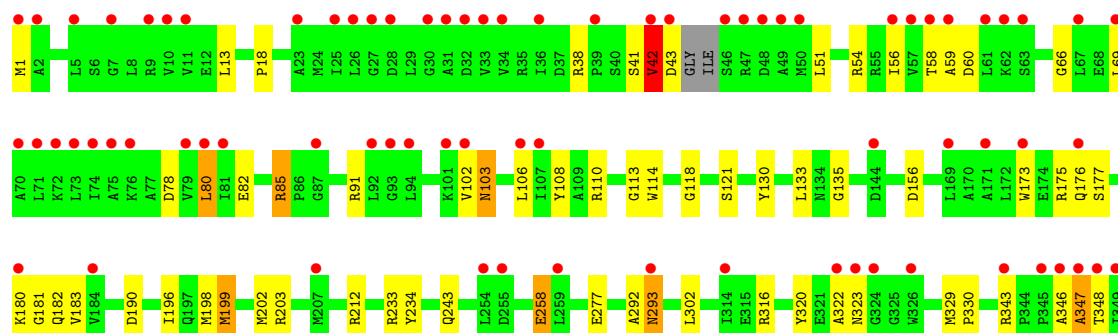
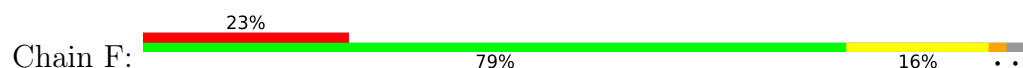
• Molecule 1: Alpha-methylacyl-CoA racemase

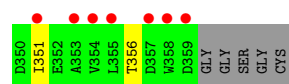


• Molecule 1: Alpha-methylacyl-CoA racemase

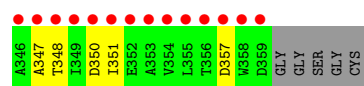
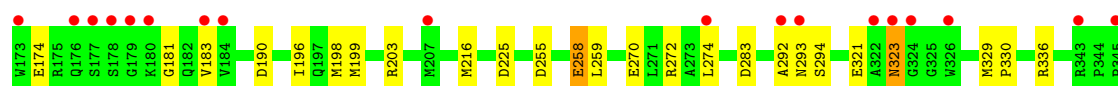
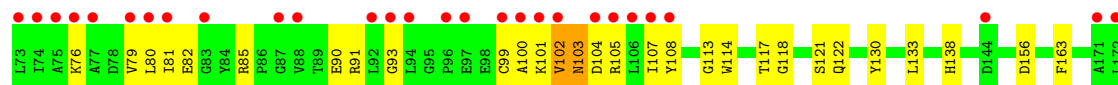
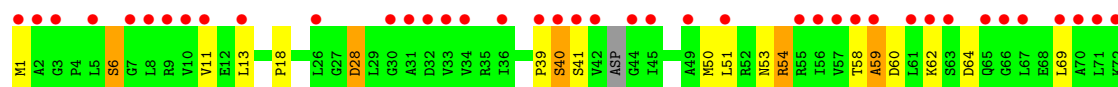
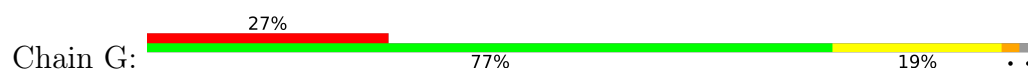


• Molecule 1: Alpha-methylacyl-CoA racemase

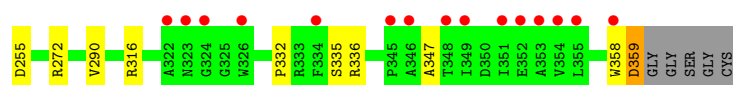
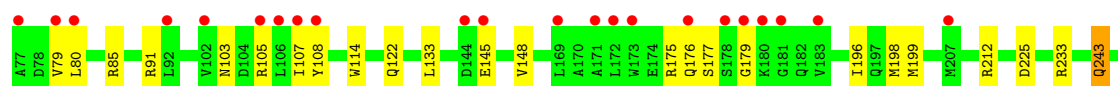
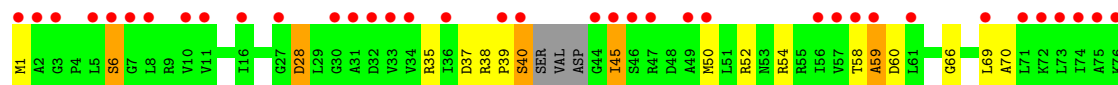
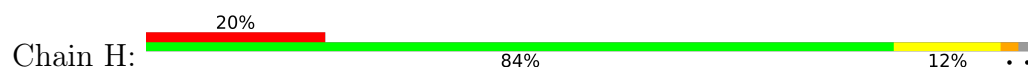




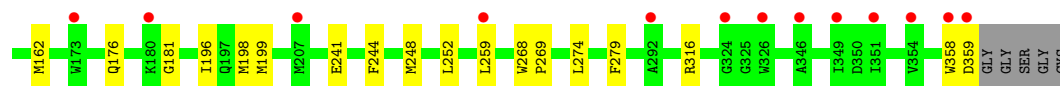
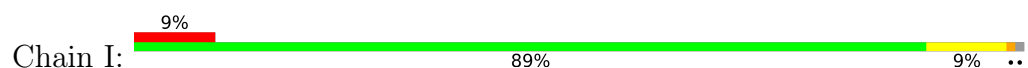
● Molecule 1: Alpha-methylacyl-CoA racemase



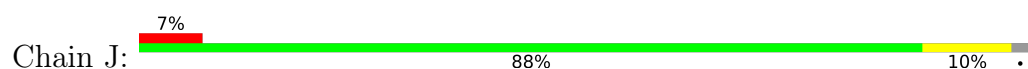
● Molecule 1: Alpha-methylacyl-CoA racemase

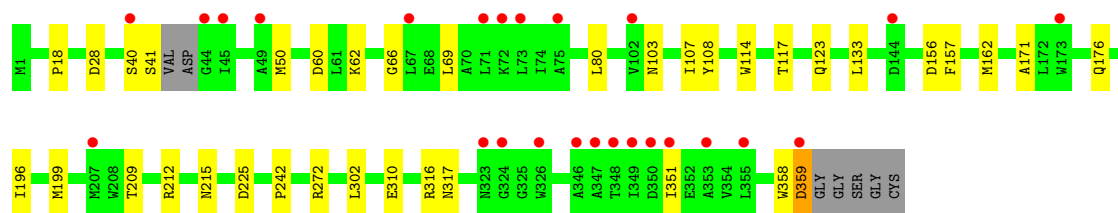


● Molecule 1: Alpha-methylacyl-CoA racemase

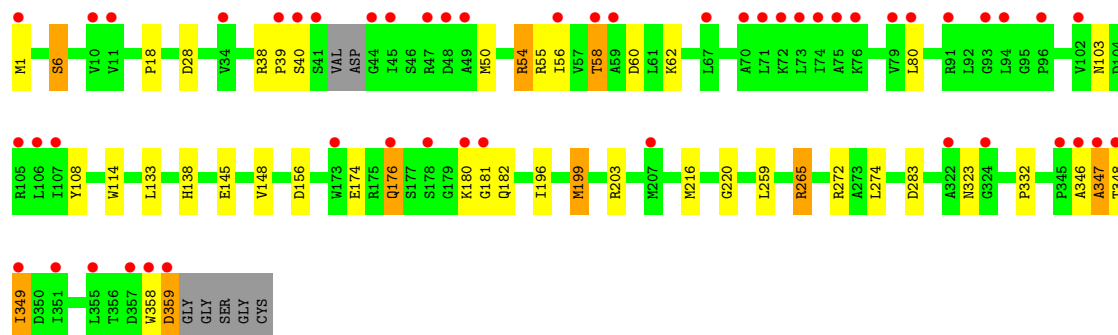
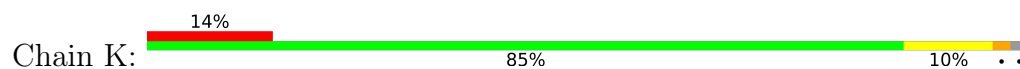


● Molecule 1: Alpha-methylacyl-CoA racemase

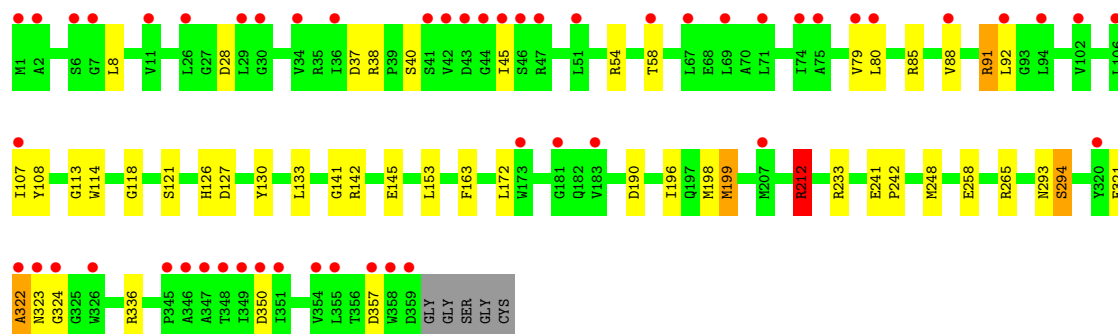
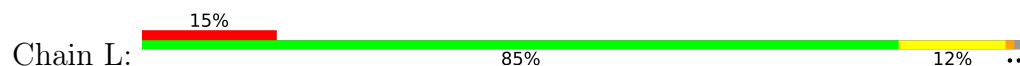




● Molecule 1: Alpha-methylacyl-CoA racemase



● 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, $\alpha$ , $\beta$ , $\gamma$	276.73Å 276.73Å 390.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	196.45 – 2.07 196.45 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (196.45-2.07) 99.9 (196.45-2.07)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, $R_{free}$	0.208 , 0.248 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	22208 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.009 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	34666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: A1IY9

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	0.63	0/2783	1.02	3/3786 (0.1%)
1	B	0.64	0/2766	1.03	5/3761 (0.1%)
1	C	0.64	0/2782	1.06	3/3783 (0.1%)
1	D	0.64	0/2782	1.09	1/3785 (0.0%)
1	E	0.63	0/2780	1.03	3/3780 (0.1%)
1	F	0.63	0/2769	1.07	3/3766 (0.1%)
1	G	0.62	0/2782	1.07	3/3783 (0.1%)
1	H	0.63	0/2760	1.08	3/3753 (0.1%)
1	I	0.63	0/2791	1.05	1/3797 (0.0%)
1	J	0.64	0/2766	1.04	3/3761 (0.1%)
1	K	0.64	0/2775	1.05	3/3773 (0.1%)
1	L	0.64	0/2782	1.05	4/3785 (0.1%)
All	All	0.64	0/33318	1.05	35/45313 (0.1%)

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	3
1	B	0	2
1	D	0	5
1	E	0	2
1	F	0	5
1	G	0	1
1	H	0	6
1	J	0	1
1	K	0	3
1	L	0	5
All	All	0	33

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ARG	CB-CA-C	-9.65	94.45	110.85
1	J	123	GLN	CB-CA-C	7.94	122.78	109.84
1	C	203	ARG	CB-CA-C	-7.75	97.68	110.85
1	L	38	ARG	CB-CA-C	7.57	120.39	109.26
1	B	203	ARG	N-CA-CB	7.53	121.30	110.16
1	L	38	ARG	N-CA-CB	-7.25	99.92	110.14
1	C	203	ARG	N-CA-CB	6.80	120.23	110.16
1	G	190	ASP	CA-CB-CG	6.63	119.23	112.60
1	E	28	ASP	CA-CB-CG	6.62	119.22	112.60
1	H	148	VAL	CB-CA-C	6.46	116.40	110.13
1	J	28	ASP	CA-CB-CG	6.46	119.06	112.60
1	G	283	ASP	CA-CB-CG	6.27	118.87	112.60
1	K	203	ARG	CB-CA-C	-6.22	100.46	110.79
1	F	203	ARG	CB-CA-C	-6.11	100.65	110.79
1	B	255	ASP	CB-CA-C	6.07	120.36	110.22
1	A	190	ASP	CA-CB-CG	6.01	118.61	112.60
1	L	190	ASP	CA-CB-CG	5.99	118.59	112.60
1	D	91	ARG	CB-CA-C	-5.97	99.58	110.63
1	K	28	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	28	ASP	CA-CB-CG	5.69	118.29	112.60
1	F	190	ASP	CA-CB-CG	5.62	118.22	112.60
1	E	190	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	28	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	190	ASP	CA-CB-CG	5.53	118.13	112.60
1	E	123	GLN	CB-CA-C	-5.45	100.68	109.72
1	G	28	ASP	CA-CB-CG	5.34	117.94	112.60
1	K	283	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	28	ASP	CA-CB-CG	5.31	117.91	112.60
1	I	91	ARG	CB-CA-C	-5.30	100.82	110.63
1	B	144	ASP	CA-CB-CG	5.24	117.83	112.60
1	L	28	ASP	CA-CB-CG	5.24	117.83	112.60
1	A	243	GLN	CB-CA-C	-5.18	102.04	110.85
1	F	258	GLU	CB-CA-C	-5.14	100.76	110.01
1	H	148	VAL	CA-C-O	5.13	122.69	119.51
1	J	123	GLN	N-CA-CB	-5.04	102.13	109.95

