



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:57 PM UTC

PDB ID : 9I31 / pdb_00009i31
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with acetyl-CoA
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on : 2025-01-22
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

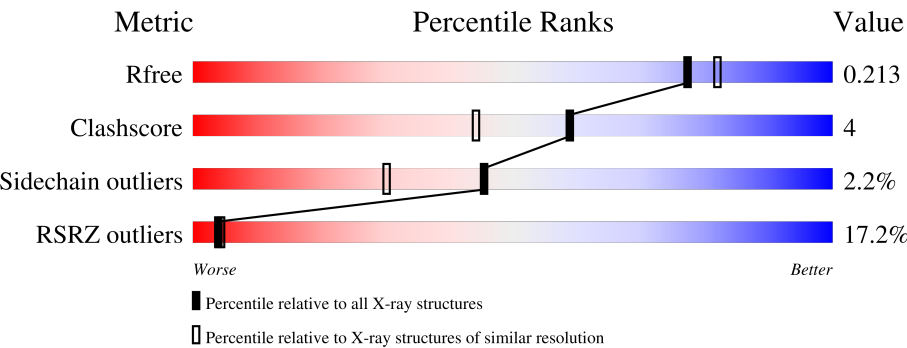
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	20% 87% 11%
1	B	364	13% 89% 8%
1	C	364	18% 87% 11%
1	D	364	20% 88% 9%
1	E	364	15% 86% 11%
1	F	364	21% 86% 12%

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Mol	Chain	Length	Quality of chain
1	G	364	25% 88% 10% ..
1	H	364	21% 88% 9% ..
1	I	364	11% 91% 7% ..
1	J	364	9% 91% 7% .
1	K	364	16% 88% 9% ..
1	L	364	15% 90% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35726 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	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	B	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	C	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	F	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	G	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	H	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	K	360	Total	C	N	O	S	0	3	0
			2728	1710	488	514	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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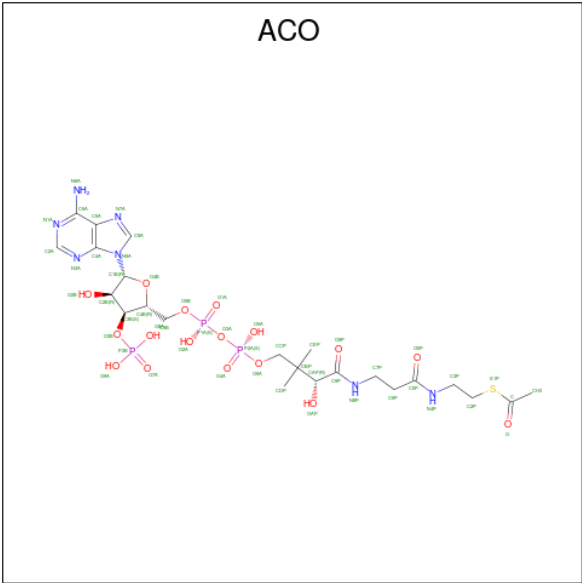
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	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 ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (la-
beled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	B	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	C	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	D	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	E	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	F	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	G	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	H	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	I	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		
2	J	1	Total	C	N	O	P	S	0	1
			102	46	14	34	6	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	
			102	46	14	34	6	2	0
2	L	1	Total	C	N	O	P	S	
			102	46	14	34	6	2	0

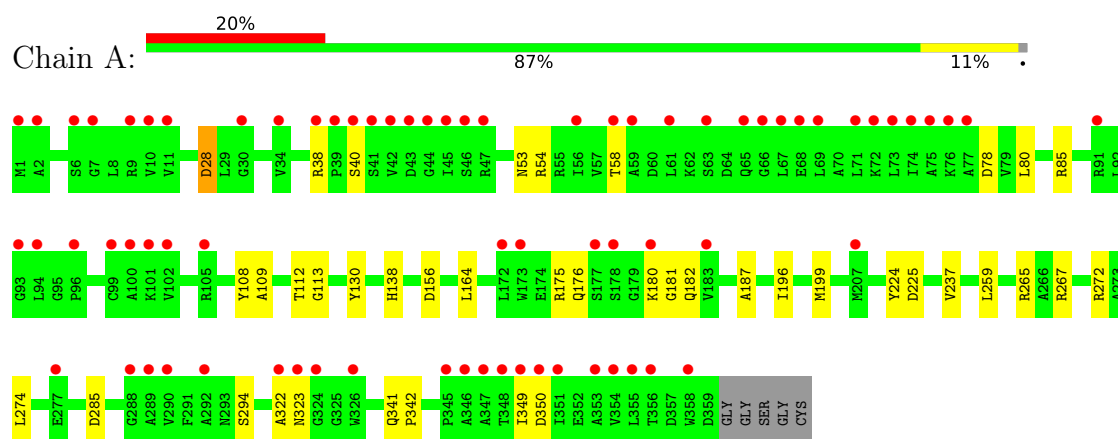
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O		
			166	166	0	0
3	B	150	Total	O		
			150	150	0	0
3	C	152	Total	O		
			152	152	0	0
3	D	162	Total	O		
			162	162	0	0
3	E	154	Total	O		
			154	154	0	0
3	F	143	Total	O		
			143	143	0	0
3	G	135	Total	O		
			135	135	0	0
3	H	144	Total	O		
			144	144	0	0
3	I	170	Total	O		
			170	170	0	0
3	J	180	Total	O		
			180	180	0	0
3	K	172	Total	O		
			172	172	0	0
3	L	166	Total	O		
			166	166	0	0

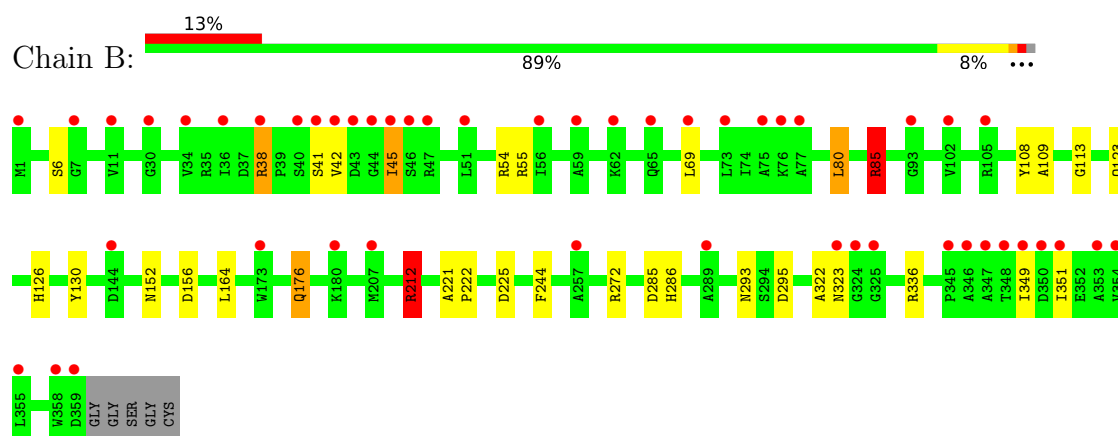
3 Residue-property plots

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.

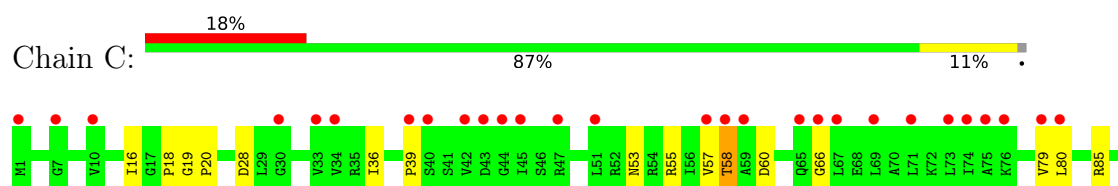
• Molecule 1: Alpha-methylacyl-CoA racemase

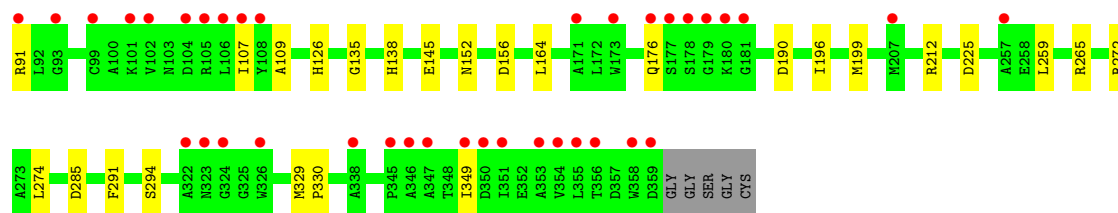


• Molecule 1: Alpha-methylacyl-CoA racemase

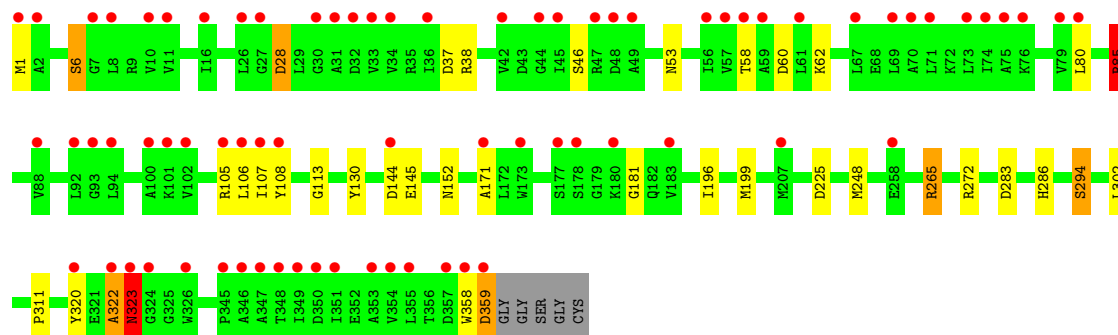
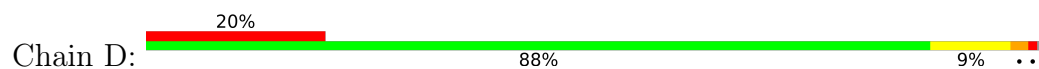