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	54	ARG	Peptide
1	B	35	ARG	Sidechain
1	B	85	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	233	ARG	Sidechain
1	D	265	ARG	Sidechain
1	D	43	ASP	Peptide
1	D	85	ARG	Sidechain
1	E	348	THR	Peptide
1	E	350	ASP	Peptide
1	F	110	ARG	Sidechain
1	F	212	ARG	Sidechain
1	F	233	ARG	Sidechain
1	F	85	ARG	Sidechain
1	F	91	ARG	Sidechain
1	G	91	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	233	ARG	Sidechain
1	H	35	ARG	Sidechain
1	H	38	ARG	Sidechain
1	H	54	ARG	Peptide
1	H	91	ARG	Sidechain
1	J	212	ARG	Sidechain
1	K	265	ARG	Sidechain
1	K	54	ARG	Sidechain,Peptide
1	L	212	ARG	Sidechain
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	2710	0	2654	23	0
1	B	2700	0	2646	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2710	0	2653	37	0
1	D	2715	0	2660	33	0
1	E	2705	0	2649	31	0
1	F	2703	0	2645	39	0
1	G	2710	0	2653	45	0
1	H	2694	0	2641	25	0
1	I	2718	0	2658	22	0
1	J	2700	0	2646	22	0
1	K	2703	0	2644	25	0
1	L	2715	0	2660	27	0
2	A	65	0	0	2	0
2	B	65	0	0	0	0
2	C	65	0	0	0	0
2	D	65	0	0	6	0
2	E	65	0	0	1	0
2	F	65	0	0	3	0
2	G	65	0	0	0	0
2	H	65	0	0	4	0
2	I	65	0	0	1	0
2	J	65	0	0	1	0
2	K	65	0	0	2	0
2	L	65	0	0	1	0
3	A	120	0	0	1	0
3	B	115	0	0	0	0
3	C	128	0	0	1	0
3	D	120	0	0	1	0
3	E	112	0	0	3	0
3	F	102	0	0	2	0
3	G	104	0	0	2	0
3	H	108	0	0	0	0
3	I	127	0	0	1	0
3	J	127	0	0	1	0
3	K	121	0	0	1	0
3	L	119	0	0	1	0
All	All	34666	0	31809	312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (312) 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:G:259:LEU:HD22	1:G:274:LEU:HD13	1.52	0.91
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.37	0.90
1:F:85:ARG:HD3	2:F:401:A1IY9:O9	1.74	0.88
1:F:320:TYR:CE2	1:F:322:ALA:HB2	2.13	0.84
1:D:85:ARG:HD3	2:D:401:A1IY9:O9	1.83	0.77
1:L:323:ASN:CG	1:L:324:GLY:H	1.93	0.76
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.70	0.74
1:J:310:GLU:OE2	3:J:501:HOH:O	2.04	0.74
1:F:85:ARG:CD	2:F:401:A1IY9:O9	2.39	0.71
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.27	0.70
1:E:105:ARG:HG2	1:E:179:GLY:O	1.93	0.69
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.76	0.69
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.29	0.67
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.28	0.67
1:D:320:TYR:CE2	1:D:322:ALA:HB2	2.30	0.67
1:G:216:MET:HE1	2:H:401:A1IY9:C32	2.25	0.67
1:G:90:GLU:O	1:G:93:GLY:N	2.26	0.65
1:L:88:VAL:O	1:L:92:LEU:HD12	1.97	0.64
1:K:346:ALA:O	1:K:347:ALA:O	2.16	0.63
1:E:358:TRP:O	1:E:359:ASP:C	2.40	0.63
1:D:320:TYR:HE2	1:D:322:ALA:HB2	1.64	0.62
1:C:138:HIS:HD2	3:C:544:HOH:O	1.81	0.62
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.80	0.62
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.35	0.62
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.35	0.62
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.82	0.61
1:F:320:TYR:HE2	1:F:322:ALA:HB2	1.66	0.61
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.35	0.60
1:G:1:MET:O	1:G:6:SER:OG	2.17	0.60
1:C:118:GLY:O	1:C:121:SER:OG	2.16	0.60
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.33	0.60
1:F:108:TYR:HB3	1:F:183:VAL:HG22	1.83	0.60
1:K:39:PRO:HA	1:K:58:THR:CG2	2.32	0.60
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.34	0.59
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.83	0.59
1:A:69:LEU:HD13	1:A:351:ILE:HG21	1.84	0.59
1:D:69:LEU:HD13	1:D:351:ILE:HG21	1.85	0.58
1:H:358:TRP:O	1:H:359:ASP:C	2.46	0.58
1:A:138:HIS:HD2	3:A:535:HOH:O	1.87	0.58
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.84	0.58
1:E:78:ASP:OD1	1:E:175:ARG:NH2	2.23	0.58
1:G:69:LEU:HB3	1:G:351:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:MET:O	1:K:6:SER:OG	2.14	0.58
1:K:138:HIS:HD2	3:K:552:HOH:O	1.86	0.58
1:F:54:ARG:O	1:F:346:ALA:HB3	2.03	0.57
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.39	0.57
1:H:60:ASP:O	1:H:66:GLY:HA3	2.03	0.57
1:C:28:ASP:HA	1:C:53:ASN:HD22	1.69	0.57
1:A:323:ASN:O	1:A:324:GLY:C	2.47	0.57
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.18	0.57
1:C:1:MET:HE2	1:C:343:ARG:NH2	2.20	0.57
1:J:358:TRP:O	1:J:359:ASP:C	2.47	0.57
1:D:85:ARG:CD	2:D:401:A1IY9:O9	2.53	0.56
1:E:85:ARG:NH1	1:E:122:GLN:O	2.34	0.56
1:I:118:GLY:O	1:I:121:SER:OG	2.23	0.56
1:E:196:ILE:HG12	1:E:199:MET:HB2	1.88	0.55
1:F:69:LEU:HD13	1:F:351:ILE:HG23	1.89	0.55
1:H:105:ARG:HG2	1:H:179:GLY:O	2.07	0.55
1:C:196:ILE:HG12	1:C:199:MET:HB2	1.89	0.55
1:D:78:ASP:OD1	1:D:175:ARG:NH2	2.30	0.55
1:G:80:LEU:CD2	1:G:108:TYR:CE1	2.89	0.55
1:C:80:LEU:HD22	1:C:108:TYR:CE2	2.41	0.55
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.13	0.55
1:G:183:VAL:H	1:H:335:SER:HG	1.54	0.55
1:H:1:MET:O	1:H:6:SER:OG	2.25	0.54
1:L:323:ASN:CG	1:L:324:GLY:N	2.62	0.54
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.43	0.54
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.34	0.53
1:G:60:ASP:OD1	1:G:62:LYS:HB2	2.09	0.53
1:D:28:ASP:HA	1:D:53:ASN:ND2	2.23	0.53
1:G:323:ASN:OD1	1:G:323:ASN:N	2.41	0.53
1:G:216:MET:HE1	2:H:401:A1IY9:C31	2.37	0.53
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.24	0.53
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.41	0.53
1:C:346:ALA:O	1:C:347:ALA:O	2.25	0.53
1:F:106:LEU:O	1:F:181:GLY:HA3	2.08	0.53
1:E:138:HIS:HD2	3:E:541:HOH:O	1.92	0.53
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.92	0.52
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.34	0.52
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.42	0.52
1:I:198:MET:HB2	1:J:50:MET:HE1	1.90	0.52
1:B:291:PHE:O	1:B:294:SER:HB3	2.10	0.52
1:F:80:LEU:HD22	1:F:108:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:TRP:CZ3	1:G:133:LEU:HD22	2.45	0.52
1:G:336:ARG:HG2	1:G:336:ARG:HH11	1.75	0.51
1:D:28:ASP:HA	1:D:53:ASN:HD22	1.74	0.51
1:F:38:ARG:HG2	3:F:519:HOH:O	2.11	0.51
1:F:181:GLY:O	1:F:182:GLN:HB3	2.10	0.51
1:J:242:PRO:HB3	1:L:91:ARG:HD3	1.93	0.51
1:A:198:MET:HB2	1:B:50:MET:HE1	1.93	0.51
1:C:320:TYR:CE2	1:C:322:ALA:HB2	2.46	0.51
1:K:50:MET:HE1	1:L:198:MET:HB2	1.92	0.51
1:F:329:MET:HE3	1:F:330:PRO:HD2	1.92	0.50
1:I:268:TRP:N	1:I:269:PRO:CD	2.73	0.50
1:C:135:GLY:HA2	1:D:302:LEU:O	2.11	0.50
1:G:58:THR:O	1:G:59:ALA:HB2	2.10	0.50
1:C:65:GLN:O	1:C:68:GLU:N	2.45	0.50
1:G:50:MET:HE1	1:H:198:MET:HB2	1.92	0.50
1:H:39:PRO:O	1:H:40:SER:C	2.53	0.50
1:C:67:LEU:HD12	1:C:67:LEU:O	2.11	0.50
1:K:39:PRO:CA	1:K:58:THR:CG2	2.90	0.49
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.94	0.49
1:G:18:PRO:HB3	1:G:156:ASP:O	2.12	0.49
2:I:401:A1IY9:S1	2:I:401:A1IY9:C26	3.00	0.49
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.93	0.49
1:F:60:ASP:O	1:F:66:GLY:HA3	2.13	0.49
1:F:198:MET:HE2	1:F:202:MET:SD	2.51	0.49
1:G:85:ARG:NH1	1:G:122:GLN:O	2.44	0.49
1:K:196:ILE:HG13	1:L:153:LEU:HD21	1.94	0.49
1:A:69:LEU:HD13	1:A:351:ILE:CG2	2.43	0.49
1:H:85:ARG:NH2	1:H:122:GLN:O	2.44	0.49
1:A:80:LEU:CD2	1:A:108:TYR:CE2	2.96	0.49
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.28	0.49
1:C:80:LEU:HD23	1:C:108:TYR:CE2	2.48	0.49
1:E:259:LEU:HD22	1:E:274:LEU:HD13	1.94	0.49
1:A:42:VAL:HG13	1:A:43:ASP:H	1.78	0.48
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.94	0.48
1:E:57:VAL:HG12	1:E:349:ILE:O	2.13	0.48
1:G:163:PHE:O	1:H:332:PRO:HG3	2.13	0.48
1:I:358:TRP:O	1:I:359:ASP:HB2	2.13	0.48
1:E:50:MET:HE1	1:F:198:MET:HB2	1.96	0.48
1:F:78:ASP:OD1	1:F:175:ARG:NH2	2.37	0.48
1:C:259:LEU:CD2	1:C:274:LEU:HD13	2.44	0.48
1:G:11:VAL:HG12	1:G:80:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:GLU:HG3	3:G:521:HOH:O	2.13	0.48
1:A:163:PHE:O	1:B:332:PRO:HG3	2.13	0.48
1:D:107:ILE:HD12	1:D:171:ALA:HB1	1.95	0.48
1:D:294:SER:HB2	1:L:293:ASN:O	2.13	0.48
1:E:243[B]:GLN:HG3	3:E:570:HOH:O	2.14	0.48
1:G:99:CYS:C	1:G:101:LYS:H	2.22	0.48
1:D:225:ASP:OD2	1:D:272:ARG:NH1	2.47	0.48
1:E:135:GLY:HA2	1:F:302:LEU:O	2.13	0.48
1:F:1:MET:HE2	1:F:343:ARG:NH2	2.29	0.48
2:K:401:A1IY9:S1	2:K:401:A1IY9:C26	3.02	0.48
1:H:28:ASP:CG	1:H:52:ARG:HH21	2.22	0.47
1:A:50:MET:HE1	1:B:198:MET:HB2	1.97	0.47
1:K:332:PRO:HG3	1:L:163:PHE:O	2.14	0.47
1:I:87:GLY:O	1:I:91:ARG:HG3	2.14	0.47
1:K:148:VAL:HG21	1:L:141:GLY:HA2	1.97	0.47
1:E:117:THR:O	1:F:316:ARG:HD2	2.14	0.47
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.98	0.47
1:A:224:TYR:HA	1:A:237:VAL:O	2.14	0.47
1:D:40:SER:OG	3:D:501:HOH:O	2.20	0.47
2:F:401:A1IY9:O3	2:F:401:A1IY9:C13	2.62	0.47
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.95	0.47
1:B:231:ASP:OD2	1:B:233:ARG:NH1	2.44	0.47
1:I:138:HIS:HD2	3:I:1217:HOH:O	1.98	0.47
1:F:51:LEU:HA	1:F:54:ARG:NH1	2.30	0.47
1:G:225:ASP:OD2	1:G:272:ARG:NH1	2.48	0.47
1:I:241:GLU:HB2	1:I:244:PHE:CD2	2.50	0.47
1:D:106:LEU:O	1:D:181:GLY:HA3	2.15	0.46
1:J:107:ILE:HD12	1:J:171:ALA:HB1	1.96	0.46
1:A:289:ALA:O	1:A:290:VAL:C	2.58	0.46
1:C:291:PHE:O	1:C:294:SER:HB3	2.16	0.46
1:G:79:VAL:HG22	1:G:107:ILE:HB	1.97	0.46
1:H:196:ILE:HG12	1:H:199:MET:HB2	1.97	0.46
1:D:318:THR:HG22	1:D:319:PHE:CE1	2.50	0.46
1:H:114:TRP:CZ3	1:H:133:LEU:HD22	2.50	0.46
1:C:19:GLY:N	1:C:20:PRO:CD	2.79	0.46
1:H:243:GLN:CD	1:H:243:GLN:H	2.23	0.46
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.51	0.46
1:G:69:LEU:HB3	1:G:351:ILE:CD1	2.46	0.46
1:H:45:ILE:HG13	1:H:347:ALA:HB2	1.98	0.46
1:A:126:HIS:ND1	2:A:401:A1IY9:C3	2.79	0.46
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG22	1:C:107:ILE:HB	1.98	0.46
1:G:181:GLY:O	1:H:336:ARG:NH2	2.41	0.46
1:K:60:ASP:OD1	1:K:62:LYS:HB2	2.16	0.45
1:C:42:VAL:HG13	1:C:44:GLY:O	2.16	0.45
1:E:241:GLU:HB2	1:E:244:PHE:CD2	2.50	0.45
1:G:80:LEU:HD22	1:G:108:TYR:CE1	2.51	0.45
1:L:79:VAL:HG22	1:L:107:ILE:HB	1.98	0.45
1:A:1:MET:HE2	1:A:343:ARG:NH2	2.32	0.45
1:E:10:VAL:HG22	1:E:79:VAL:HB	1.97	0.45
1:F:196:ILE:HG12	1:F:199:MET:HB2	1.98	0.45
1:H:175:ARG:C	1:H:177:SER:N	2.75	0.45
1:I:117:THR:O	1:J:316:ARG:HD2	2.17	0.45
1:E:272:ARG:NH1	3:E:510:HOH:O	2.49	0.45
1:I:38:ARG:HH21	1:I:38:ARG:HG3	1.81	0.44
1:C:176:GLN:HG3	1:D:176:GLN:NE2	2.33	0.44
1:G:39:PRO:C	1:G:41:SER:H	2.25	0.44
1:K:80:LEU:HD23	1:K:108:TYR:CE2	2.53	0.44
1:K:358:TRP:O	1:K:359:ASP:C	2.60	0.44
1:C:39:PRO:HG3	1:C:58:THR:HG23	1.99	0.44
1:E:223:TYR:O	1:E:237:VAL:HG12	2.18	0.44
2:H:401:A1IY9:C31	2:H:401:A1IY9:C28	2.94	0.44
1:L:142:ARG:O	1:L:212:ARG:HD2	2.18	0.44
1:D:126:HIS:ND1	2:D:401:A1IY9:C3	2.81	0.44
1:K:346:ALA:O	1:K:347:ALA:C	2.60	0.44
1:A:89:THR:OG1	1:A:110:ARG:NH2	2.50	0.44
1:B:69:LEU:HD13	1:B:351:ILE:CG2	2.47	0.44
1:G:117:THR:O	1:H:316:ARG:HD2	2.18	0.44
1:G:255:ASP:HB3	1:G:258:GLU:HG2	2.00	0.44
1:K:114:TRP:CZ3	1:K:133:LEU:HD22	2.52	0.44
1:E:39:PRO:HA	1:E:58:THR:HG23	1.99	0.44
1:L:37:ASP:O	1:L:58:THR:HA	2.18	0.44
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.53	0.44
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.53	0.43
1:F:346:ALA:O	1:F:347:ALA:O	2.36	0.43
1:J:18:PRO:HB3	1:J:156:ASP:O	2.17	0.43
1:J:196:ILE:HG12	1:J:199:MET:HB2	2.00	0.43
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.53	0.43
1:C:19:GLY:N	1:C:20:PRO:HD2	2.34	0.43
1:H:58:THR:O	1:H:59:ALA:HB2	2.18	0.43
1:I:106:LEU:O	1:I:181:GLY:HA3	2.19	0.43
1:K:55:ARG:HD2	1:K:349:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:TRP:CZ3	1:E:133:LEU:HD22	2.54	0.43
1:G:196:ILE:HG12	1:G:199:MET:HB2	2.00	0.43
1:H:69:LEU:O	1:H:70:ALA:C	2.61	0.43
1:D:126:HIS:O	1:D:127:ASP:C	2.61	0.43
1:F:18:PRO:HB3	1:F:156:ASP:O	2.19	0.43
1:G:118:GLY:O	1:G:121:SER:OG	2.35	0.43
1:K:145:GLU:OE1	1:L:145:GLU:OE1	2.37	0.43
2:D:401:A1IY9:C26	2:D:401:A1IY9:S1	3.07	0.43
1:G:51:LEU:HA	1:G:54:ARG:NH1	2.33	0.43
1:G:80:LEU:HG	1:G:81:ILE:N	2.33	0.43
2:H:401:A1IY9:O3	2:H:401:A1IY9:C12	2.66	0.43
1:L:114:TRP:CZ3	1:L:133:LEU:HD22	2.53	0.43
1:H:37:ASP:O	1:H:58:THR:HA	2.19	0.43
1:J:62:LYS:NZ	2:J:401:A1IY9:O16	2.52	0.43
1:A:28:ASP:HA	1:A:53:ASN:ND2	2.33	0.43
1:D:87:GLY:O	1:D:91:ARG:HG3	2.19	0.43
1:E:255:ASP:HB3	1:E:258:GLU:HG3	2.00	0.43
1:E:181:GLY:O	1:E:182:GLN:HB3	2.19	0.42
1:J:69:LEU:HB3	1:J:351:ILE:HD13	2.01	0.42
1:D:118:GLY:O	1:D:121:SER:OG	2.21	0.42
1:G:198:MET:HE3	1:H:50:MET:HE1	1.99	0.42
1:I:316:ARG:HD2	1:J:117:THR:O	2.19	0.42
1:L:80:LEU:CD2	1:L:108:TYR:CE2	3.02	0.42
1:A:348:THR:HG22	1:A:349:ILE:H	1.83	0.42
1:D:126:HIS:ND1	2:D:401:A1IY9:C2	2.83	0.42
2:E:401:A1IY9:C27	1:F:198:MET:HE1	2.49	0.42
1:E:174:GLU:OE1	1:E:174:GLU:C	2.63	0.42
1:F:13:LEU:HD12	1:F:82:GLU:HB3	2.02	0.42
1:I:196:ILE:HG12	1:I:199:MET:HB2	2.01	0.42
1:B:19:GLY:N	1:B:20:PRO:CD	2.82	0.42
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.55	0.42
1:K:174:GLU:C	1:K:174:GLU:OE1	2.63	0.42
1:L:233:ARG:CD	3:L:542:HOH:O	2.67	0.42
1:L:336:ARG:HH11	1:L:336:ARG:HG2	1.85	0.42
1:A:175:ARG:HG2	1:A:175:ARG:O	2.20	0.42
1:K:196:ILE:HG12	1:K:199:MET:HB2	2.02	0.42
1:C:50:MET:HE1	1:D:198:MET:HB2	2.00	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.82	0.42
1:G:102:VAL:O	1:G:103:ASN:HB2	2.19	0.42
1:E:353:ALA:O	1:E:356:THR:HB	2.19	0.42
1:F:293:ASN:HB3	1:G:294:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:GLN:HA	1:K:176:GLN:HE21	1.85	0.42
1:C:13:LEU:O	1:C:14:ALA:C	2.63	0.41
1:G:105:ARG:O	1:G:181:GLY:CA	2.68	0.41
1:I:18:PRO:HB3	1:I:156:ASP:O	2.20	0.41
1:J:316:ARG:O	1:J:317:ASN:C	2.62	0.41
2:K:401:A1IY9:C28	2:K:401:A1IY9:C35	2.98	0.41
1:C:322:ALA:O	1:C:323:ASN:C	2.63	0.41
1:E:322:ALA:O	1:E:324:GLY:N	2.53	0.41
1:L:118:GLY:O	1:L:121:SER:OG	2.28	0.41
1:L:241:GLU:HA	1:L:242:PRO:HD3	1.92	0.41
1:D:293:ASN:O	1:L:294:SER:HB2	2.20	0.41
1:E:302:LEU:O	1:F:135:GLY:HA2	2.20	0.41
1:F:42:VAL:HG11	1:F:58:THR:CG2	2.50	0.41
1:F:42:VAL:O	1:F:43:ASP:HB2	2.20	0.41
1:F:102:VAL:O	1:F:103:ASN:HB2	2.20	0.41
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.56	0.41
1:I:176:GLN:NE2	1:J:176:GLN:HG2	2.35	0.41
1:G:13:LEU:HD12	1:G:82:GLU:HB3	2.03	0.41
1:C:316:ARG:HD2	1:D:117:THR:O	2.21	0.41
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.35	0.41
1:J:60:ASP:O	1:J:66:GLY:HA3	2.21	0.41
1:L:322:ALA:O	1:L:323:ASN:C	2.64	0.41
1:D:11:VAL:O	1:D:80:LEU:HA	2.20	0.41
1:G:39:PRO:HB3	1:G:58:THR:HG23	2.03	0.41
1:G:255:ASP:HB3	1:G:258:GLU:CG	2.51	0.41
1:J:209:THR:HG22	1:J:215:ASN:OD1	2.21	0.41
1:A:67:LEU:HD13	1:A:92:LEU:O	2.21	0.41
1:C:51:LEU:HA	1:C:54:ARG:NH1	2.35	0.41
1:D:80:LEU:CD2	1:D:108:TYR:CE2	3.04	0.41
1:E:39:PRO:CA	1:E:58:THR:HG23	2.50	0.41
1:F:58:THR:O	1:F:59:ALA:HB2	2.20	0.41
1:F:196:ILE:HG23	1:F:196:ILE:O	2.20	0.41
1:K:216:MET:HE1	2:L:401:A1IY9:C35	2.51	0.41
1:L:113:GLY:HA3	1:L:130:TYR:CE1	2.56	0.41
1:G:138:HIS:HD2	3:G:528:HOH:O	2.03	0.41
1:G:199:MET:O	1:G:203:ARG:HB2	2.20	0.41
1:H:80:LEU:CD2	1:H:108:TYR:CE2	3.02	0.41
1:I:252:LEU:HD21	1:I:279:PHE:CE1	2.56	0.41
1:K:50:MET:CE	1:L:198:MET:HB2	2.51	0.41
1:C:69:LEU:HD13	1:C:351:ILE:CG2	2.51	0.41
1:K:18:PRO:HB3	1:K:156:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ALA:O	1:C:347:ALA:C	2.63	0.40
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.56	0.40
1:E:13:LEU:O	1:E:14:ALA:C	2.64	0.40
1:G:174:GLU:OE1	1:G:174:GLU:C	2.64	0.40
1:K:220:GLY:O	1:K:272:ARG:NH2	2.54	0.40
1:L:8:LEU:HD11	1:L:172:LEU:HD11	2.03	0.40
2:A:401:A1IY9:O3	2:A:401:A1IY9:C13	2.69	0.40
1:B:174:GLU:OE1	1:B:174:GLU:C	2.64	0.40
1:F:113:GLY:HA3	1:F:130:TYR:CZ	2.56	0.40
1:G:329:MET:HE3	1:G:330:PRO:HD2	2.04	0.40
1:I:135:GLY:HA2	1:J:302:LEU:O	2.21	0.40
1:K:181:GLY:O	1:K:182:GLN:HB3	2.21	0.40
2:D:401:A1IY9:O15	2:D:401:A1IY9:O13	2.39	0.40
1:F:118:GLY:O	1:F:121:SER:OG	2.37	0.40
1:I:198:MET:HE3	1:J:157:PHE:HZ	1.86	0.40
1:E:291:PHE:O	1:E:294:SER:OG	2.35	0.40
1:F:114:TRP:CZ3	1:F:133:LEU:HD22	2.57	0.40
1:F:234:TYR:OH	3:F:501:HOH:O	2.21	0.40
1:C:295:ASP:CG	1:D:85:ARG:HH22	2.29	0.40
1:D:60:ASP:OD1	1:D:62:LYS:HB2	2.22	0.40
1:E:113:GLY:HA3	1:E:130:TYR:CZ	2.57	0.40
1:I:162:MET:HB3	1:J:162:MET:HB3	2.04	0.40
1:J:114:TRP:CZ3	1:J:133:LEU:HD22	2.56	0.40
1:L:126:HIS:O	1:L:127:ASP:C	2.64	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	358/364 (98%)	332 (93%)	21 (6%)	5 (1%)	<b>9</b> <b>3</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	354/364 (97%)	338 (96%)	11 (3%)	5 (1%)	9	3
1	C	356/364 (98%)	332 (93%)	21 (6%)	3 (1%)	16	8
1	D	358/364 (98%)	338 (94%)	18 (5%)	2 (1%)	22	13
1	E	355/364 (98%)	334 (94%)	18 (5%)	3 (1%)	16	8
1	F	354/364 (97%)	326 (92%)	21 (6%)	7 (2%)	6	1
1	G	356/364 (98%)	327 (92%)	23 (6%)	6 (2%)	7	2
1	H	353/364 (97%)	327 (93%)	24 (7%)	2 (1%)	22	13
1	I	359/364 (99%)	346 (96%)	12 (3%)	1 (0%)	37	31
1	J	354/364 (97%)	341 (96%)	12 (3%)	1 (0%)	37	31
1	K	355/364 (98%)	333 (94%)	18 (5%)	4 (1%)	12	4
1	L	358/364 (98%)	339 (95%)	19 (5%)	0	100	100
All	All	4270/4368 (98%)	4013 (94%)	218 (5%)	39 (1%)	14	7

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	C	347	ALA
1	D	103	ASN
1	F	41	SER
1	F	103	ASN
1	G	103	ASN
1	K	347	ALA
1	C	103	ASN
1	F	292	ALA
1	F	347	ALA
1	G	40	SER
1	G	59	ALA
1	G	292	ALA
1	G	347	ALA
1	H	103	ASN
1	I	103	ASN
1	K	103	ASN
1	B	40	SER
1	G	100	ALA
1	H	59	ALA
1	J	103	ASN
1	B	103	ASN

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Mol	Chain	Res	Type
1	C	66	GLY
1	D	323	ASN
1	E	103	ASN
1	E	151	LEU
1	E	356	THR
1	F	323	ASN
1	A	42	VAL
1	A	43	ASP
1	A	59	ALA
1	B	59	ALA
1	F	356	THR
1	K	323	ASN
1	K	348	THR
1	B	151	LEU
1	B	290	VAL
1	A	290	VAL
1	F	42	VAL

### 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%)	268 (97%)	8 (3%)	37	32
1	B	274/277 (99%)	268 (98%)	6 (2%)	47	43
1	C	276/277 (100%)	269 (98%)	7 (2%)	42	38
1	D	276/277 (100%)	264 (96%)	12 (4%)	25	18
1	E	276/277 (100%)	270 (98%)	6 (2%)	47	43
1	F	275/277 (99%)	263 (96%)	12 (4%)	24	18
1	G	276/277 (100%)	262 (95%)	14 (5%)	20	13
1	H	273/277 (99%)	264 (97%)	9 (3%)	33	27
1	I	277/277 (100%)	271 (98%)	6 (2%)	47	43
1	J	274/277 (99%)	271 (99%)	3 (1%)	70	70
1	K	275/277 (99%)	263 (96%)	12 (4%)	24	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	276/277 (100%)	265 (96%)	11 (4%)	27	21
All	All	3304/3324 (99%)	3198 (97%)	106 (3%)	34	28

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	56	ILE
1	A	91	ARG
1	A	243	GLN
1	A	294	SER
1	A	323	ASN
1	A	349	ILE
1	A	350	ASP
1	B	6	SER
1	B	40	SER
1	B	177	SER
1	B	248	MET
1	B	258	GLU
1	B	356	THR
1	C	40	SER
1	C	54	ARG
1	C	58	THR
1	C	91	ARG
1	C	121	SER
1	C	176	GLN
1	C	258	GLU
1	D	6	SER
1	D	40	SER
1	D	41	SER
1	D	43	ASP
1	D	85	ARG
1	D	91	ARG
1	D	176	GLN
1	D	199	MET
1	D	248	MET
1	D	294	SER
1	D	348	THR
1	D	357	ASP
1	E	6	SER
1	E	54	ARG
1	E	144	ASP

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Mol	Chain	Res	Type
1	E	176	GLN
1	E	177	SER
1	E	248	MET
1	F	42	VAL
1	F	56	ILE
1	F	80	LEU
1	F	173	TRP
1	F	176	GLN
1	F	177	SER
1	F	199	MET
1	F	243	GLN
1	F	258	GLU
1	F	277	GLU
1	F	293	ASN
1	F	348	THR
1	G	6	SER
1	G	40	SER
1	G	54	ARG
1	G	64	ASP
1	G	76	LYS
1	G	102	VAL
1	G	104	ASP
1	G	258	GLU
1	G	293	ASN
1	G	321	GLU
1	G	323	ASN
1	G	348	THR
1	G	350	ASP
1	G	357	ASP
1	H	6	SER
1	H	40	SER
1	H	45	ILE
1	H	145	GLU
1	H	176	GLN
1	H	243	GLN
1	H	255	ASP
1	H	290	VAL
1	H	359	ASP
1	I	42	VAL
1	I	54	ARG
1	I	58	THR
1	I	68	GLU

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Mol	Chain	Res	Type
1	I	121	SER
1	I	248	MET
1	J	40	SER
1	J	41	SER
1	J	359	ASP
1	K	6	SER
1	K	38	ARG
1	K	40	SER
1	K	54	ARG
1	K	56	ILE
1	K	58	THR
1	K	176	GLN
1	K	180	LYS
1	K	199	MET
1	K	265	ARG
1	K	349	ILE
1	K	359	ASP
1	L	40	SER
1	L	45	ILE
1	L	85	ARG
1	L	199	MET
1	L	212	ARG
1	L	248	MET
1	L	258	GLU
1	L	294	SER
1	L	321	GLU
1	L	350	ASP
1	L	357	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	286	HIS
1	A	323	ASN
1	A	327	GLN
1	B	176	GLN
1	B	293	ASN
1	C	116	GLN
1	C	138	HIS
1	C	176	GLN
1	C	263	ASN

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Mol	Chain	Res	Type
1	C	282	HIS
1	C	327	GLN
1	D	176	GLN
1	D	286	HIS
1	E	116	GLN
1	E	134	ASN
1	E	138	HIS
1	E	263	ASN
1	E	293	ASN
1	F	116	GLN
1	F	293	ASN
1	F	308	HIS
1	F	323	ASN
1	G	138	HIS
1	G	176	GLN
1	G	282	HIS
1	G	286	HIS
1	G	293	ASN
1	G	327	GLN
1	H	116	GLN
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	327	GLN
1	J	286	HIS
1	K	138	HIS
1	K	176	GLN
1	K	293	ASN
1	K	327	GLN
1	L	122	GLN
1	L	176	GLN
1	L	308	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	A1IY9	D	401	-	61,69,69	0.81	2 (3%)	78,101,101	1.48	8 (10%)
2	A1IY9	F	401	-	61,69,69	0.88	3 (4%)	78,101,101	1.82	11 (14%)
2	A1IY9	A	401	-	61,69,69	0.81	3 (4%)	78,101,101	1.75	15 (19%)
2	A1IY9	I	401	-	61,69,69	0.86	2 (3%)	78,101,101	1.40	10 (12%)
2	A1IY9	G	401	-	61,69,69	0.77	2 (3%)	78,101,101	1.74	13 (16%)
2	A1IY9	K	401	-	61,69,69	0.83	1 (1%)	78,101,101	1.49	9 (11%)
2	A1IY9	J	401	-	61,69,69	0.86	3 (4%)	78,101,101	1.53	11 (14%)
2	A1IY9	L	401	-	61,69,69	0.86	3 (4%)	78,101,101	1.45	7 (8%)
2	A1IY9	E	401	-	61,69,69	0.90	4 (6%)	78,101,101	1.80	11 (14%)
2	A1IY9	C	401	-	61,69,69	0.84	2 (3%)	78,101,101	1.28	10 (12%)
2	A1IY9	B	401	-	61,69,69	0.81	2 (3%)	78,101,101	1.76	13 (16%)
2	A1IY9	H	401	-	61,69,69	1.19	4 (6%)	78,101,101	1.55	14 (17%)

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	A1IY9	D	401	-	-	9/59/79/79	0/5/5/5
2	A1IY9	F	401	-	-	20/59/79/79	0/5/5/5
2	A1IY9	A	401	-	-	18/59/79/79	0/5/5/5
2	A1IY9	I	401	-	-	10/59/79/79	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IY9	G	401	-	-	9/59/79/79	0/5/5/5
2	A1IY9	K	401	-	-	10/59/79/79	0/5/5/5
2	A1IY9	J	401	-	-	12/59/79/79	0/5/5/5
2	A1IY9	L	401	-	-	11/59/79/79	0/5/5/5
2	A1IY9	E	401	-	-	17/59/79/79	0/5/5/5
2	A1IY9	C	401	-	-	8/59/79/79	0/5/5/5
2	A1IY9	B	401	-	-	12/59/79/79	0/5/5/5
2	A1IY9	H	401	-	-	16/59/79/79	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	A1IY9	C2-C3	6.52	1.58	1.53
2	I	401	A1IY9	O1-C3	3.66	1.26	1.20
2	E	401	A1IY9	C2-C3	3.28	1.56	1.53
2	J	401	A1IY9	C2-C3	-3.22	1.51	1.53
2	H	401	A1IY9	O1-C3	3.14	1.25	1.20
2	F	401	A1IY9	O1-C3	3.04	1.25	1.20
2	C	401	A1IY9	O1-C3	3.03	1.25	1.20
2	D	401	A1IY9	P3-O14	2.98	1.64	1.59
2	K	401	A1IY9	O1-C3	2.93	1.25	1.20
2	E	401	A1IY9	O1-C3	2.86	1.25	1.20
2	L	401	A1IY9	O1-C3	2.85	1.25	1.20
2	L	401	A1IY9	P3-O14	2.85	1.64	1.59
2	H	401	A1IY9	C3-S1	2.66	1.83	1.75
2	B	401	A1IY9	P3-O14	2.59	1.64	1.59
2	A	401	A1IY9	P3-O14	2.59	1.64	1.59
2	F	401	A1IY9	O2-C6	2.52	1.28	1.23
2	E	401	A1IY9	P3-O14	2.50	1.64	1.59
2	G	401	A1IY9	P3-O14	2.43	1.63	1.59
2	B	401	A1IY9	O1-C3	2.42	1.24	1.20
2	E	401	A1IY9	C3-S1	2.27	1.82	1.75
2	H	401	A1IY9	P3-O14	2.25	1.63	1.59
2	F	401	A1IY9	P3-O14	2.25	1.63	1.59
2	J	401	A1IY9	P3-O14	2.23	1.63	1.59
2	A	401	A1IY9	C2-C3	2.18	1.55	1.53
2	C	401	A1IY9	P3-O14	2.14	1.63	1.59
2	J	401	A1IY9	O12-C17	2.10	1.44	1.41
2	G	401	A1IY9	O1-C3	2.09	1.23	1.20
2	L	401	A1IY9	O12-C17	2.07	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1IY9	O1-C3	2.07	1.23	1.20
2	D	401	A1IY9	O12-C17	2.06	1.44	1.41
2	I	401	A1IY9	P3-O14	2.02	1.63	1.59

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1IY9	C2-C3-S1	9.11	121.69	111.81
2	G	401	A1IY9	C2-C3-S1	7.99	120.48	111.81
2	D	401	A1IY9	C2-C3-S1	7.94	120.43	111.81
2	E	401	A1IY9	C2-C3-S1	7.94	120.42	111.81
2	B	401	A1IY9	C2-C3-S1	7.81	120.28	111.81
2	E	401	A1IY9	C30-O18-C29	7.34	135.97	118.80
2	K	401	A1IY9	C2-C3-S1	7.11	119.52	111.81
2	F	401	A1IY9	C2-C3-S1	6.76	119.14	111.81
2	H	401	A1IY9	C2-C3-S1	6.75	119.13	111.81
2	J	401	A1IY9	C2-C3-S1	6.46	118.82	111.81
2	L	401	A1IY9	C2-C3-S1	6.41	118.77	111.81
2	B	401	A1IY9	C30-O18-C29	6.32	133.57	118.80
2	F	401	A1IY9	C30-O18-C29	6.19	133.28	118.80
2	F	401	A1IY9	C23-C24-C16	-5.41	93.64	103.22
2	G	401	A1IY9	C30-O18-C29	5.00	130.50	118.80
2	E	401	A1IY9	O1-C3-C2	-4.99	116.11	124.12
2	G	401	A1IY9	O7-P1-O6	4.94	136.68	112.24
2	A	401	A1IY9	O1-C3-C2	-4.79	116.42	124.12
2	L	401	A1IY9	C23-C24-C16	-4.74	94.81	103.22
2	I	401	A1IY9	C2-C3-S1	4.74	116.95	111.81
2	L	401	A1IY9	O1-C3-C2	-4.72	116.54	124.12
2	G	401	A1IY9	O1-C3-C2	-4.66	116.63	124.12
2	J	401	A1IY9	C30-O18-C29	4.60	129.57	118.80
2	A	401	A1IY9	C13-C11-C14	-4.55	100.82	108.23
2	D	401	A1IY9	C23-C24-C16	-4.44	95.36	103.22
2	I	401	A1IY9	C23-C24-C16	-4.30	95.60	103.22
2	K	401	A1IY9	C23-C24-C16	-4.25	95.68	103.22
2	B	401	A1IY9	O1-C3-C2	-4.22	117.33	124.12
2	J	401	A1IY9	C23-C24-C16	-4.13	95.91	103.22
2	H	401	A1IY9	O1-C3-C2	-4.07	117.58	124.12
2	H	401	A1IY9	C8-C7-C6	4.05	119.10	112.36
2	F	401	A1IY9	O1-C3-C2	-4.00	117.70	124.12
2	G	401	A1IY9	C23-C24-C16	-3.90	96.32	103.22
2	F	401	A1IY9	O7-P1-O6	3.88	131.45	112.24
2	J	401	A1IY9	O1-C3-C2	-3.88	117.88	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	A1IY9	C13-C11-C14	-3.86	101.94	108.23
2	B	401	A1IY9	C23-C24-C16	-3.81	96.47	103.22
2	H	401	A1IY9	C13-C11-C14	3.77	114.39	108.23
2	A	401	A1IY9	O7-P1-O6	3.73	130.70	112.24
2	E	401	A1IY9	C23-C24-C16	-3.71	96.65	103.22
2	E	401	A1IY9	O13-C23-C24	3.70	121.67	111.17
2	C	401	A1IY9	C2-C3-S1	3.66	115.79	111.81
2	K	401	A1IY9	O16-P3-O14	-3.63	89.73	105.99
2	C	401	A1IY9	O1-C3-C2	-3.54	118.43	124.12
2	A	401	A1IY9	C23-C24-C16	-3.50	97.02	103.22
2	F	401	A1IY9	O13-C23-C24	3.47	121.03	111.17
2	C	401	A1IY9	C25-C2-C3	3.45	117.33	109.90
2	I	401	A1IY9	O7-P1-O6	3.43	129.20	112.24
2	C	401	A1IY9	C23-C24-C16	-3.38	97.24	103.22
2	D	401	A1IY9	O1-C3-S1	-3.32	119.33	123.80
2	L	401	A1IY9	O7-P1-O6	3.31	128.58	112.24
2	B	401	A1IY9	O17-P3-O15	-3.29	97.79	110.68
2	A	401	A1IY9	C4-S1-C3	3.28	111.63	101.75
2	I	401	A1IY9	O1-C3-C2	-3.28	118.84	124.12
2	K	401	A1IY9	O17-P3-O16	3.17	119.75	107.64
2	I	401	A1IY9	C5-N1-C6	-3.13	117.02	122.84
2	L	401	A1IY9	C1-C2-C25	3.12	120.40	112.92
2	D	401	A1IY9	O7-P1-O6	3.10	127.56	112.24
2	K	401	A1IY9	O1-C3-C2	-3.08	119.16	124.12
2	H	401	A1IY9	C19-C20-N5	3.08	125.04	120.35
2	K	401	A1IY9	O7-P1-O6	2.97	126.91	112.24
2	F	401	A1IY9	C1-C2-C25	2.96	120.02	112.92
2	H	401	A1IY9	C12-C11-C14	-2.95	103.43	108.23
2	I	401	A1IY9	C30-O18-C29	2.94	125.67	118.80
2	K	401	A1IY9	O5-P1-O6	-2.92	97.67	109.07
2	D	401	A1IY9	C30-O18-C29	2.90	125.58	118.80
2	F	401	A1IY9	C12-C11-C14	2.89	112.95	108.23
2	J	401	A1IY9	C13-C11-C10	2.89	113.82	108.82
2	H	401	A1IY9	C23-C24-C16	-2.79	98.28	103.22
2	C	401	A1IY9	O5-P1-O6	-2.79	98.17	109.07
2	I	401	A1IY9	C19-C20-N5	2.79	124.59	120.35
2	G	401	A1IY9	C19-C20-N5	2.77	124.56	120.35
2	B	401	A1IY9	O17-P3-O16	2.75	118.14	107.64
2	K	401	A1IY9	C19-C20-N5	2.74	124.52	120.35
2	E	401	A1IY9	C19-C20-N5	2.72	124.48	120.35
2	B	401	A1IY9	O18-C29-C36	-2.67	110.71	119.10
2	C	401	A1IY9	O7-P1-O6	2.63	125.25	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	A1IY9	O17-P3-O14	-2.62	94.25	105.99
2	F	401	A1IY9	C19-C20-N5	2.61	124.31	120.35
2	B	401	A1IY9	O18-C29-C28	2.59	128.51	119.38
2	C	401	A1IY9	C19-C20-N5	2.56	124.25	120.35
2	I	401	A1IY9	O17-P3-O16	2.53	117.30	107.64
2	G	401	A1IY9	O5-P1-O6	-2.50	99.29	109.07
2	A	401	A1IY9	C19-C20-N5	2.50	124.15	120.35
2	E	401	A1IY9	C25-C2-C3	2.46	115.20	109.90
2	B	401	A1IY9	C19-C20-N5	2.44	124.06	120.35
2	D	401	A1IY9	O1-C3-C2	-2.44	120.20	124.12
2	C	401	A1IY9	C30-O18-C29	-2.43	113.12	118.80
2	G	401	A1IY9	C25-C2-C3	2.41	115.09	109.90
2	J	401	A1IY9	O18-C29-C36	-2.40	111.56	119.10
2	A	401	A1IY9	C13-C11-C10	2.37	112.93	108.82
2	H	401	A1IY9	P2-O8-P1	2.36	140.94	132.83
2	J	401	A1IY9	O18-C29-C28	2.34	127.62	119.38
2	E	401	A1IY9	O18-C29-C36	-2.34	111.76	119.10
2	J	401	A1IY9	O7-P1-O6	2.33	123.77	112.24
2	A	401	A1IY9	O7-P1-O5	2.33	118.56	107.75
2	F	401	A1IY9	C13-C11-C10	2.32	112.85	108.82
2	B	401	A1IY9	O7-P1-O6	2.31	123.67	112.24
2	E	401	A1IY9	O16-P3-O14	2.29	116.27	105.99
2	G	401	A1IY9	O17-P3-O16	2.29	116.39	107.64
2	H	401	A1IY9	O16-P3-O14	2.29	116.23	105.99
2	I	401	A1IY9	C25-C2-C3	2.26	114.78	109.90
2	J	401	A1IY9	C19-C20-N5	2.26	123.79	120.35
2	E	401	A1IY9	O18-C29-C28	2.25	127.29	119.38
2	D	401	A1IY9	O5-P1-O6	-2.24	100.32	109.07
2	A	401	A1IY9	O16-P3-O14	2.24	116.02	105.99
2	G	401	A1IY9	O18-C29-C28	2.23	127.24	119.38
2	A	401	A1IY9	C12-C11-C14	2.20	111.82	108.23
2	L	401	A1IY9	C19-C20-N5	2.20	123.69	120.35
2	H	401	A1IY9	O7-P1-O6	2.18	123.00	112.24
2	E	401	A1IY9	C12-C11-C14	-2.17	104.69	108.23
2	J	401	A1IY9	O5-C14-C11	-2.17	107.06	110.55
2	D	401	A1IY9	C19-C20-N5	2.14	123.61	120.35
2	G	401	A1IY9	O5-C14-C11	-2.14	107.11	110.55
2	C	401	A1IY9	C13-C11-C10	2.14	112.53	108.82
2	H	401	A1IY9	C12-C11-C10	2.14	112.52	108.82
2	G	401	A1IY9	O18-C29-C36	-2.09	112.55	119.10
2	J	401	A1IY9	C12-C11-C14	2.09	111.64	108.23
2	H	401	A1IY9	C8-N2-C9	2.07	126.28	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1IY9	C15-C16-C24	2.07	121.26	114.40
2	B	401	A1IY9	C25-C2-C3	2.07	114.36	109.90
2	L	401	A1IY9	C1-C2-C3	-2.07	105.47	111.88
2	G	401	A1IY9	C13-C11-C14	2.06	111.59	108.23
2	A	401	A1IY9	C1-C2-C25	2.06	117.85	112.92
2	H	401	A1IY9	O17-P3-O15	2.05	118.72	110.68
2	A	401	A1IY9	O5-P1-O6	-2.05	101.08	109.07
2	B	401	A1IY9	C1-C2-C25	2.04	117.81	112.92
2	A	401	A1IY9	C5-N1-C6	2.03	126.61	122.84
2	C	401	A1IY9	C15-C16-C24	2.02	121.09	114.40
2	I	401	A1IY9	C12-C11-C14	2.01	111.51	108.23
2	K	401	A1IY9	C1-C2-C25	2.01	117.73	112.92
2	B	401	A1IY9	O13-C23-C24	2.00	116.86	111.17

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1IY9	C9-C10-C11-C14
2	A	401	A1IY9	C9-C10-C11-C12
2	A	401	A1IY9	C9-C10-C11-C13
2	A	401	A1IY9	C6-C7-C8-N2
2	A	401	A1IY9	C25-C2-C3-O1
2	A	401	A1IY9	C25-C2-C3-S1
2	A	401	A1IY9	C2-C3-S1-C4
2	A	401	A1IY9	O1-C3-S1-C4
2	A	401	A1IY9	C14-O5-P1-O6
2	A	401	A1IY9	C14-O5-P1-O8
2	A	401	A1IY9	C15-O11-P2-O8
2	B	401	A1IY9	C25-C2-C3-O1
2	B	401	A1IY9	C25-C2-C3-S1
2	B	401	A1IY9	C15-O11-P2-O8
2	B	401	A1IY9	C24-O14-P3-O17
2	C	401	A1IY9	C25-C2-C3-O1
2	C	401	A1IY9	C25-C2-C3-S1
2	C	401	A1IY9	C15-O11-P2-O8
2	C	401	A1IY9	C15-O11-P2-O10
2	D	401	A1IY9	C25-C2-C3-O1
2	D	401	A1IY9	C25-C2-C3-S1
2	D	401	A1IY9	C15-O11-P2-O8
2	E	401	A1IY9	C9-C10-C11-C14
2	E	401	A1IY9	C6-C7-C8-N2