• Molecule 1: Alpha-methylacyl-CoA racemase

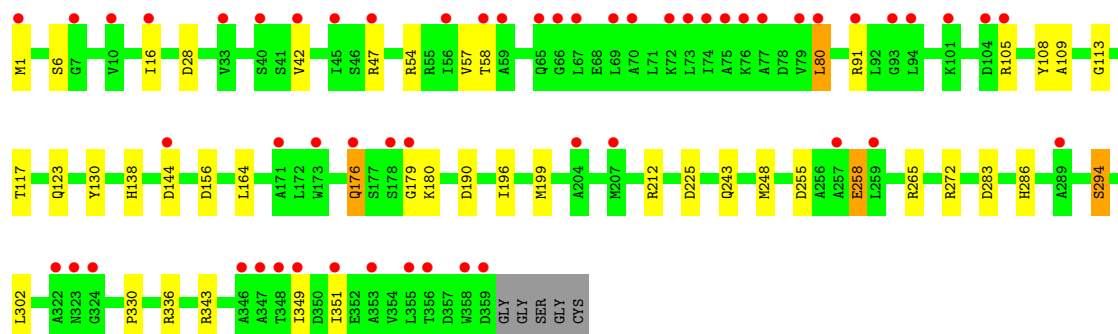
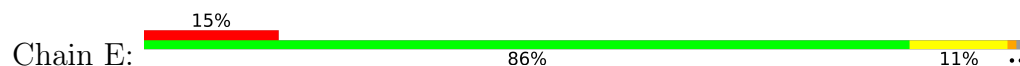




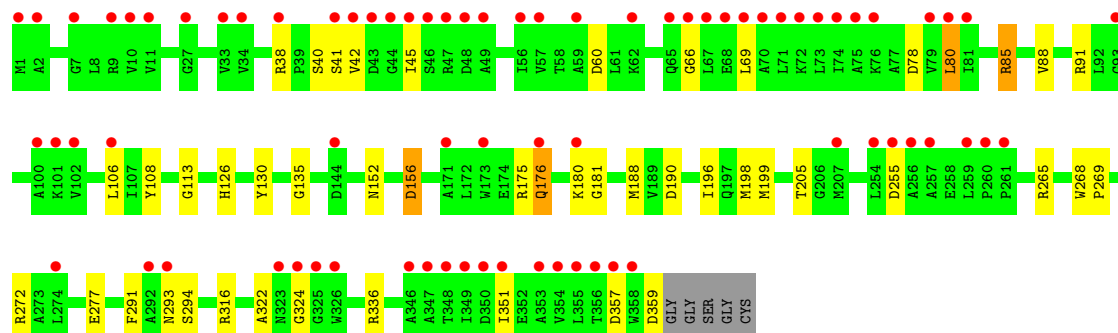
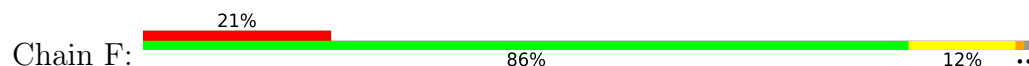
● Molecule 1: Alpha-methylacyl-CoA racemase



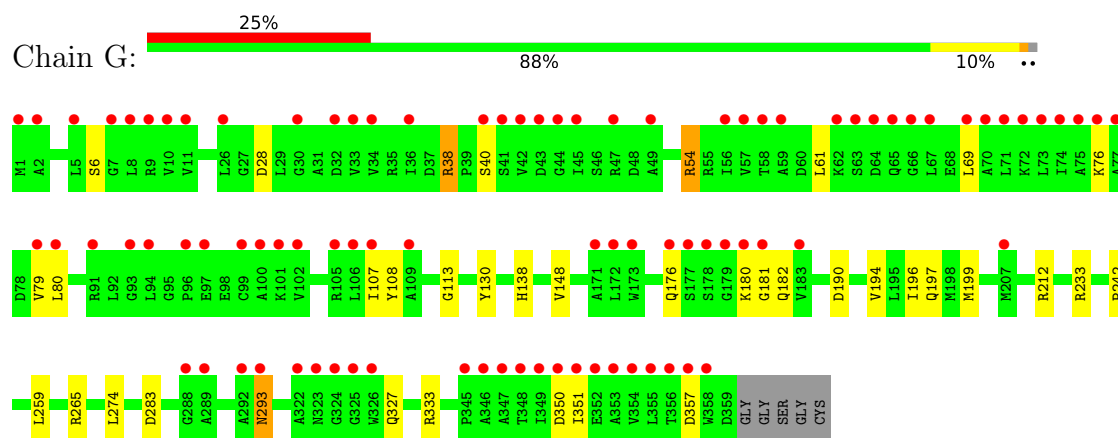
● Molecule 1: Alpha-methylacyl-CoA racemase