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Mol	Chain	Res	Type	Atoms
2	E	401	A1IY9	C14-O5-P1-O8
2	E	401	A1IY9	C15-O11-P2-O10
2	E	401	A1IY9	O11-C15-C16-O12
2	F	401	A1IY9	C9-C10-C11-C14
2	F	401	A1IY9	C9-C10-C11-C12
2	F	401	A1IY9	O4-C10-C11-C12
2	F	401	A1IY9	C9-C10-C11-C13
2	F	401	A1IY9	C25-C2-C3-S1
2	F	401	A1IY9	C14-O5-P1-O6
2	F	401	A1IY9	C14-O5-P1-O7
2	F	401	A1IY9	C15-O11-P2-O8
2	F	401	A1IY9	C24-O14-P3-O15
2	F	401	A1IY9	C24-O14-P3-O17
2	G	401	A1IY9	C6-C7-C8-N2
2	G	401	A1IY9	C15-O11-P2-O8
2	G	401	A1IY9	C15-O11-P2-O10
2	H	401	A1IY9	C9-C10-C11-C14
2	H	401	A1IY9	C6-C7-C8-N2
2	H	401	A1IY9	C25-C2-C3-S1
2	H	401	A1IY9	C14-O5-P1-O6
2	H	401	A1IY9	C14-O5-P1-O7
2	H	401	A1IY9	O11-C15-C16-O12
2	I	401	A1IY9	C25-C2-C3-S1
2	I	401	A1IY9	C2-C3-S1-C4
2	I	401	A1IY9	C14-O5-P1-O6
2	I	401	A1IY9	C15-O11-P2-O8
2	J	401	A1IY9	C15-O11-P2-O8
2	J	401	A1IY9	C24-O14-P3-O15
2	K	401	A1IY9	C6-C7-C8-N2
2	K	401	A1IY9	C15-O11-P2-O8
2	L	401	A1IY9	C25-C2-C3-S1
2	L	401	A1IY9	C15-O11-P2-O8
2	A	401	A1IY9	C7-C6-N1-C5
2	H	401	A1IY9	C16-C24-O14-P3
2	H	401	A1IY9	C23-C24-O14-P3
2	A	401	A1IY9	O2-C6-N1-C5
2	C	401	A1IY9	C6-C7-C8-N2
2	D	401	A1IY9	C6-C7-C8-N2
2	F	401	A1IY9	C6-C7-C8-N2
2	I	401	A1IY9	C6-C7-C8-N2
2	J	401	A1IY9	C6-C7-C8-N2
2	L	401	A1IY9	C6-C7-C8-N2

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Mol	Chain	Res	Type	Atoms
2	E	401	A1IY9	C2-C3-S1-C4
2	G	401	A1IY9	C2-C3-S1-C4
2	K	401	A1IY9	C2-C3-S1-C4
2	A	401	A1IY9	O4-C10-C11-C12
2	F	401	A1IY9	O4-C10-C11-C13
2	I	401	A1IY9	O11-C15-C16-O12
2	H	401	A1IY9	C25-C2-C3-O1
2	H	401	A1IY9	C9-C10-C11-C12
2	D	401	A1IY9	C24-O14-P3-O16
2	H	401	A1IY9	C14-O5-P1-O8
2	L	401	A1IY9	C24-O14-P3-O16
2	C	401	A1IY9	O11-C15-C16-O12
2	B	401	A1IY9	C15-O11-P2-O9
2	B	401	A1IY9	C15-O11-P2-O10
2	D	401	A1IY9	C15-O11-P2-O9
2	D	401	A1IY9	C15-O11-P2-O10
2	E	401	A1IY9	C14-O5-P1-O6
2	F	401	A1IY9	C15-O11-P2-O9
2	F	401	A1IY9	C15-O11-P2-O10
2	I	401	A1IY9	C15-O11-P2-O9
2	I	401	A1IY9	C15-O11-P2-O10
2	J	401	A1IY9	C15-O11-P2-O9
2	J	401	A1IY9	C15-O11-P2-O10
2	K	401	A1IY9	C15-O11-P2-O9
2	K	401	A1IY9	C15-O11-P2-O10
2	L	401	A1IY9	C15-O11-P2-O9
2	L	401	A1IY9	C15-O11-P2-O10
2	I	401	A1IY9	O1-C3-S1-C4
2	K	401	A1IY9	O1-C3-S1-C4
2	A	401	A1IY9	O4-C10-C11-C14
2	E	401	A1IY9	O4-C10-C11-C14
2	F	401	A1IY9	O4-C10-C11-C14
2	H	401	A1IY9	O4-C10-C11-C14
2	E	401	A1IY9	C25-C2-C3-O1
2	F	401	A1IY9	C25-C2-C3-O1
2	G	401	A1IY9	C25-C2-C3-O1
2	I	401	A1IY9	C25-C2-C3-O1
2	J	401	A1IY9	C25-C2-C3-O1
2	K	401	A1IY9	C25-C2-C3-O1
2	L	401	A1IY9	C25-C2-C3-O1
2	C	401	A1IY9	P1-O8-P2-O9
2	J	401	A1IY9	P1-O8-P2-O9

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Mol	Chain	Res	Type	Atoms
2	K	401	A1IY9	P1-O8-P2-O9
2	B	401	A1IY9	C6-C7-C8-N2
2	G	401	A1IY9	O11-C15-C16-O12
2	K	401	A1IY9	O11-C15-C16-O12
2	L	401	A1IY9	O11-C15-C16-O12
2	E	401	A1IY9	C13-C11-C14-O5
2	H	401	A1IY9	C11-C10-C9-N2
2	E	401	A1IY9	C25-C2-C3-S1
2	G	401	A1IY9	C25-C2-C3-S1
2	J	401	A1IY9	C25-C2-C3-S1
2	K	401	A1IY9	C25-C2-C3-S1
2	A	401	A1IY9	O11-C15-C16-O12
2	B	401	A1IY9	O11-C15-C16-O12
2	F	401	A1IY9	O11-C15-C16-O12
2	A	401	A1IY9	C5-C4-S1-C3
2	G	401	A1IY9	O1-C3-S1-C4
2	C	401	A1IY9	C2-C3-S1-C4
2	F	401	A1IY9	C2-C3-S1-C4
2	J	401	A1IY9	C2-C3-S1-C4
2	B	401	A1IY9	P1-O8-P2-O9
2	B	401	A1IY9	P1-O8-P2-O10
2	G	401	A1IY9	P1-O8-P2-O9
2	E	401	A1IY9	C24-O14-P3-O15
2	A	401	A1IY9	C4-C5-N1-C6
2	E	401	A1IY9	C9-C10-C11-C12
2	E	401	A1IY9	C16-C24-O14-P3
2	B	401	A1IY9	C24-O14-P3-O16
2	E	401	A1IY9	O4-C10-C11-C13
2	F	401	A1IY9	C14-O5-P1-O8
2	J	401	A1IY9	C24-O14-P3-O17
2	L	401	A1IY9	C24-O14-P3-O17
2	D	401	A1IY9	O11-C15-C16-O12
2	J	401	A1IY9	O11-C15-C16-O12
2	D	401	A1IY9	P1-O8-P2-O10
2	E	401	A1IY9	P1-O8-P2-O9
2	E	401	A1IY9	P1-O8-P2-O10
2	F	401	A1IY9	P1-O8-P2-O10
2	H	401	A1IY9	P1-O8-P2-O9
2	J	401	A1IY9	P1-O8-P2-O10
2	L	401	A1IY9	P1-O8-P2-O10
2	H	401	A1IY9	C11-C10-C9-O3
2	L	401	A1IY9	C16-C24-O14-P3

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Mol	Chain	Res	Type	Atoms
2	B	401	A1IY9	C2-C3-S1-C4
2	H	401	A1IY9	C2-C3-S1-C4

There are no ring outliers.

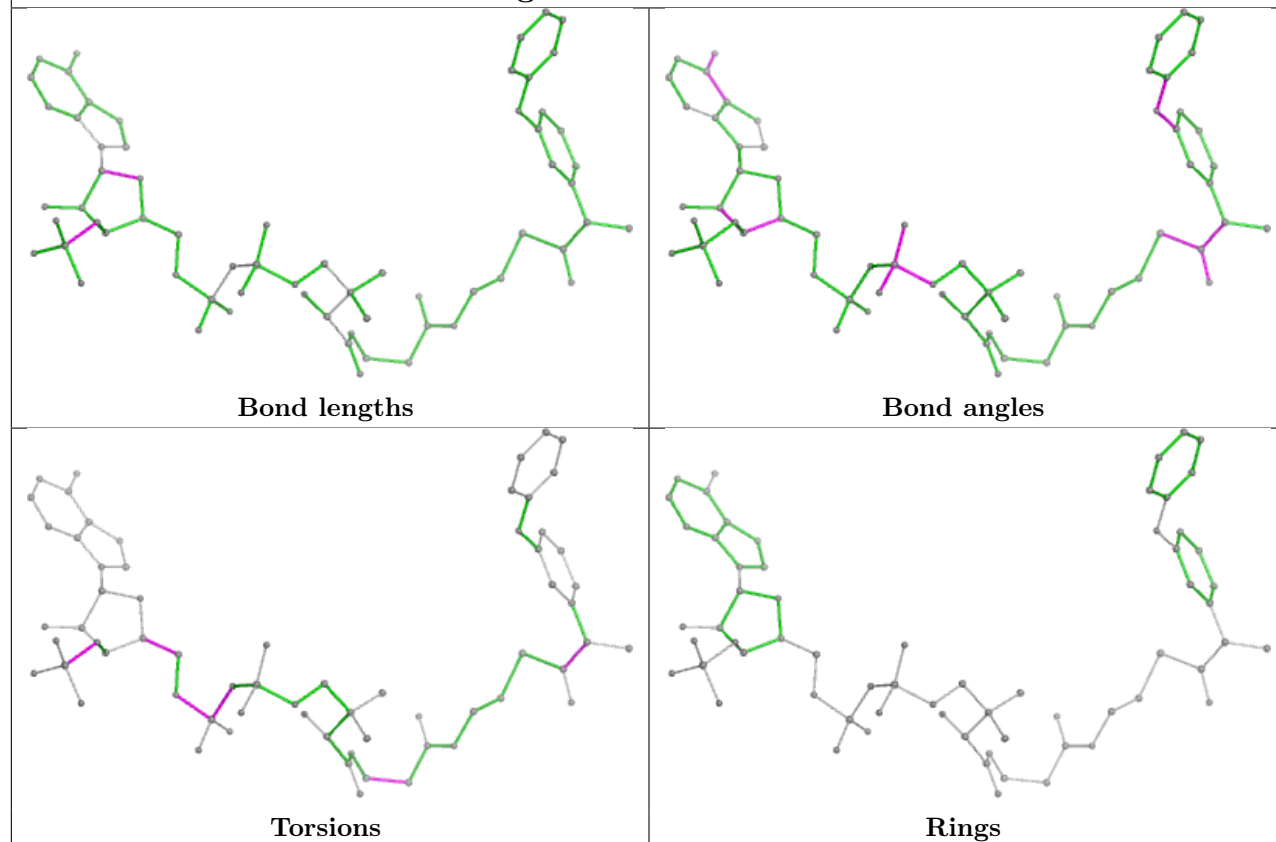
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	A1IY9	6	0
2	F	401	A1IY9	3	0
2	A	401	A1IY9	2	0
2	I	401	A1IY9	1	0
2	K	401	A1IY9	2	0
2	J	401	A1IY9	1	0
2	L	401	A1IY9	1	0
2	E	401	A1IY9	1	0
2	H	401	A1IY9	4	0

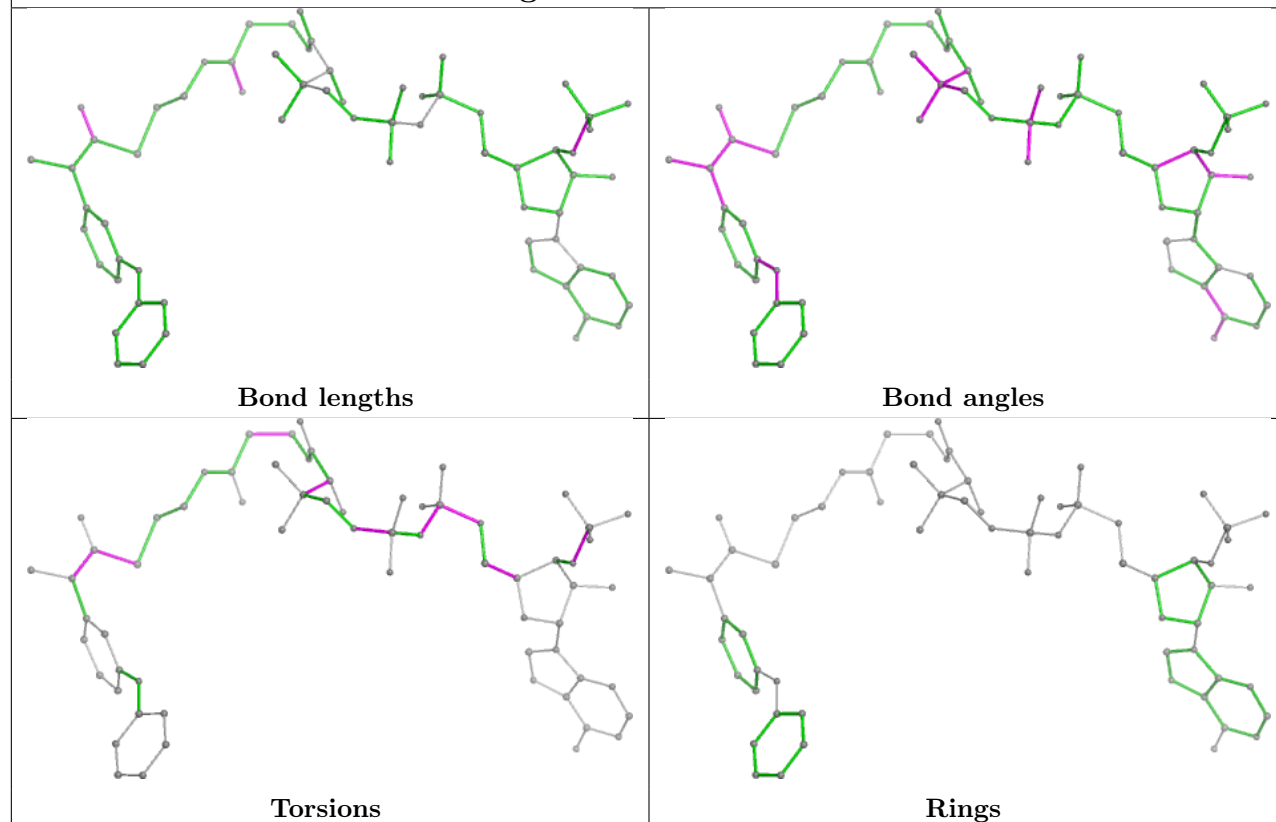
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



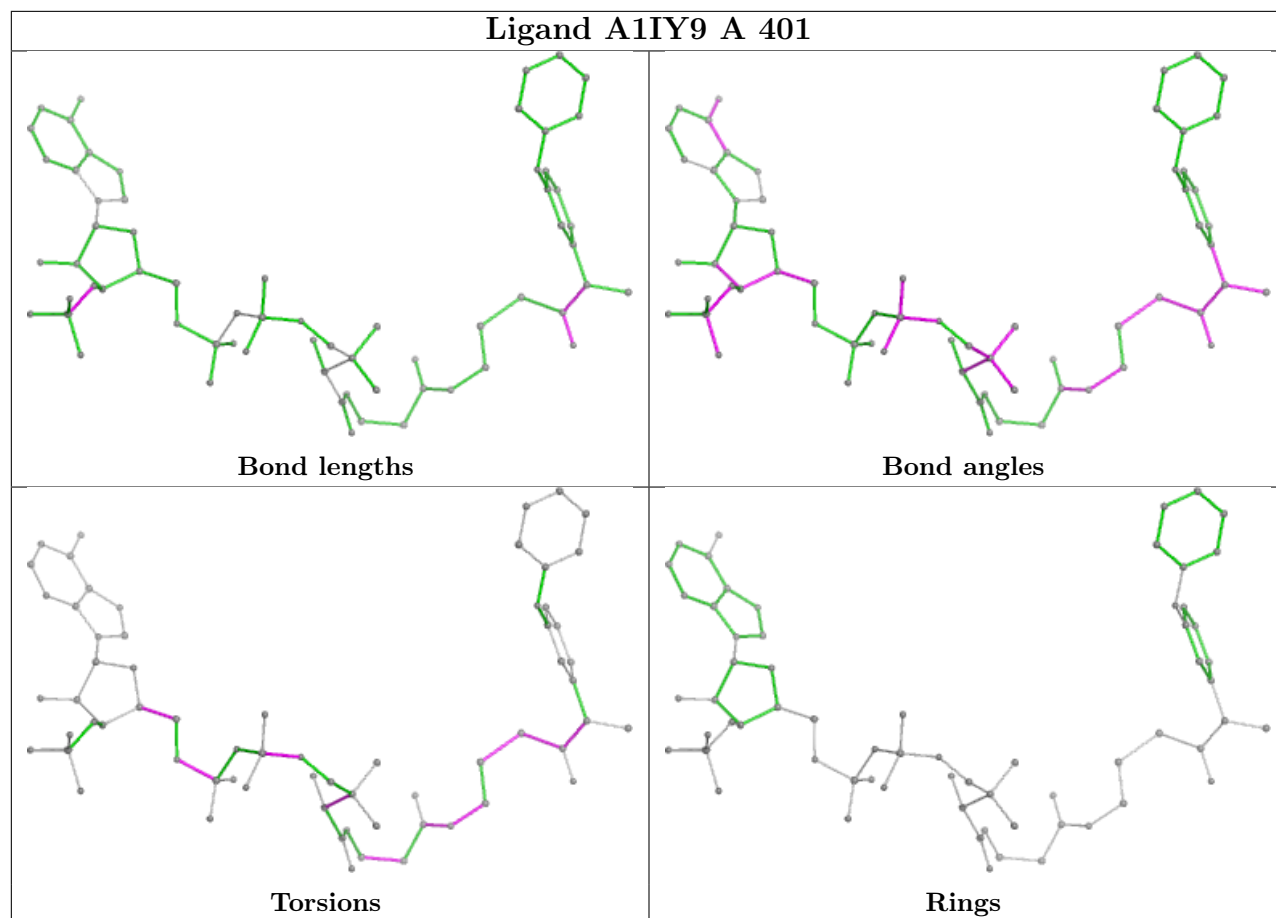
## Ligand A1IY9 D 401

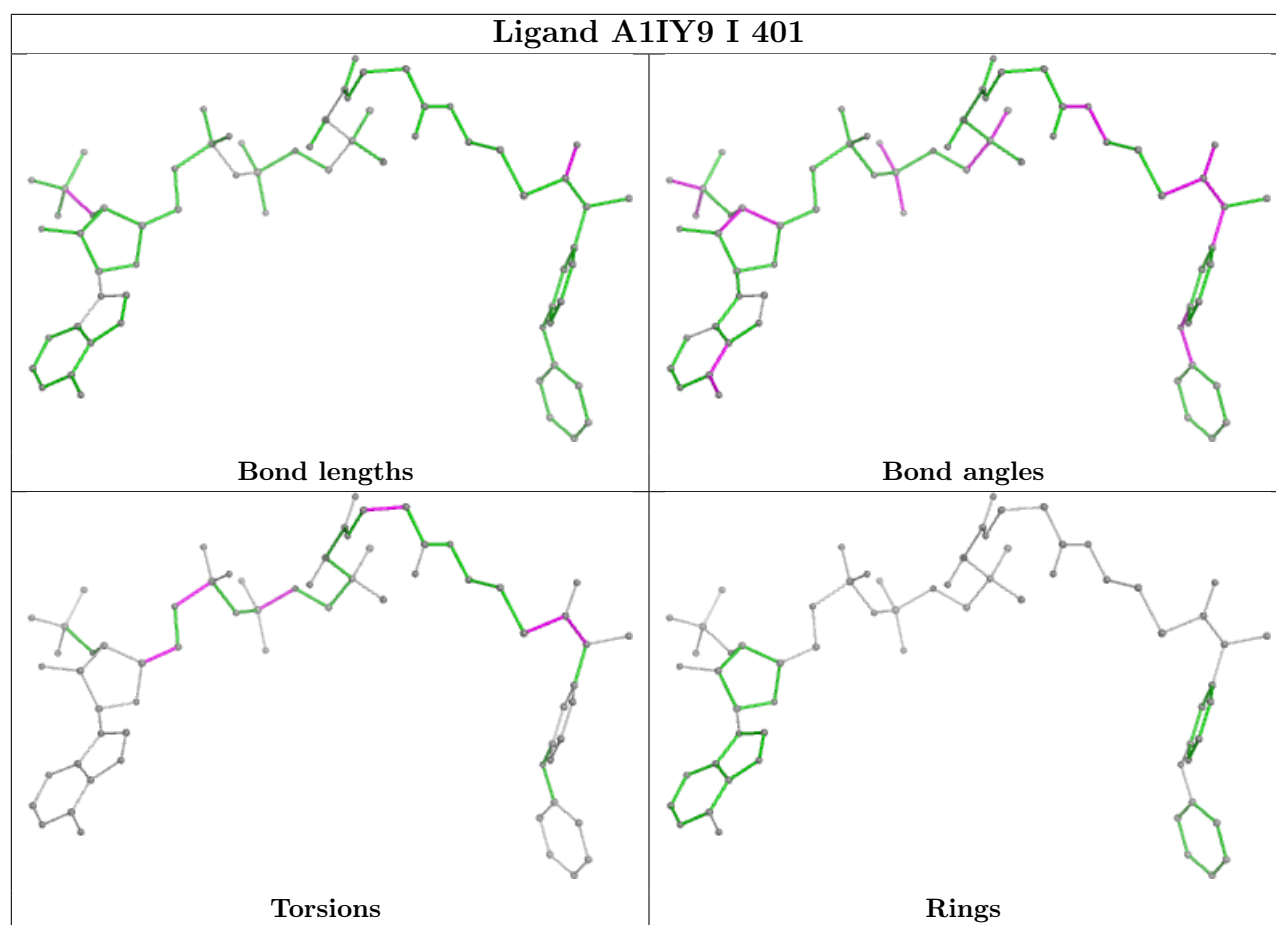


## Ligand A1IY9 F 401

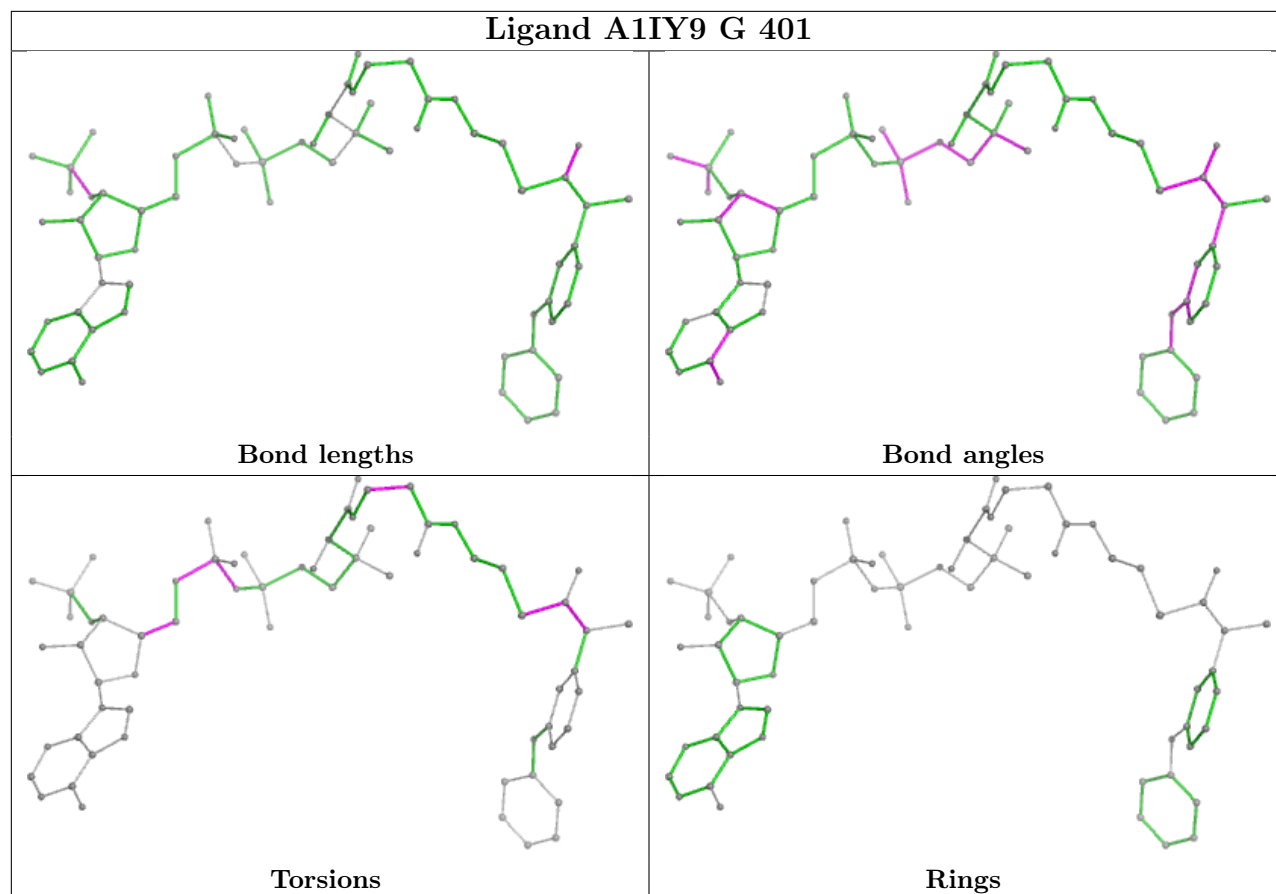


## Ligand A1IY9 A 401

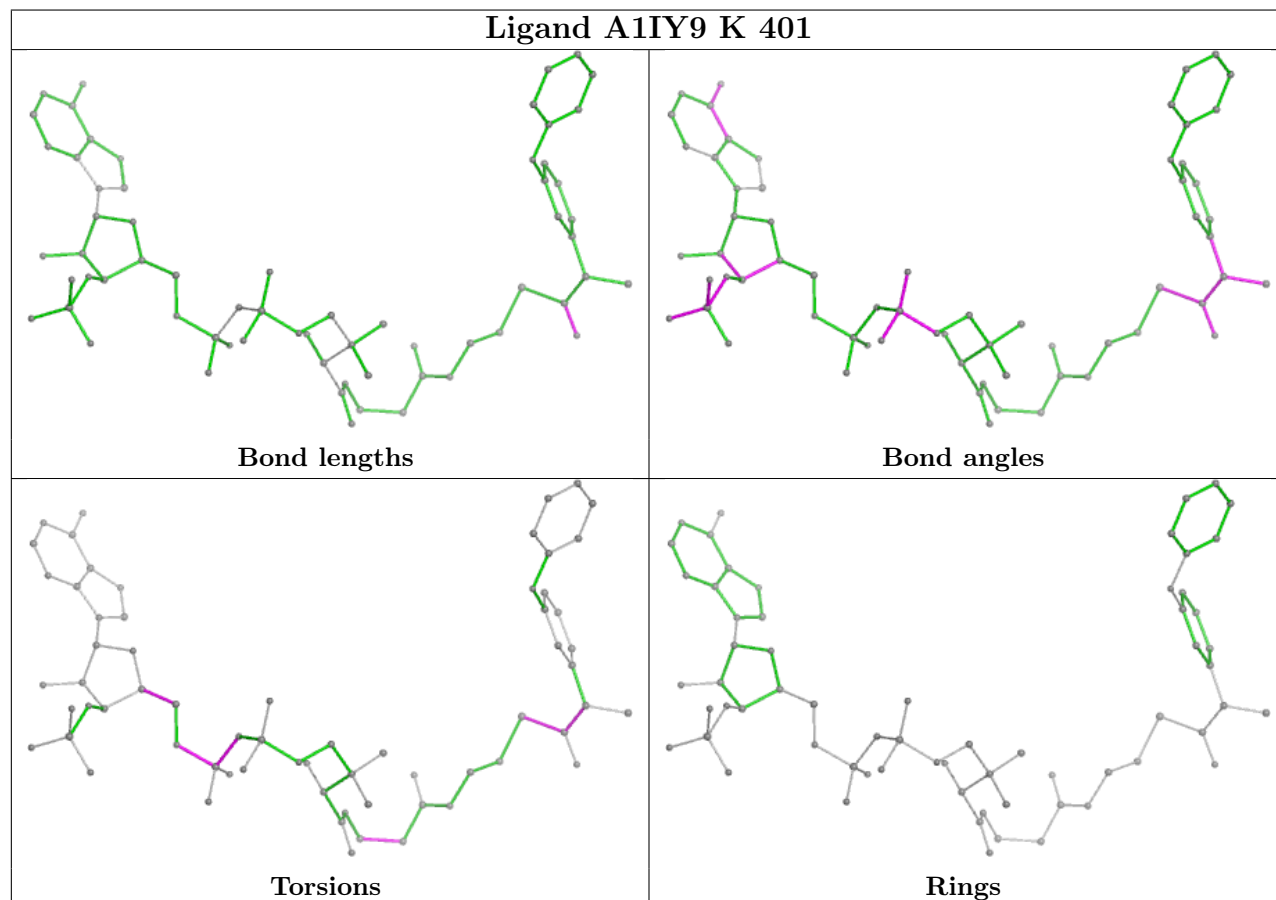




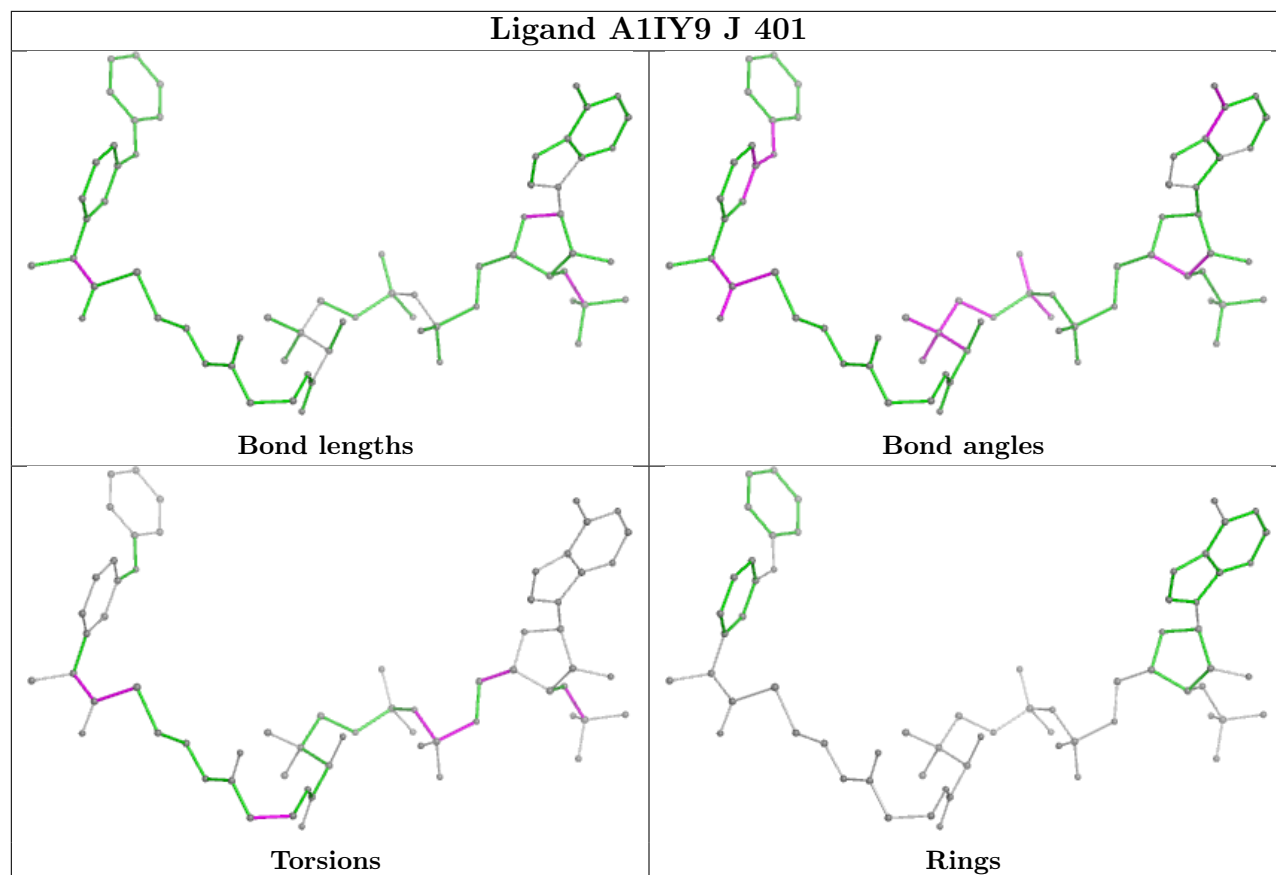
## Ligand A1IY9 G 401



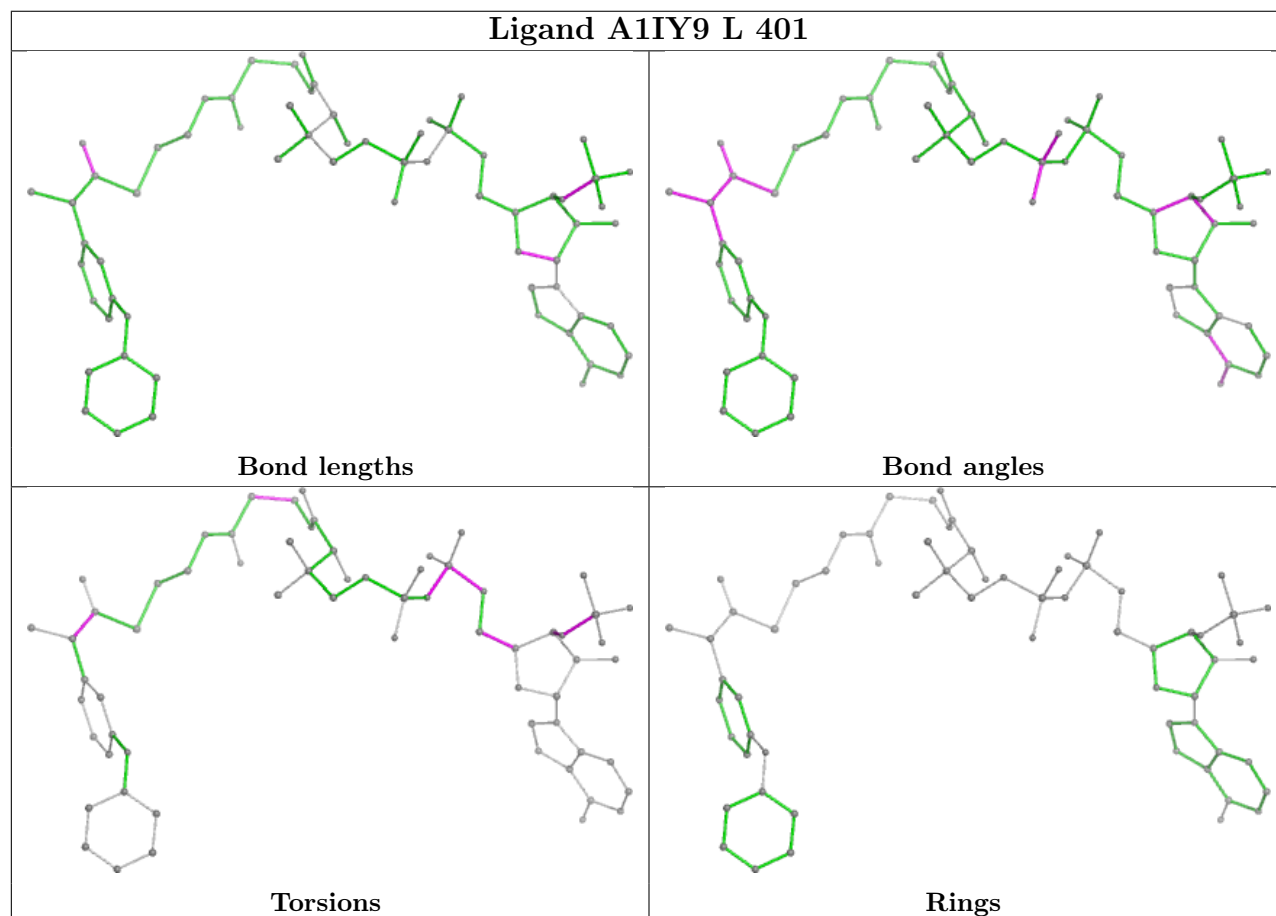
## Ligand A1IY9 K 401



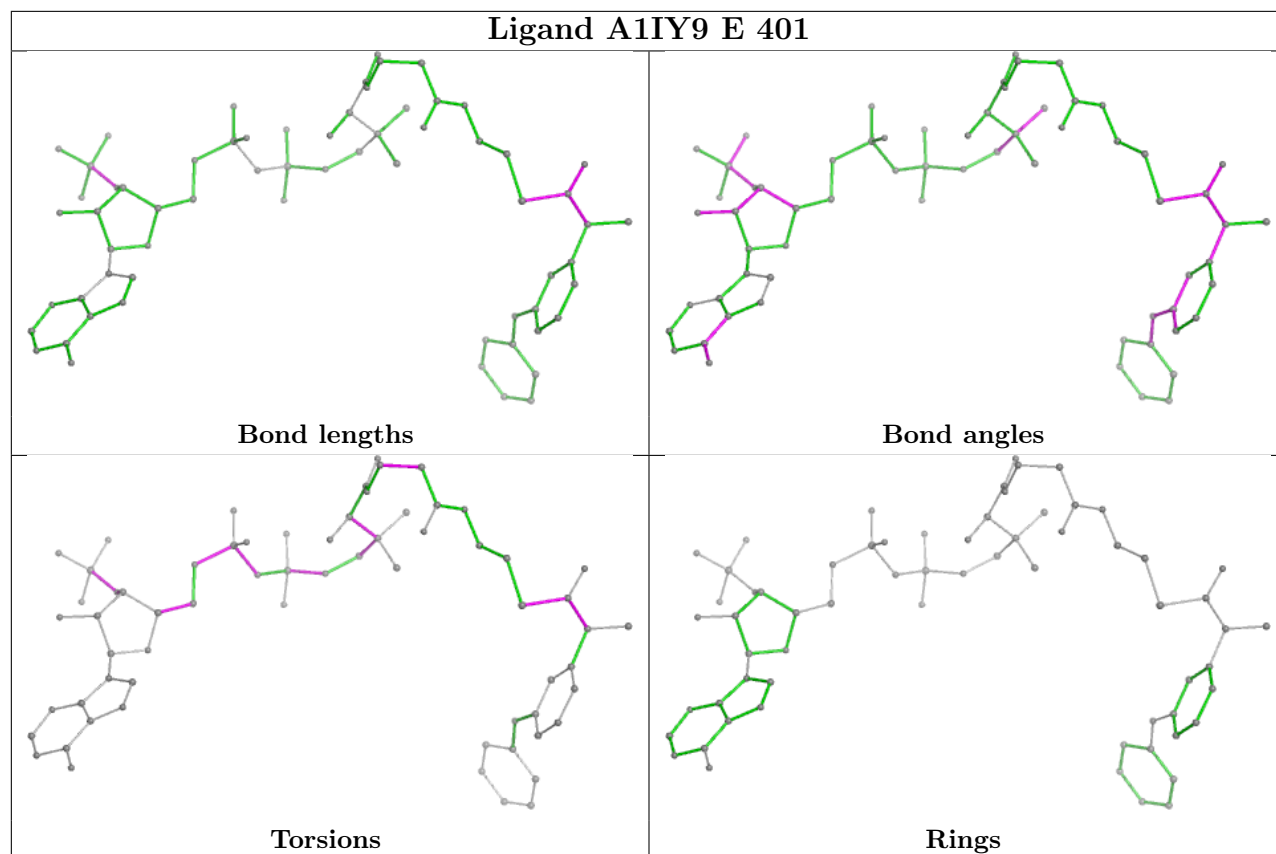
## Ligand A1IY9 J 401



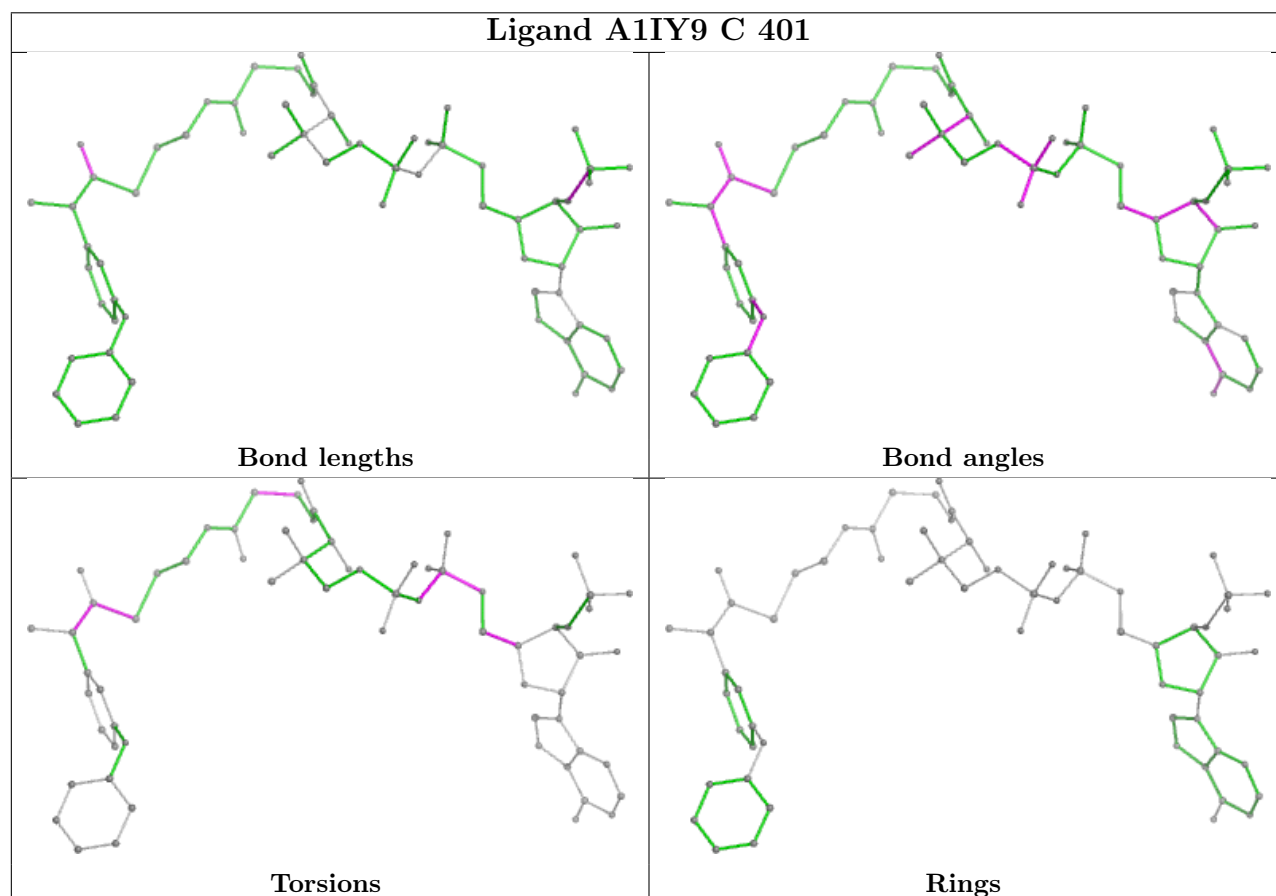
## Ligand A1IY9 L 401



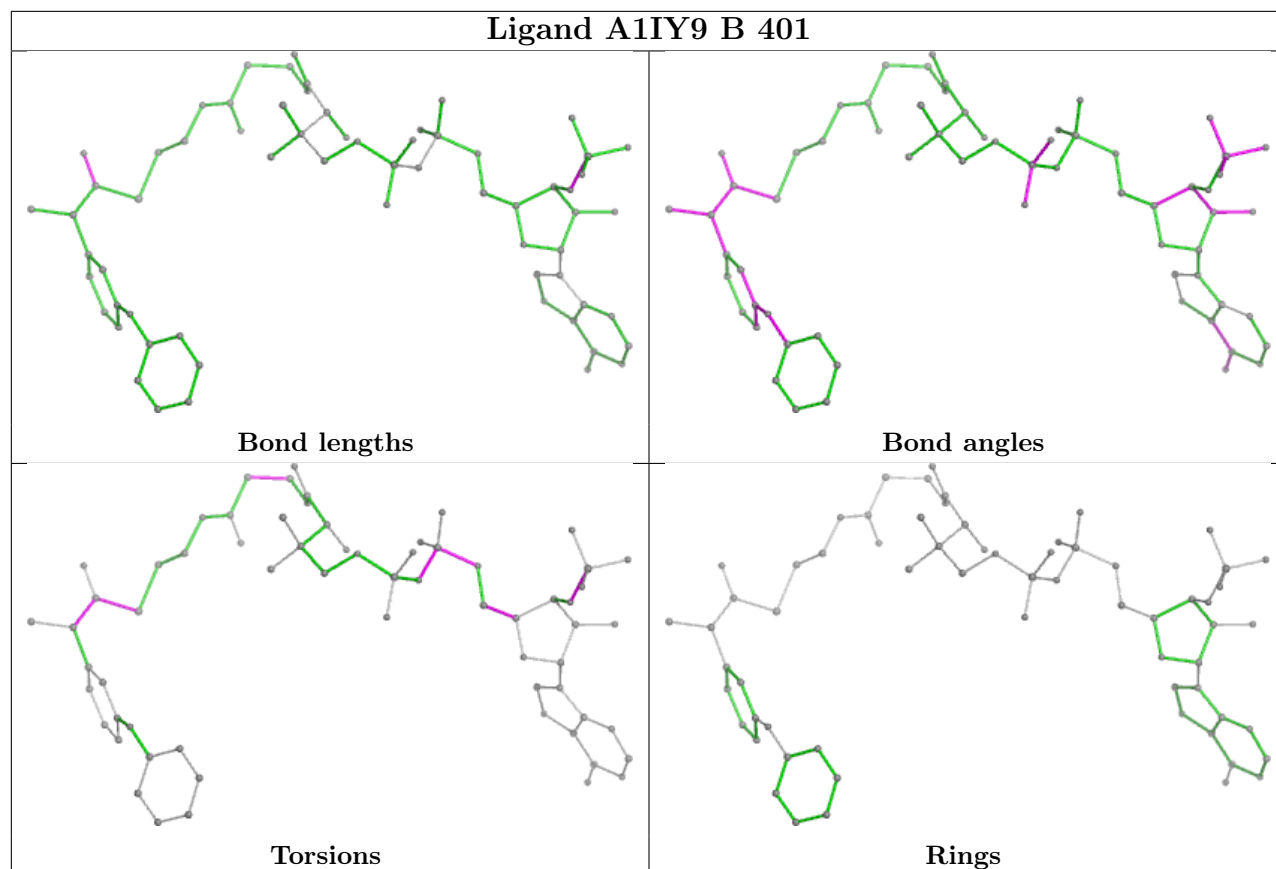
## Ligand A1IY9 E 401



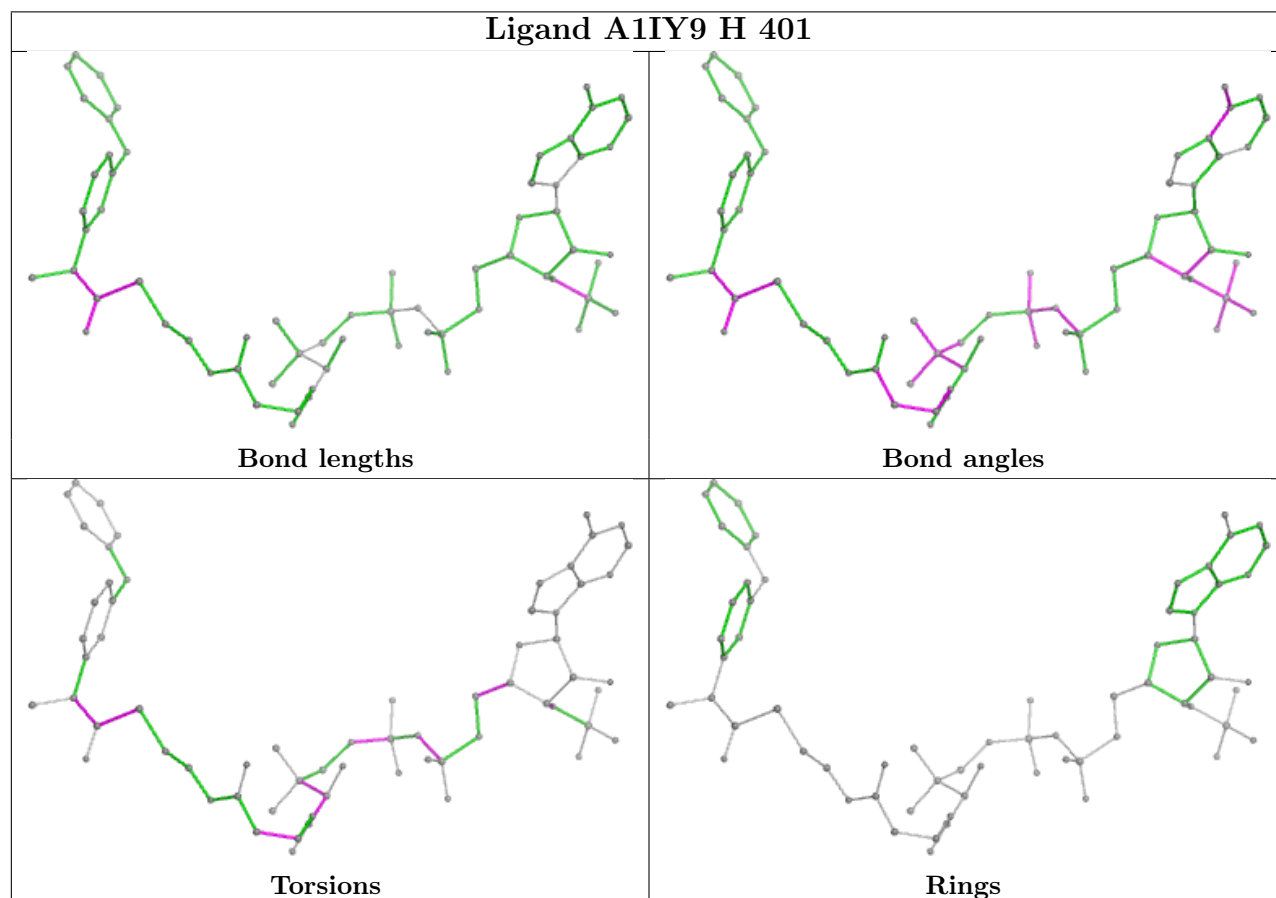
## Ligand A1IY9 C 401



## Ligand A1IY9 B 401



## Ligand A1IY9 H 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	358/364 (98%)	0.87	62 (17%) <b>5</b> <b>4</b>	27, 42, 83, 112	2 (0%)
1	B	357/364 (98%)	0.64	30 (8%) <b>18</b> <b>20</b>	26, 42, 82, 114	1 (0%)