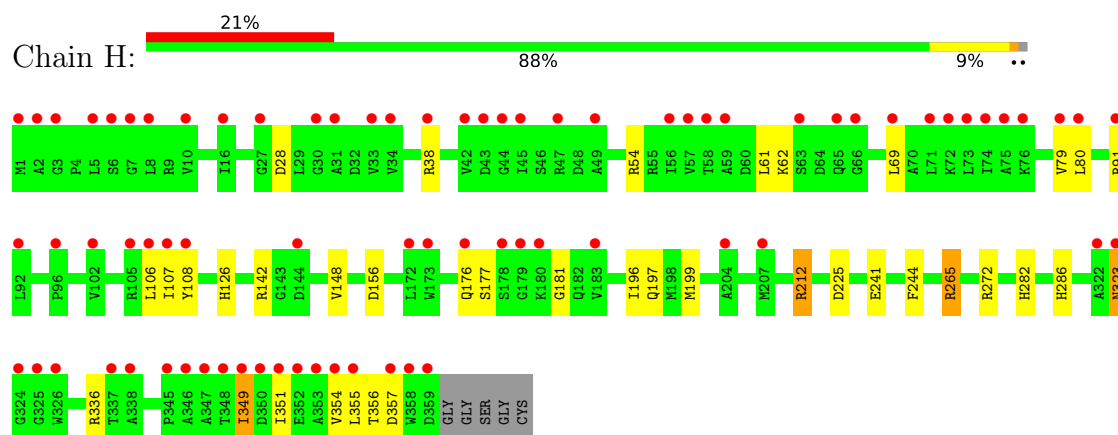
● Molecule 1: Alpha-methylacyl-CoA racemase



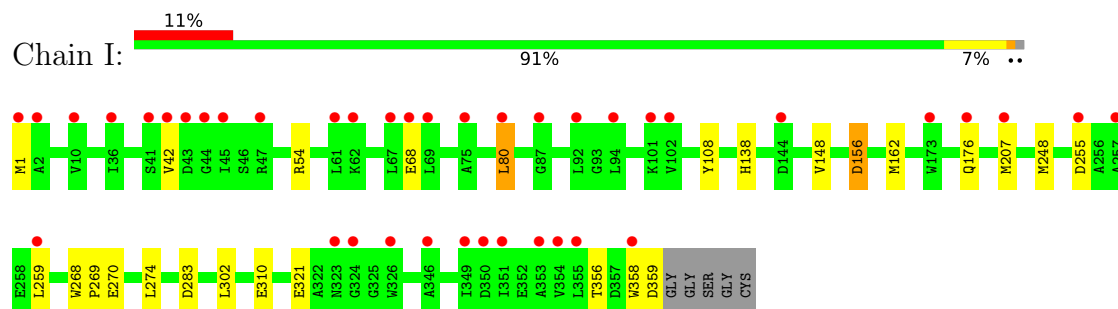
- Molecule 1: Alpha-methylacyl-CoA racemase



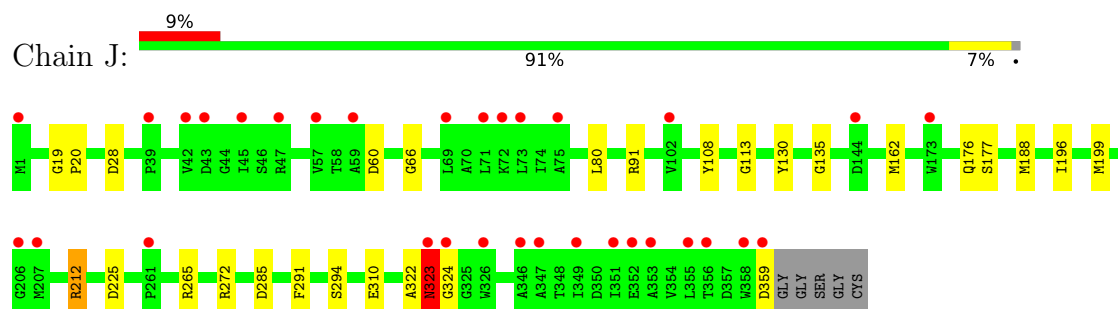
- Molecule 1: Alpha-methylacyl-CoA racemase



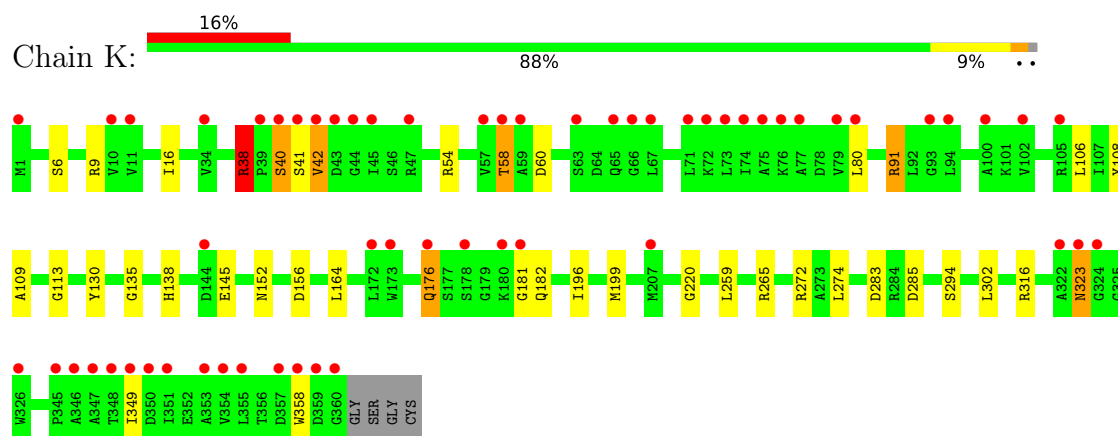
- Molecule 1: Alpha-methylacyl-CoA racemase