1	C	358/364 (98%)	0.86	68 (18%) <b>4</b> <b>3</b>	26, 43, 84, 113	2 (0%)
1	D	359/364 (98%)	0.91	59 (16%) <b>5</b> <b>5</b>	27, 43, 82, 121	1 (0%)
1	E	356/364 (97%)	1.03	79 (22%) <b>3</b> <b>2</b>	21, 44, 90, 118	3 (0%)
1	F	357/364 (98%)	1.11	83 (23%) <b>2</b> <b>2</b>	27, 46, 86, 120	1 (0%)
1	G	358/364 (98%)	1.28	100 (27%) <b>2</b> <b>1</b>	28, 47, 96, 119	2 (0%)
1	H	356/364 (97%)	1.02	74 (20%) <b>3</b> <b>3</b>	26, 46, 93, 122	1 (0%)
1	I	359/364 (98%)	0.69	32 (8%) <b>17</b> <b>18</b>	26, 41, 76, 115	2 (0%)
1	J	357/364 (98%)	0.60	25 (7%) <b>24</b> <b>25</b>	27, 41, 75, 114	1 (0%)
1	K	357/364 (98%)	0.79	51 (14%) <b>7</b> <b>7</b>	26, 42, 82, 109	2 (0%)
1	L	359/364 (98%)	0.87	53 (14%) <b>7</b> <b>7</b>	27, 43, 80, 118	1 (0%)
All	All	4291/4368 (98%)	0.89	716 (16%) <b>5</b> <b>5</b>	21, 43, 85, 122	19 (0%)