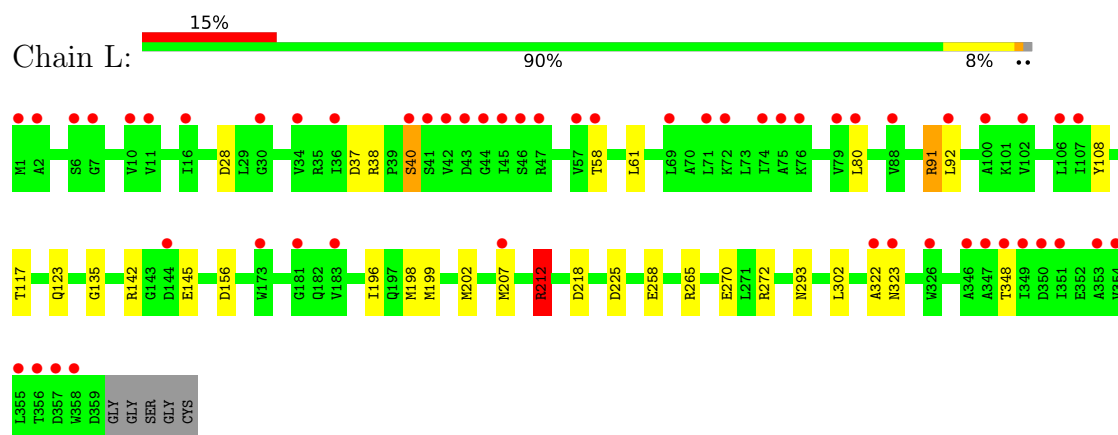
- Molecule 1: Alpha-methylacyl-CoA racemase



● 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, α , β , γ	276.63Å 276.63Å 390.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.69 – 1.88 225.69 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.69-1.88) 99.9 (225.69-1.88)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.203 , 0.234 (Not available) , 0.213	Depositor DCC
R_{free} test set	30186 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 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	0.96	EDS
Total number of atoms	35726	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.66	0/2791	1.02	2/3797 (0.1%)
1	B	0.67	0/2782	1.02	1/3785 (0.0%)
1	C	0.65	0/2791	1.05	1/3797 (0.0%)
1	D	0.68	0/2782	1.08	7/3785 (0.2%)
1	E	0.68	0/2791	1.06	5/3797 (0.1%)
1	F	0.66	0/2782	1.02	3/3785 (0.1%)
1	G	0.65	0/2791	1.06	4/3797 (0.1%)
1	H	0.68	0/2782	1.07	5/3785 (0.1%)
1	I	0.67	0/2791	1.07	6/3797 (0.2%)
1	J	0.68	1/2782 (0.0%)	1.05	3/3785 (0.1%)
1	K	0.66	1/2804 (0.0%)	1.04	3/3814 (0.1%)
1	L	0.67	0/2782	1.03	2/3785 (0.1%)
All	All	0.67	2/33451 (0.0%)	1.05	42/45509 (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	4
1	D	0	3
1	E	0	2
1	G	0	5
1	H	0	4
1	I	0	1
1	J	0	2
1	K	0	2
1	L	0	4
All	All	0	30

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	285	ASP	CG-OD1	6.46	1.37	1.25
1	K	285	ASP	CG-OD1	5.28	1.35	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	ASP	CA-CB-CG	6.97	119.57	112.60
1	G	283	ASP	CA-CB-CG	6.96	119.56	112.60
1	E	28	ASP	CA-CB-CG	6.82	119.42	112.60
1	D	265	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	H	148	VAL	CA-C-O	6.44	123.76	119.38
1	I	255	ASP	CB-CA-C	6.20	120.57	110.22
1	F	156	ASP	CB-CA-C	-6.15	101.23	110.88
1	L	218	ASP	CA-CB-CG	6.11	118.71	112.60
1	I	156	ASP	CA-CB-CG	6.06	118.66	112.60
1	H	28	ASP	CA-CB-CG	6.01	118.61	112.60
1	I	156	ASP	CB-CA-C	-5.92	101.58	110.88
1	K	58	THR	CB-CA-C	5.87	119.34	109.48
1	A	28	ASP	CA-CB-CG	5.83	118.42	112.60
1	H	323	ASN	CB-CA-C	-5.78	108.91	115.79
1	F	190	ASP	CA-CB-CG	5.71	118.31	112.60
1	L	28	ASP	CA-CB-CG	5.61	118.21	112.60
1	K	156	ASP	CB-CA-C	-5.58	102.09	110.90
1	D	38	ARG	CB-CA-C	5.57	117.45	109.26
1	I	148	VAL	CA-C-O	5.55	122.95	119.51
1	H	265	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	G	190	ASP	CA-CB-CG	5.50	118.10	112.60
1	E	190	ASP	CA-CB-CG	5.47	118.07	112.60
1	J	323	ASN	CB-CA-C	5.41	121.19	110.42
1	D	265	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	D	283	ASP	CA-CB-CG	5.38	117.97	112.60
1	H	357	ASP	CA-CB-CG	5.36	117.96	112.60
1	J	285	ASP	CB-CA-C	5.33	120.90	110.67
1	D	265	ARG	CB-CG-CD	5.30	123.50	111.30
1	B	38	ARG	CB-CA-C	5.27	116.68	108.61
1	J	28	ASP	CA-CB-CG	5.26	117.86	112.60
1	K	283	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	190	ASP	CA-CB-CG	5.24	117.84	112.60
1	I	283	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	144	ASP	CA-CB-CG	5.21	117.81	112.60
1	G	148	VAL	CA-C-O	5.18	122.72	119.51
1	E	123	GLN	CB-CA-C	-5.13	101.68	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	255	ASP	CB-CA-C	5.08	118.62	110.29
1	D	28	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	285	ASP	CB-CA-C	5.06	120.38	110.67
1	G	28	ASP	CA-CB-CG	5.04	117.64	112.60
1	I	321	GLU	CB-CA-C	-5.01	102.54	110.81
1	E	144	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (30) 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	212	ARG	Sidechain
1	B	322	ALA	Peptide
1	B	54	ARG	Peptide
1	B	85	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	323	ASN	Peptide
1	D	85	ARG	Sidechain
1	E	265	ARG	Sidechain
1	E	54	ARG	Peptide
1	G	233	ARG	Sidechain
1	G	265	ARG	Sidechain
1	G	333	ARG	Sidechain
1	G	38	ARG	Sidechain
1	G	54	ARG	Peptide
1	H	212	ARG	Sidechain
1	H	265	ARG	Sidechain
1	H	323	ASN	Peptide
1	H	54	ARG	Peptide
1	I	54	ARG	Peptide
1	J	212	ARG	Sidechain
1	J	265	ARG	Sidechain
1	K	38	ARG	Sidechain
1	K	54	ARG	Peptide
1	L	212	ARG	Sidechain
1	L	265	ARG	Sidechain
1	L	322	ALA	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	2718	0	2658	21	0
1	B	2715	0	2660	27	0
1	C	2718	0	2658	29	0
1	D	2715	0	2660	25	0
1	E	2718	0	2658	27	0
1	F	2715	0	2660	40	0
1	G	2718	0	2658	20	0
1	H	2715	0	2660	25	0
1	I	2718	0	2658	14	0
1	J	2715	0	2660	16	0
1	K	2728	0	2669	30	0
1	L	2715	0	2660	20	0
2	A	102	0	68	9	0
2	B	102	0	68	15	0
2	C	102	0	68	8	0
2	D	102	0	68	5	0
2	E	102	0	68	13	0
2	F	102	0	68	15	0
2	G	102	0	68	4	0
2	H	102	0	68	10	0
2	I	102	0	68	1	0
2	J	102	0	68	2	0
2	K	102	0	68	8	0
2	L	102	0	68	6	0
3	A	166	0	0	4	0
3	B	150	0	0	3	0
3	C	152	0	0	2	0
3	D	162	0	0	3	0
3	E	154	0	0	3	0
3	F	143	0	0	4	0
3	G	135	0	0	1	0
3	H	144	0	0	3	0
3	I	170	0	0	4	0
3	J	180	0	0	1	0