All (716) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	ALA	8.2
1	C	346	ALA	7.5
1	G	346	ALA	6.7
1	F	351	ILE	6.7
1	J	346	ALA	6.4
1	A	346	ALA	6.3
1	L	45	ILE	6.2
1	K	45	ILE	6.1
1	A	42	VAL	6.0
1	G	42	VAL	5.8
1	C	42	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	349	ILE	5.5
1	F	346	ALA	5.3
1	H	358	TRP	5.3
1	D	42	VAL	5.3
1	L	323	ASN	5.3
1	H	351	ILE	5.2
1	G	102	VAL	5.2
1	E	346	ALA	5.1
1	H	45	ILE	5.0
1	D	346	ALA	5.0
1	F	42	VAL	5.0
1	E	351	ILE	4.9
1	G	355	LEU	4.8
1	H	349	ILE	4.8
1	L	351	ILE	4.8
1	K	347	ALA	4.7
1	F	49	ALA	4.6
1	I	45	ILE	4.5
1	G	358	TRP	4.5
1	H	7	GLY	4.5
1	J	45	ILE	4.5
1	A	351	ILE	4.5
1	G	351	ILE	4.5
1	J	144	ASP	4.5
1	I	351	ILE	4.4
1	D	322	ALA	4.4
1	K	49	ALA	4.4
1	G	10	VAL	4.4
1	L	46	SER	4.4
1	L	92	LEU	4.3
1	J	351	ILE	4.3
1	H	144	ASP	4.3
1	H	59	ALA	4.3
1	A	45	ILE	4.3
1	C	45	ILE	4.3
1	C	66	GLY	4.2
1	G	69	LEU	4.2
1	C	75	ALA	4.2
1	D	44	GLY	4.2
1	B	351	ILE	4.2
1	A	324	GLY	4.2
1	E	7	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	33	VAL	4.2
1	A	322	ALA	4.1
1	D	59	ALA	4.1
1	J	347	ALA	4.1
1	K	349	ILE	4.1
1	F	173	TRP	4.1
1	F	48	ASP	4.1
1	I	41	SER	4.1
1	H	355	LEU	4.1
1	G	61	LEU	4.1
1	G	354	VAL	4.1
1	H	34	VAL	4.1
1	A	180	LYS	4.0
1	B	45	ILE	4.0
1	C	171	ALA	4.0
1	L	346	ALA	4.0
1	F	47	ARG	4.0
1	L	173	TRP	4.0
1	E	207	MET	4.0
1	H	346	ALA	4.0
1	H	40	SER	4.0
1	G	56	ILE	4.0
1	A	323	ASN	4.0
1	H	44	GLY	4.0
1	L	80	LEU	4.0
1	F	27	GLY	3.9
1	G	79	VAL	3.9
1	A	348	THR	3.9
1	K	180	LYS	3.9
1	J	324	GLY	3.9
1	G	349	ILE	3.9
1	A	355	LEU	3.9
1	L	94	LEU	3.9
1	G	322	ALA	3.9
1	C	351	ILE	3.8
1	G	7	GLY	3.8
1	F	57	VAL	3.8
1	D	45	ILE	3.8
1	C	347	ALA	3.7
1	G	178	SER	3.7
1	G	8	LEU	3.7
1	G	347	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	96	PRO	3.7
1	C	323	ASN	3.7
1	F	7	GLY	3.7
1	L	324	GLY	3.7
1	G	59	ALA	3.7
1	G	348	THR	3.7
1	F	345	PRO	3.7
1	G	57	VAL	3.7
1	G	45	ILE	3.7
1	E	355	LEU	3.7
1	E	77	ALA	3.7
1	K	345	PRO	3.6
1	H	5	LEU	3.6
1	H	73	LEU	3.6
1	K	324	GLY	3.6
1	F	348	THR	3.6
1	I	58	THR	3.6
1	D	347	ALA	3.6
1	F	43	ASP	3.6
1	E	173	TRP	3.6
1	G	11	VAL	3.6
1	C	177	SER	3.6
1	I	180	LYS	3.6
1	G	71	LEU	3.6
1	G	70	ALA	3.6
1	D	345	PRO	3.6
1	A	358	TRP	3.6
1	E	358	TRP	3.6
1	H	57	VAL	3.6
1	D	355	LEU	3.6
1	G	94	LEU	3.6
1	G	1	MET	3.6
1	E	10	VAL	3.6
1	E	75	ALA	3.5
1	C	176	GLN	3.5
1	D	48	ASP	3.5
1	D	351	ILE	3.5
1	F	349	ILE	3.5
1	G	34	VAL	3.5
1	G	107	ILE	3.5
1	C	69	LEU	3.5
1	D	94	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	2	ALA	3.5
1	H	39	PRO	3.5
1	G	93	GLY	3.5
1	L	30	GLY	3.5
1	F	358	TRP	3.5
1	G	173	TRP	3.5
1	G	73	LEU	3.5
1	F	347	ALA	3.4
1	C	76	LYS	3.4
1	G	324	GLY	3.4
1	E	56	ILE	3.4
1	I	349	ILE	3.4
1	F	71	LEU	3.4
1	H	8	LEU	3.4
1	E	347	ALA	3.4
1	I	346	ALA	3.4
1	K	47	ARG	3.4
1	A	173	TRP	3.4
1	A	349	ILE	3.4
1	G	144	ASP	3.4
1	F	354	VAL	3.4
1	G	88	VAL	3.4
1	E	204	ALA	3.4
1	H	322	ALA	3.4
1	G	97	GLU	3.4
1	A	93	GLY	3.4
1	K	44	GLY	3.4
1	L	7	GLY	3.4
1	E	79	VAL	3.3
1	D	56	ILE	3.3
1	B	346	ALA	3.3
1	B	358	TRP	3.3
1	G	353	ALA	3.3
1	I	358	TRP	3.3
1	L	47	ARG	3.3
1	L	44	GLY	3.3
1	F	33	VAL	3.3
1	F	176	GLN	3.3
1	D	348	THR	3.3
1	D	92	LEU	3.3
1	F	67	LEU	3.3
1	I	61	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	3.3
1	H	353	ALA	3.3
1	D	27	GLY	3.3
1	D	323	ASN	3.3
1	F	323	ASN	3.3
1	H	58	THR	3.3
1	B	40	SER	3.3
1	E	45	ILE	3.3
1	E	59	ALA	3.3
1	H	105	ARG	3.3
1	H	6	SER	3.3
1	D	107	ILE	3.2
1	E	345	PRO	3.2
1	A	49	ALA	3.2
1	I	292	ALA	3.2
1	H	176	GLN	3.2
1	F	106	LEU	3.2
1	K	71	LEU	3.2
1	B	345	PRO	3.2
1	H	345	PRO	3.2
1	G	36	ILE	3.2
1	K	322	ALA	3.2
1	A	44	GLY	3.2
1	H	173	TRP	3.2
1	F	79	VAL	3.2
1	F	355	LEU	3.2
1	G	76	LYS	3.2
1	G	180	LYS	3.2
1	F	10	VAL	3.2
1	I	42	VAL	3.2
1	F	69	LEU	3.2
1	H	61	LEU	3.2
1	L	345	PRO	3.2
1	B	75	ALA	3.2
1	B	204	ALA	3.2
1	D	2	ALA	3.2
1	K	351	ILE	3.2
1	L	207	MET	3.2
1	E	34	VAL	3.1
1	G	183	VAL	3.1
1	C	358	TRP	3.1
1	I	144	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	76	LYS	3.1
1	A	347	ALA	3.1
1	H	107	ILE	3.1
1	G	58	THR	3.1
1	B	76	LYS	3.1
1	E	73	LEU	3.1
1	D	324	GLY	3.1
1	I	1	MET	3.1
1	E	16	ILE	3.1
1	G	75	ALA	3.1
1	L	349	ILE	3.1
1	K	102	VAL	3.1
1	G	359	ASP	3.1
1	C	180	LYS	3.1
1	K	348	THR	3.1
1	D	358	TRP	3.0
1	A	74	ILE	3.0
1	H	56	ILE	3.0
1	H	352	GLU	3.0
1	A	69	LEU	3.0
1	A	92	LEU	3.0
1	G	80	LEU	3.0
1	H	92	LEU	3.0
1	I	69	LEU	3.0
1	I	259	LEU	3.0
1	C	173	TRP	3.0
1	D	173	TRP	3.0
1	E	47	ARG	3.0
1	H	207	MET	3.0
1	A	345	PRO	3.0
1	D	30	GLY	3.0
1	F	34	VAL	3.0
1	H	323	ASN	3.0
1	I	324	GLY	3.0
1	L	355	LEU	3.0
1	F	59	ALA	3.0
1	F	70	ALA	3.0
1	I	47	ARG	3.0
1	C	349	ILE	3.0
1	D	74	ILE	3.0
1	F	74	ILE	3.0
1	J	349	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	324	GLY	3.0
1	E	39	PRO	3.0
1	F	39	PRO	3.0
1	L	88	VAL	3.0
1	L	102	VAL	3.0
1	K	355	LEU	3.0
1	A	76	LYS	3.0
1	B	144	ASP	2.9
1	G	357	ASP	2.9
1	I	207	MET	2.9
1	K	56	ILE	2.9
1	L	41	SER	2.9
1	B	65	GLN	2.9
1	F	11	VAL	2.9
1	L	79	VAL	2.9
1	L	71	LEU	2.9
1	G	62	LYS	2.9
1	G	101	LYS	2.9
1	B	77	ALA	2.9
1	G	77	ALA	2.9
1	G	292	ALA	2.9
1	B	207	MET	2.9
1	G	177	SER	2.9
1	I	173	TRP	2.9
1	E	176	GLN	2.9
1	G	176	GLN	2.9
1	B	324	GLY	2.9
1	K	96	PRO	2.9
1	D	8	LEU	2.9
1	K	72	LYS	2.9
1	E	322	ALA	2.9
1	A	40	SER	2.9
1	E	323	ASN	2.9
1	H	10	VAL	2.9
1	H	102	VAL	2.9
1	L	69	LEU	2.9
1	A	77	ALA	2.9
1	G	100	ALA	2.9
1	H	77	ALA	2.9
1	L	75	ALA	2.9
1	L	322	ALA	2.9
1	L	74	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	323	ASN	2.9
1	D	7	GLY	2.9
1	G	30	GLY	2.9
1	F	73	LEU	2.8
1	G	106	LEU	2.8
1	C	77	ALA	2.8
1	D	31	ALA	2.8
1	A	30	GLY	2.8
1	H	180	LYS	2.8
1	J	207	MET	2.8
1	E	172	LEU	2.8
1	F	80	LEU	2.8
1	L	357	ASP	2.8
1	D	102	VAL	2.8
1	H	49	ALA	2.8
1	F	107	ILE	2.8
1	E	179	GLY	2.8
1	E	67	LEU	2.8
1	H	106	LEU	2.8
1	H	31	ALA	2.8
1	K	40	SER	2.8
1	G	323	ASN	2.8
1	A	56	ILE	2.8
1	E	30	GLY	2.8
1	G	66	GLY	2.8
1	G	207	MET	2.8
1	H	50	MET	2.8
1	G	99	CYS	2.8
1	F	357	ASP	2.8
1	C	61	LEU	2.8
1	E	69	LEU	2.8
1	E	80	LEU	2.8
1	G	92	LEU	2.8
1	H	69	LEU	2.8
1	K	73	LEU	2.8
1	E	11	VAL	2.8
1	H	354	VAL	2.8
1	A	6	SER	2.8
1	A	177	SER	2.8
1	B	44	GLY	2.7
1	C	144	ASP	2.7
1	F	26	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	92	LEU	2.7
1	G	63	SER	2.7
1	H	79	VAL	2.7
1	F	322	ALA	2.7
1	F	326	TRP	2.7
1	D	95	GLY	2.7
1	A	356	THR	2.7
1	F	101	LYS	2.7
1	K	80	LEU	2.7
1	E	178	SER	2.7
1	A	354	VAL	2.7
1	H	326	TRP	2.7
1	K	176	GLN	2.7
1	F	56	ILE	2.7
1	C	350	ASP	2.7
1	L	359	ASP	2.7
1	E	5	LEU	2.7
1	G	67	LEU	2.7
1	G	293	ASN	2.7
1	E	46	SER	2.7
1	D	79	VAL	2.7
1	F	75	ALA	2.7
1	J	102	VAL	2.7
1	L	2	ALA	2.7
1	E	66	GLY	2.7
1	F	93	GLY	2.7
1	G	87	GLY	2.7
1	G	55	ARG	2.7
1	J	173	TRP	2.7
1	K	173	TRP	2.7
1	C	56	ILE	2.7
1	C	74	ILE	2.7
1	C	107	ILE	2.7
1	H	16	ILE	2.7
1	B	72	LYS	2.6
1	F	1	MET	2.6
1	K	1	MET	2.6
1	B	41	SER	2.6
1	D	40	SER	2.6
1	A	34	VAL	2.6
1	C	10	VAL	2.6
1	I	2	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	83	GLY	2.6
1	D	144	ASP	2.6
1	K	359	ASP	2.6
1	B	173	TRP	2.6
1	B	1	MET	2.6
1	E	1	MET	2.6
1	D	80	LEU	2.6
1	G	5	LEU	2.6
1	C	11	VAL	2.6
1	C	30	GLY	2.6
1	K	34	VAL	2.6
1	D	349	ILE	2.6
1	G	345	PRO	2.6
1	A	46	SER	2.6
1	F	46	SER	2.6
1	H	178	SER	2.6
1	B	73	LEU	2.6
1	C	80	LEU	2.6
1	C	106	LEU	2.6
1	E	106	LEU	2.6
1	F	5	LEU	2.6
1	C	93	GLY	2.6
1	E	100	ALA	2.6
1	G	49	ALA	2.6
1	C	57	VAL	2.6
1	G	72	LYS	2.6
1	J	72	LYS	2.6
1	E	58	THR	2.6
1	C	178	SER	2.6
1	C	8	LEU	2.6
1	F	61	LEU	2.6
1	G	172	LEU	2.6
1	C	353	ALA	2.5
1	E	76	LYS	2.5
1	F	72	LYS	2.5
1	H	183	VAL	2.5
1	L	320	TYR	2.5
1	H	74	ILE	2.5
1	D	6	SER	2.5
1	F	259	LEU	2.5
1	H	80	LEU	2.5
1	H	179	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	44	GLY	2.5
1	K	75	ALA	2.5
1	F	184	VAL	2.5
1	C	105	ARG	2.5
1	A	39	PRO	2.5
1	H	334	PHE	2.5
1	E	62	LYS	2.5
1	E	93	GLY	2.5
1	G	326	TRP	2.5
1	K	358	TRP	2.5
1	D	32	ASP	2.5
1	D	1	MET	2.5
1	L	1	MET	2.5
1	C	102	VAL	2.5
1	H	47	ARG	2.5
1	G	356	THR	2.5
1	L	348	THR	2.5
1	A	96	PRO	2.5
1	E	74	ILE	2.5
1	F	81	ILE	2.5
1	E	72	LYS	2.5
1	H	72	LYS	2.5
1	C	167	GLY	2.5
1	D	5	LEU	2.5
1	E	359	ASP	2.5
1	C	99	CYS	2.5
1	A	75	ALA	2.5
1	C	49	ALA	2.5
1	C	345	PRO	2.4
1	E	40	SER	2.4
1	K	76	LYS	2.4
1	F	25	ILE	2.4
1	K	107	ILE	2.4
1	H	324	GLY	2.4
1	A	80	LEU	2.4
1	G	9	ARG	2.4
1	J	71	LEU	2.4
1	L	67	LEU	2.4
1	C	59	ALA	2.4
1	E	31	ALA	2.4
1	J	75	ALA	2.4
1	J	353	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	352	GLU	2.4
1	I	10	VAL	2.4
1	G	74	ILE	2.4
1	L	107	ILE	2.4
1	C	44	GLY	2.4
1	D	93	GLY	2.4
1	I	44	GLY	2.4
1	L	181	GLY	2.4
1	D	357	ASP	2.4
1	F	28	ASP	2.4
1	F	359	ASP	2.4
1	F	293	ASN	2.4
1	C	348	THR	2.4
1	K	58	THR	2.4
1	A	72	LYS	2.4
1	C	101	LYS	2.4
1	K	10	VAL	2.4
1	L	34	VAL	2.4
1	L	354	VAL	2.4
1	H	46	SER	2.4
1	K	41	SER	2.4
1	H	108	TYR	2.4
1	A	7	GLY	2.4
1	E	87	GLY	2.4
1	H	36	ILE	2.4
1	K	74	ILE	2.4
1	K	181	GLY	2.4
1	B	350	ASP	2.4
1	C	67	LEU	2.4
1	C	71	LEU	2.4
1	F	94	LEU	2.4
1	G	26	LEU	2.4
1	D	49	ALA	2.4
1	E	70	ALA	2.4
1	E	171	ALA	2.4
1	G	171	ALA	2.4
1	I	77	ALA	2.4
1	B	356	THR	2.4
1	C	72	LYS	2.4
1	A	10	VAL	2.4
1	D	11	VAL	2.4
1	H	11	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	40	SER	2.4
1	A	1	MET	2.4
1	A	9	ARG	2.4
1	D	43	ASP	2.4
1	F	144	ASP	2.4
1	C	355	LEU	2.3
1	F	169	LEU	2.3
1	J	355	LEU	2.3
1	B	323	ASN	2.3
1	A	59	ALA	2.3
1	C	100	ALA	2.3
1	G	31	ALA	2.3
1	H	75	ALA	2.3
1	E	348	THR	2.3
1	L	58	THR	2.3
1	A	178	SER	2.3
1	B	46	SER	2.3
1	F	50	MET	2.3
1	K	207	MET	2.3
1	I	326	TRP	2.3
1	E	350	ASP	2.3
1	F	36	ILE	2.3
1	C	94	LEU	2.3
1	E	26	LEU	2.3
1	H	172	LEU	2.3
1	J	73	LEU	2.3
1	C	170	ALA	2.3
1	E	257	ALA	2.3
1	F	58	THR	2.3
1	C	1	MET	2.3
1	K	39	PRO	2.3
1	A	79	VAL	2.3
1	C	79	VAL	2.3
1	D	88	VAL	2.3
1	D	176	GLN	2.3
1	A	68	GLU	2.3
1	C	87	GLY	2.3
1	G	3	GLY	2.3
1	G	32	ASP	2.3
1	I	359	ASP	2.3
1	L	350	ASP	2.3
1	L	358	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	62	LYS	2.3
1	A	94	LEU	2.3
1	J	67	LEU	2.3
1	F	9	ARG	2.3
1	C	322	ALA	2.3
1	D	75	ALA	2.3
1	J	49	ALA	2.3
1	K	59	ALA	2.3
1	L	6	SER	2.3
1	A	102	VAL	2.3
1	I	354	VAL	2.3
1	K	11	VAL	2.3
1	L	42	VAL	2.3
1	E	37	ASP	2.3
1	F	87	GLY	2.3
1	C	108	TYR	2.3
1	G	108	TYR	2.3
1	D	51	LEU	2.3
1	D	106	LEU	2.3
1	K	67	LEU	2.3
1	H	1	MET	2.3
1	K	178	SER	2.3
1	C	39	PRO	2.2
1	E	104	ASP	2.2
1	E	88	VAL	2.2
1	H	3	GLY	2.2
1	K	93	GLY	2.2
1	E	180	LYS	2.2
1	F	62	LYS	2.2
1	F	180	LYS	2.2
1	A	326	TRP	2.2
1	D	47	ARG	2.2
1	D	334	PHE	2.2
1	L	326	TRP	2.2
1	D	108	TYR	2.2
1	E	92	LEU	2.2
1	E	94	LEU	2.2
1	D	65	GLN	2.2
1	F	23	ALA	2.2
1	H	145	GLU	2.2
1	H	171	ALA	2.2
1	F	63	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	350	ASP	2.2
1	K	48	ASP	2.2
1	C	33	VAL	2.2
1	D	290	VAL	2.2
1	E	354	VAL	2.2
1	L	183	VAL	2.2
1	A	47	ARG	2.2
1	A	67	LEU	2.2
1	A	71	LEU	2.2
1	D	69	LEU	2.2
1	G	51	LEU	2.2
1	H	71	LEU	2.2
1	L	26	LEU	2.2
1	A	70	ALA	2.2
1	E	41	SER	2.2
1	F	31	ALA	2.2
1	G	41	SER	2.2
1	H	2	ALA	2.2
1	F	255	ASP	2.2
1	A	62	LYS	2.2
1	G	179	GLY	2.2
1	C	34	VAL	2.2
1	E	33	VAL	2.2
1	G	184	VAL	2.2
1	F	92	LEU	2.2
1	I	8	LEU	2.2
1	A	41	SER	2.2
1	C	40	SER	2.2
1	C	41	SER	2.2
1	F	2	ALA	2.2
1	F	32	ASP	2.2
1	H	32	ASP	2.2
1	G	39	PRO	2.2
1	A	288	GLY	2.2
1	B	7	GLY	2.2
1	C	47	ARG	2.2
1	K	79	VAL	2.2
1	F	207	MET	2.2
1	K	106	LEU	2.1
1	L	29	LEU	2.1
1	E	101	LYS	2.1
1	F	76	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	104	ASP	2.1
1	L	43	ASP	2.1
1	K	91	ARG	2.1
1	F	30	GLY	2.1
1	G	44	GLY	2.1
1	H	27	GLY	2.1
1	H	30	GLY	2.1
1	C	65	GLN	2.1
1	G	81	ILE	2.1
1	G	274	LEU	2.1
1	I	76	LYS	2.1
1	A	350	ASP	2.1
1	J	40	SER	2.1
1	C	2	ALA	2.1
1	E	2	ALA	2.1
1	E	353	ALA	2.1
1	K	70	ALA	2.1
1	A	66	GLY	2.1
1	E	108	TYR	2.1
1	E	324	GLY	2.1
1	D	34	VAL	2.1
1	F	102	VAL	2.1
1	B	62	LYS	2.1
1	E	105	ARG	2.1
1	C	51	LEU	2.1
1	B	348	THR	2.1
1	E	81	ILE	2.1
1	G	13	LEU	2.1
1	H	169	LEU	2.1
1	I	94	LEU	2.1
1	L	347	ALA	2.1
1	H	181	GLY	2.1
1	G	65	GLN	2.1
1	D	326	TRP	2.1
1	A	11	VAL	2.1
1	H	33	VAL	2.1
1	L	11	VAL	2.1
1	K	105	ARG	2.1
1	G	350	ASP	2.1
1	E	169	LEU	2.1
1	F	254	LEU	2.1
1	I	80	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	107	ILE	2.1
1	E	205	THR	2.1
1	H	348	THR	2.1
1	E	65	GLN	2.1
1	B	353	ALA	2.0
1	C	7	GLY	2.0
1	E	181	GLY	2.0
1	F	171	ALA	2.0
1	F	353	ALA	2.0
1	D	76	LYS	2.0
1	F	343	ARG	2.0
1	G	105	ARG	2.0
1	I	101	LYS	2.0
1	A	88	VAL	2.0
1	E	57	VAL	2.0
1	J	359	ASP	2.0
1	K	357	ASP	2.0
1	D	73	LEU	2.0
1	E	71	LEU	2.0
1	J	348	THR	2.0
1	K	94	LEU	2.0
1	L	51	LEU	2.0
1	L	106	LEU	2.0
1	F	314	ILE	2.0
1	L	36	ILE	2.0
1	A	95	GLY	2.0
1	D	53	ASN	2.0
1	B	59	ALA	2.0
1	C	91	ARG	2.0
1	G	343	ARG	2.0
1	J	326	TRP	2.0
1	A	43	ASP	2.0
1	A	48	ASP	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands

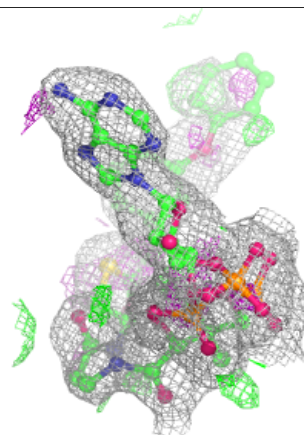
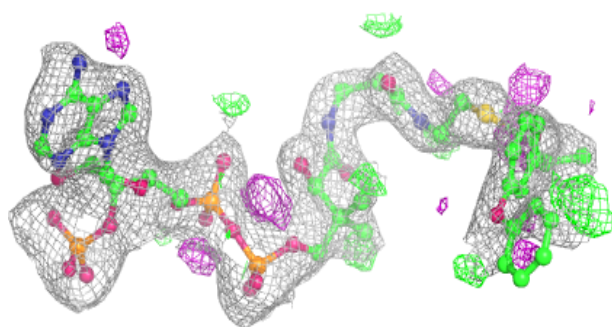
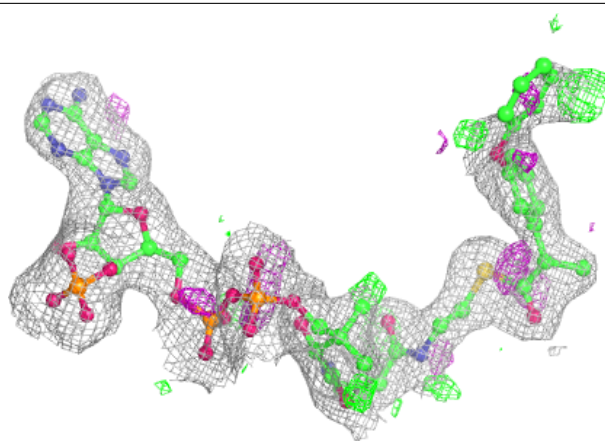
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1IY9	H	401	65/65	0.88	0.16	53,70,98,115	0
2	A1IY9	E	401	65/65	0.89	0.16	48,69,91,116	0
2	A1IY9	F	401	65/65	0.92	0.13	34,56,90,107	0
2	A1IY9	C	401	65/65	0.93	0.13	35,50,92,107	0
2	A1IY9	G	401	65/65	0.93	0.14	35,57,101,115	0
2	A1IY9	A	401	65/65	0.93	0.14	40,58,94,106	0
2	A1IY9	B	401	65/65	0.95	0.11	36,55,88,101	0
2	A1IY9	D	401	65/65	0.95	0.11	29,51,90,104	0
2	A1IY9	I	401	65/65	0.95	0.12	30,50,111,116	0
2	A1IY9	J	401	65/65	0.95	0.11	33,49,94,113	0
2	A1IY9	L	401	65/65	0.95	0.12	33,49,103,109	0
2	A1IY9	K	401	65/65	0.96	0.10	33,51,99,105	0

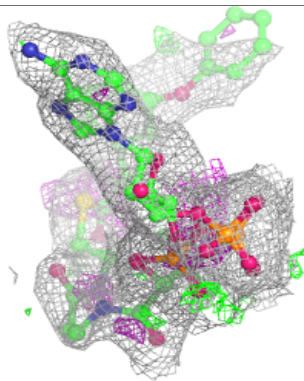
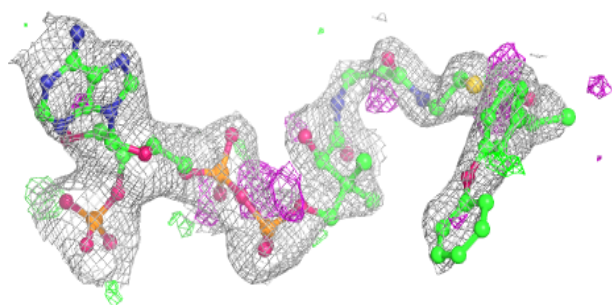
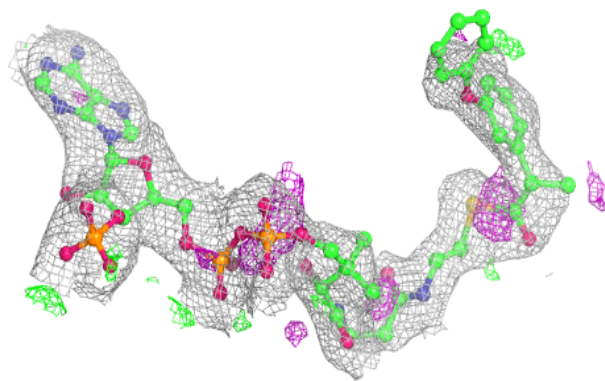
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IY9 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)