3	K	172	0	0	2	0
3	L	166	0	0	3	0
All	All	35726	0	32735	295	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 (295) 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)
2:A:401[B]:ACO:H71	2:A:401[B]:ACO:CDP	2.00	0.90
2:A:401[B]:ACO:H71	2:A:401[B]:ACO:H131	1.50	0.89
1:D:85:ARG:HD3	2:D:401[A]:ACO:O2A	1.71	0.89
1:B:85:ARG:HD3	2:B:401[A]:ACO:O2A	1.77	0.83
1:H:62:LYS:NZ	2:H:401[B]:ACO:O8A	2.10	0.83
1:H:156:ASP:OD2	2:H:401[A]:ACO:HH33	1.79	0.82
2:A:401[A]:ACO:H141	2:A:401[A]:ACO:O9P	1.81	0.78
1:K:91:ARG:HH22	2:K:401[A]:ACO:P3B	2.06	0.77
1:A:85:ARG:NH2	2:A:401[A]:ACO:O5A	2.16	0.77
1:J:322:ALA:O	1:J:324:GLY:N	2.18	0.76
1:C:152:ASN:HD22	2:C:401[B]:ACO:HH33	1.51	0.76
2:E:401[A]:ACO:OAP	2:E:401[A]:ACO:H71	1.83	0.76
1:K:40:SER:OG	3:K:501:HOH:O	2.03	0.75
1:B:152:ASN:HD22	2:B:401[B]:ACO:HH33	1.51	0.75
2:B:401[B]:ACO:H71	2:B:401[B]:ACO:OAP	1.85	0.74
2:E:401[A]:ACO:O9P	2:E:401[A]:ACO:H141	1.86	0.74
1:L:156:ASP:OD2	2:L:401[B]:ACO:HH33	1.88	0.72
1:K:152:ASN:HD22	2:K:401[B]:ACO:HH33	1.53	0.71
2:A:401[B]:ACO:H131	2:A:401[B]:ACO:C7P	2.20	0.71
1:A:40:SER:OG	3:A:501:HOH:O	2.09	0.71
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.74	0.70
2:B:401[B]:ACO:H141	2:B:401[B]:ACO:O9P	1.90	0.69
1:E:16:ILE:HD13	2:E:401[A]:ACO:S1P	2.32	0.69
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.27	0.68
1:C:285:ASP:OD1	3:C:501:HOH:O	2.13	0.67
1:D:152:ASN:HD22	2:D:401[B]:ACO:HH33	1.59	0.67
2:E:401[B]:ACO:H71	2:E:401[B]:ACO:OAP	1.95	0.67
1:F:85:ARG:HD3	2:F:401[B]:ACO:O2A	1.95	0.66
1:E:156:ASP:OD2	2:E:401[B]:ACO:HH33	1.96	0.66
1:B:85:ARG:CD	2:B:401[A]:ACO:O2A	2.43	0.65
2:L:401[A]:ACO:OAP	3:L:501:HOH:O	2.07	0.64
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.79	0.64
1:J:310:GLU:OE2	3:J:1901:HOH:O	2.15	0.64
2:E:401[A]:ACO:O9P	2:E:401[A]:ACO:CEP	2.45	0.64
2:G:401[A]:ACO:O5P	2:G:401[A]:ACO:H22	1.95	0.63
1:B:69:LEU:HD13	1:B:351:ILE:HG21	1.80	0.63
1:F:85:ARG:CD	2:F:401[B]:ACO:O2A	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.30	0.63
2:A:401[A]:ACO:O9P	2:A:401[A]:ACO:CEP	2.46	0.62
1:B:85:ARG:NH1	2:B:401[A]:ACO:O5A	2.32	0.62
1:F:152:ASN:HD22	2:F:401[A]:ACO:HH33	1.65	0.62
1:F:322:ALA:O	1:F:324:GLY:N	2.32	0.62
1:K:138:HIS:HD2	3:K:578:HOH:O	1.82	0.61
1:B:126:HIS:HB3	2:B:401[B]:ACO:O	2.01	0.61
1:L:207:MET:HE2	1:L:207:MET:HA	1.82	0.61
1:G:69:LEU:HD13	1:G:351:ILE:HG21	1.82	0.61
1:K:91:ARG:NH2	2:K:401[B]:ACO:O8A	2.33	0.61
1:B:285:ASP:HB2	3:B:515:HOH:O	2.00	0.60
2:B:401[B]:ACO:OAP	2:B:401[B]:ACO:C7P	2.48	0.60
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.19	0.60
1:L:270:GLU:HG3	3:L:536:HOH:O	2.01	0.60
1:D:294:SER:HB2	1:L:293:ASN:O	2.02	0.60
1:C:85:ARG:NH2	2:C:401[A]:ACO:O4A	2.22	0.59
2:B:401[B]:ACO:O9P	2:B:401[B]:ACO:CEP	2.50	0.59
1:I:156:ASP:OD1	2:I:401[B]:ACO:S1P	2.61	0.59
1:L:40:SER:OG	3:L:502:HOH:O	2.17	0.59
1:D:265:ARG:HD2	3:D:554:HOH:O	2.02	0.58
1:E:176:GLN:HG3	1:F:176:GLN:NE2	2.18	0.58
1:A:138:HIS:HD2	3:A:528:HOH:O	1.87	0.58
1:C:156:ASP:OD2	2:C:401[B]:ACO:HH33	2.02	0.58
2:H:401[A]:ACO:O9P	2:H:401[A]:ACO:H131	2.02	0.58
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.39	0.58
1:D:85:ARG:HD3	2:D:401[A]:ACO:P1A	2.44	0.57
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.87	0.57
1:C:138:HIS:HD2	3:C:589:HOH:O	1.86	0.56
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.86	0.56
1:I:310:GLU:OE2	3:I:501:HOH:O	2.17	0.56