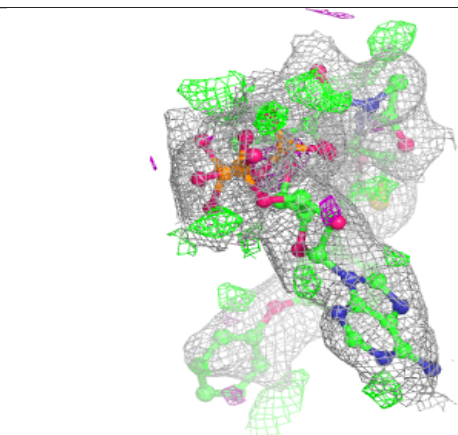
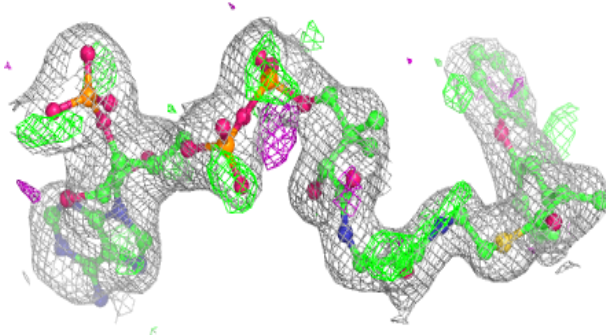
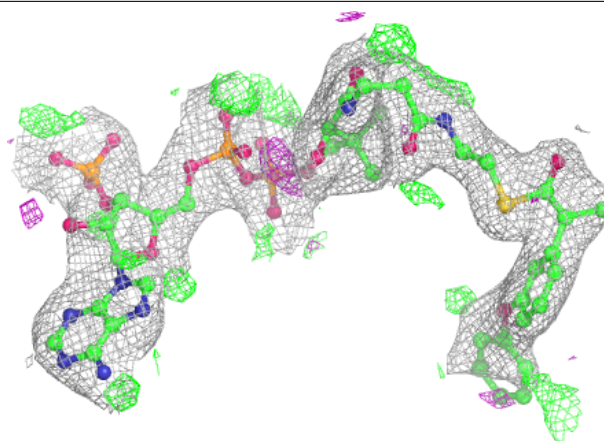
**Electron density around A1IY9 E 401:**

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

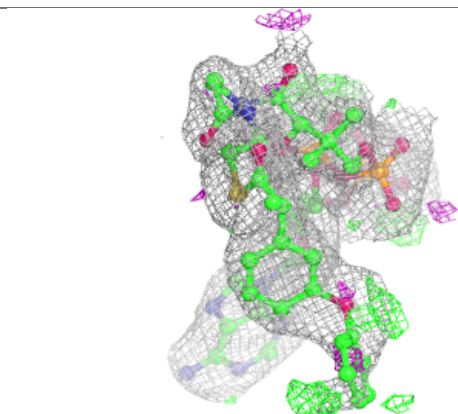
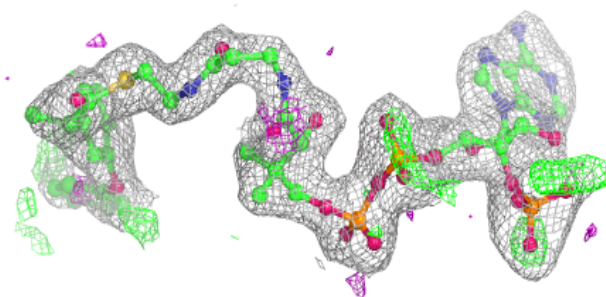
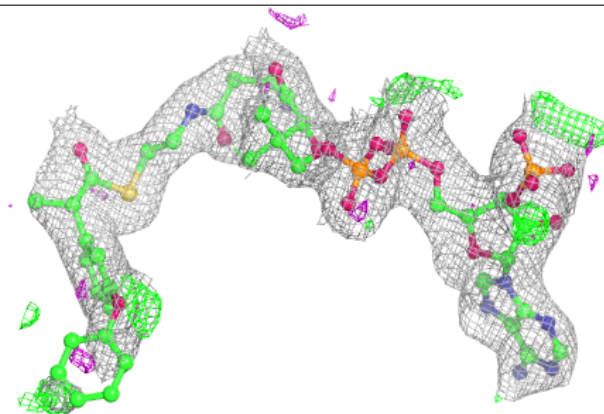


**Electron density around A1IY9 F 401:**

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

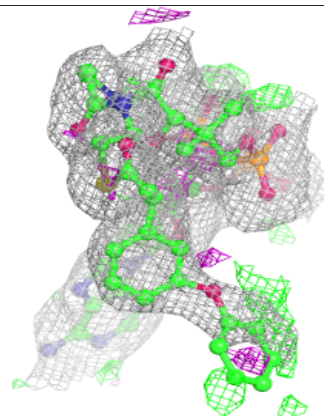
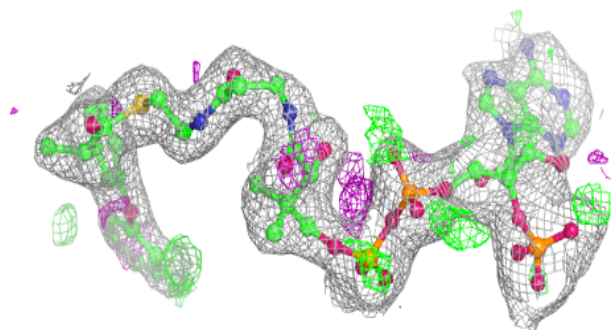
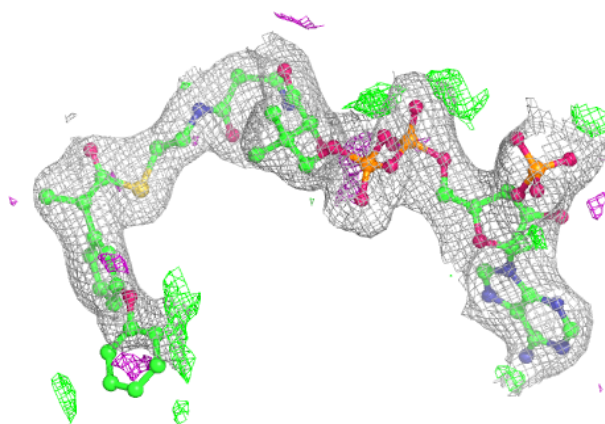
**Electron density around A1IY9 C 401:**

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



**Electron density around A1IY9 G 401:**

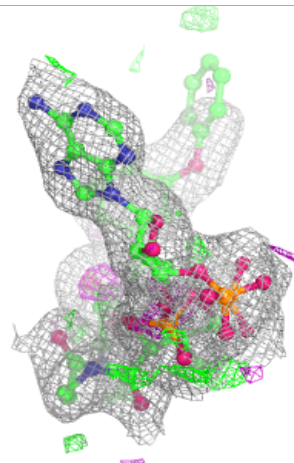
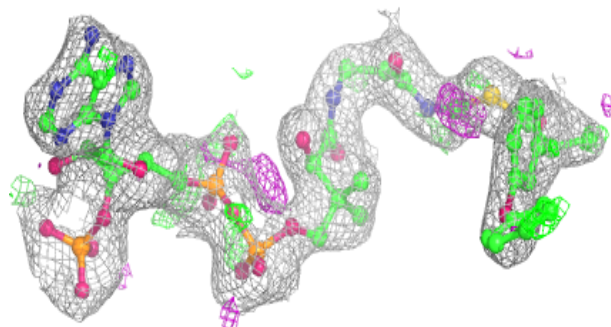
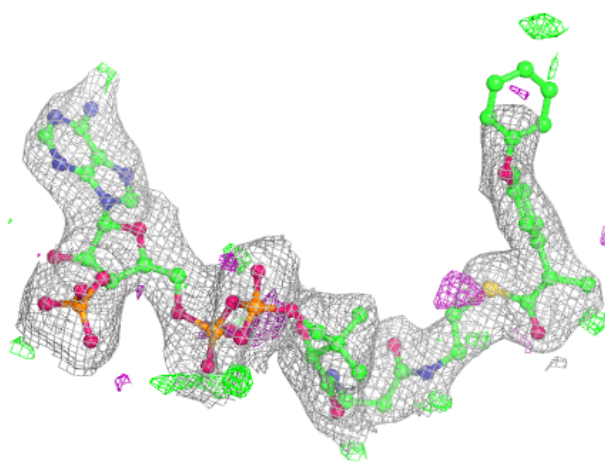
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





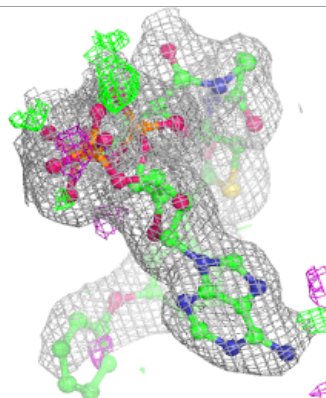
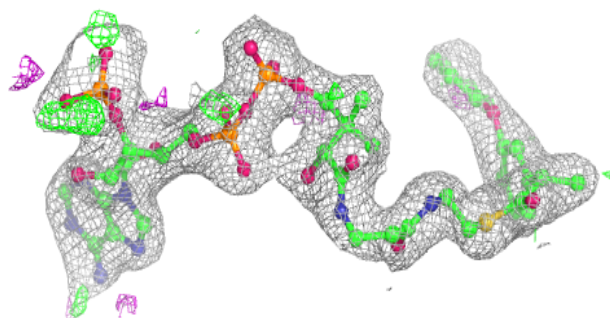
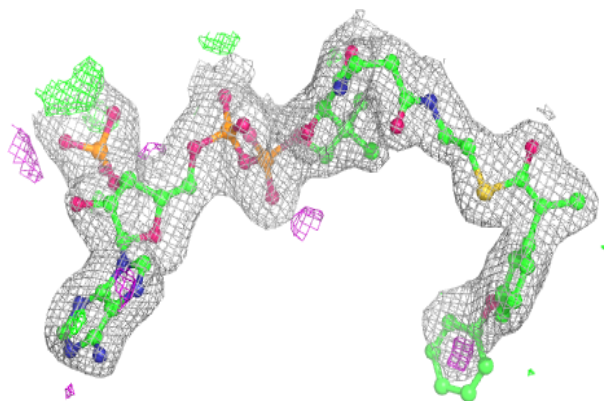
**Electron density around A1IY9 A 401:**

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

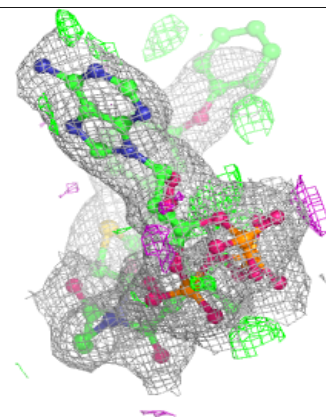
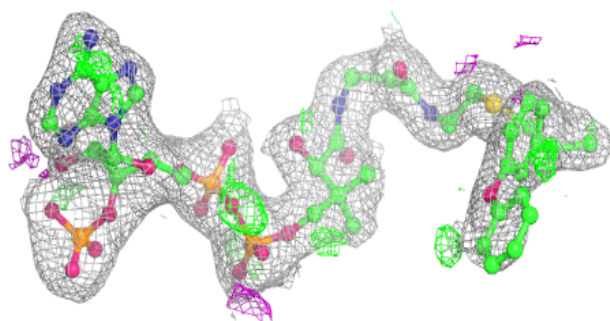
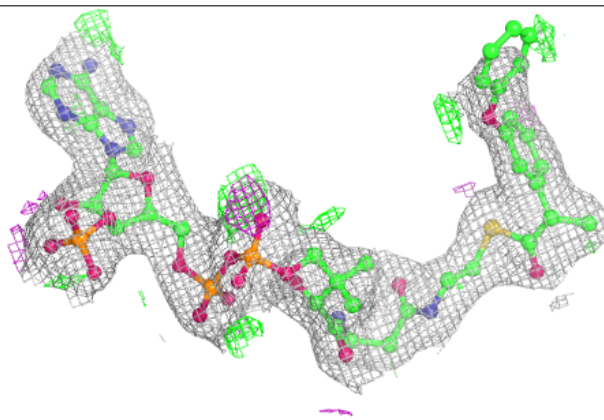


**Electron density around A1IY9 B 401:**

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

**Electron density around A1IY9 D 401:**

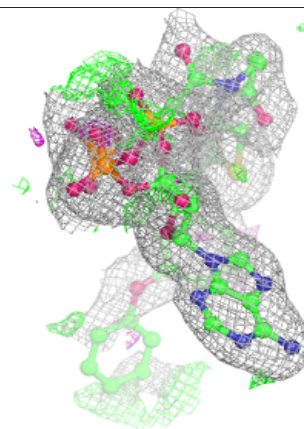
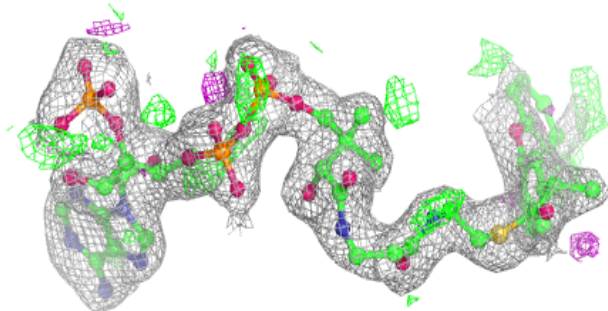
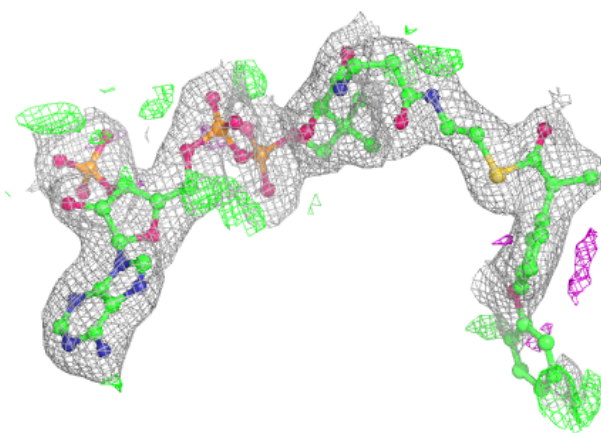
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



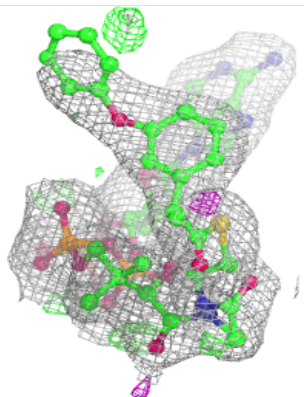
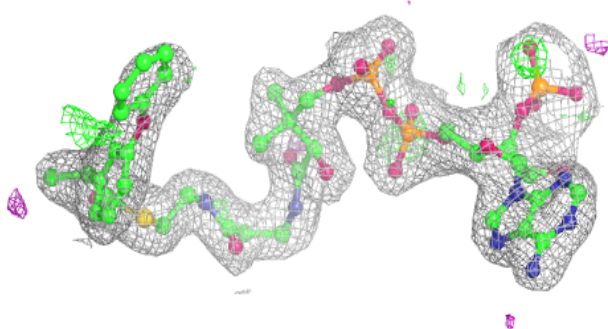
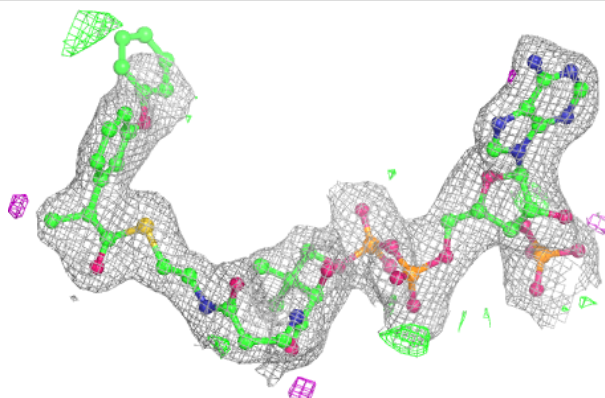


**Electron density around A1IY9 I 401:**

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

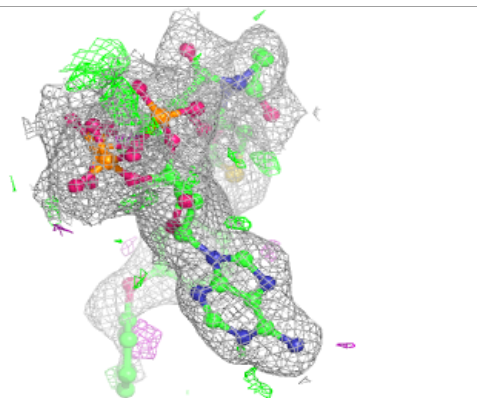
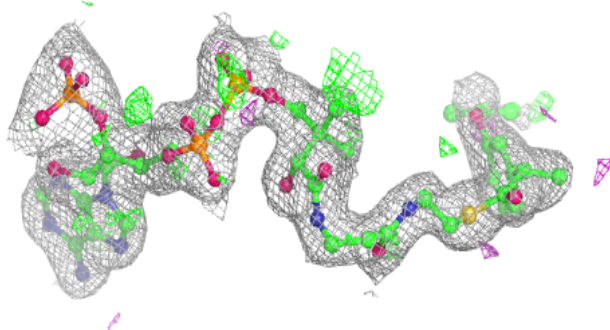
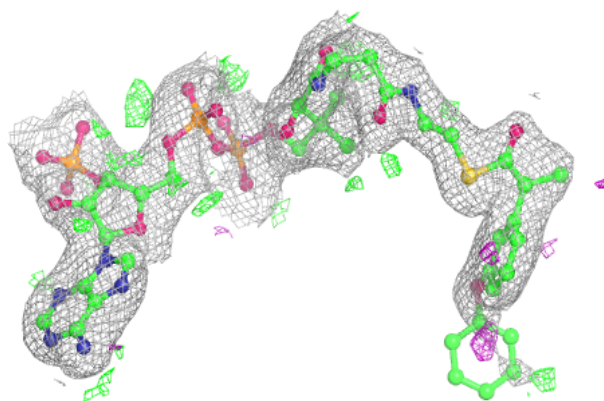
**Electron density around A1IY9 J 401:**

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

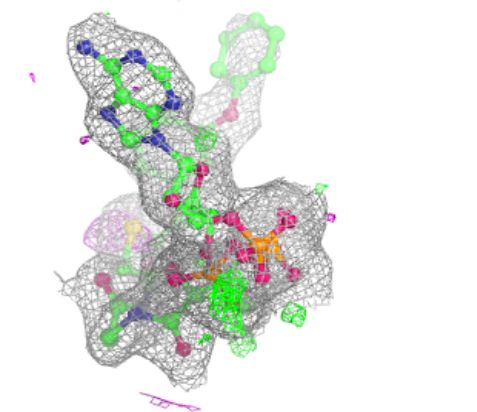
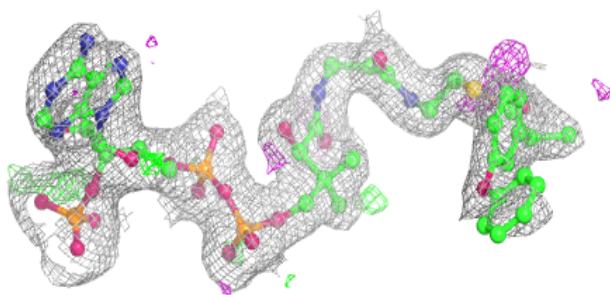
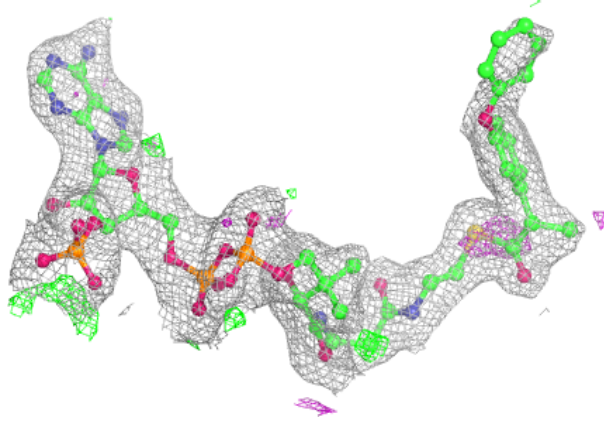


**Electron density around A1IY9 L 401:**

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

**Electron density around A1IY9 K 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.