1:E:138:HIS:HD2	3:E:589:HOH:O	1.89	0.56
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.40	0.56
1:H:349:ILE:HD11	1:H:354:VAL:HG22	1.88	0.56
1:A:156:ASP:OD2	2:A:401[B]:ACO:HH33	2.04	0.56
2:A:401[B]:ACO:H71	2:A:401[B]:ACO:H133	1.83	0.56
1:B:45:ILE:HD12	1:B:45:ILE:H	1.69	0.56
1:D:85:ARG:CD	2:D:401[A]:ACO:O2A	2.51	0.56
1:D:37:ASP:O	1:D:58:THR:HA	2.06	0.56
1:B:126:HIS:HA	2:B:401[B]:ACO:H31	1.88	0.55
1:K:176:GLN:HA	1:K:176:GLN:HE21	1.70	0.55
1:F:78:ASP:OD1	1:F:175:ARG:NH2	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.41	0.55
1:K:145:GLU:OE2	1:L:145:GLU:OE1	2.24	0.55
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.88	0.55
1:H:126:HIS:CE1	2:H:401[B]:ACO:HH32	2.42	0.55
1:F:38:ARG:HG2	3:F:501:HOH:O	2.07	0.54
1:E:47:ARG:HG2	1:F:205:THR:HG22	1.90	0.54
1:F:291:PHE:O	1:F:293:ASN:N	2.41	0.54
1:K:91:ARG:NH2	2:K:401[A]:ACO:O9A	2.41	0.53
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.41	0.53
1:I:358:TRP:O	1:I:359:ASP:HB2	2.09	0.53
1:F:126:HIS:HB3	2:F:401[A]:ACO:O	2.08	0.53
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.91	0.53
1:H:196:ILE:HG12	1:H:199:MET:HB2	1.90	0.53
1:B:212:ARG:HG2	3:B:561:HOH:O	2.09	0.53
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.91	0.52
1:C:152:ASN:HD22	2:C:401[B]:ACO:CH3	2.20	0.52
1:E:57:VAL:HG12	1:E:349:ILE:O	2.09	0.52
1:F:60:ASP:O	1:F:66:GLY:HA3	2.09	0.52
1:B:156:ASP:OD2	2:B:401[B]:ACO:S1P	2.68	0.52
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.45	0.52
1:F:106:LEU:O	1:F:181:GLY:HA3	2.11	0.51
2:B:401[A]:ACO:O9P	2:B:401[A]:ACO:H141	2.10	0.51
1:A:78:ASP:OD1	1:A:175:ARG:NH2	2.30	0.51
1:G:69:LEU:HB3	1:G:351:ILE:HD13	1.92	0.51
1:J:91:ARG:NH2	2:J:401[A]:ACO:O8A	2.39	0.51
1:A:322:ALA:O	1:A:323:ASN:C	2.54	0.51
1:F:80:LEU:HD22	1:F:108:TYR:CE2	2.46	0.50
1:F:293:ASN:ND2	3:F:503:HOH:O	2.43	0.50
1:C:19:GLY:N	1:C:20:PRO:HD2	2.27	0.50
1:C:60:ASP:O	1:C:66:GLY:HA3	2.10	0.50
1:F:188:MET:HE1	2:F:401[A]:ACO:H21	1.92	0.50
1:C:39:PRO:HG3	1:C:58:THR:HG23	1.92	0.50
1:F:85:ARG:HD2	2:F:401[A]:ACO:O2A	2.11	0.50
2:F:401[B]:ACO:O9P	2:F:401[B]:ACO:H141	2.11	0.50
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.25	0.50
2:H:401[B]:ACO:H131	2:H:401[B]:ACO:O9P	2.12	0.50
1:F:85:ARG:NH1	2:F:401[B]:ACO:O5A	2.44	0.50
1:K:91:ARG:NH2	2:K:401[A]:ACO:P3B	2.82	0.50
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.36	0.50
1:E:176:GLN:CD	1:F:176:GLN:HG2	2.37	0.50
1:F:91:ARG:HH12	2:F:401[B]:ACO:P3B	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:657:HOH:O	1:E:243:GLN:HG3	2.12	0.49
2:E:401[A]:ACO:H61	3:E:570:HOH:O	2.12	0.49
1:I:270:GLU:HG3	3:I:601:HOH:O	2.10	0.49
1:L:198:MET:HE2	1:L:202:MET:SD	2.52	0.49
1:F:85:ARG:HD2	2:F:401[B]:ACO:O2A	2.12	0.49
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.37	0.49
1:D:225:ASP:OD2	1:D:272:ARG:NH1	2.46	0.49
1:D:286:HIS:HE1	3:D:645:HOH:O	1.96	0.49
2:E:401[A]:ACO:OAP	2:E:401[A]:ACO:C7P	2.57	0.49
1:F:294:SER:HB3	1:G:293:ASN:HB3	1.93	0.49
1:K:196:ILE:HG12	1:K:199:MET:HB2	1.95	0.49
1:L:91:ARG:NH2	2:L:401[B]:ACO:O9A	2.30	0.49
1:I:80:LEU:HD22	1:I:108:TYR:CE2	2.48	0.49
1:F:69:LEU:HD13	1:F:351:ILE:HG23	1.94	0.49
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.46	0.48
1:C:55:ARG:HG2	1:C:349:ILE:CD1	2.43	0.48
1:D:320:TYR:CE2	1:D:322:ALA:HB2	2.48	0.48
1:I:138:HIS:HD2	3:I:540:HOH:O	1.97	0.48
1:C:19:GLY:N	1:C:20:PRO:CD	2.77	0.48
1:L:61:LEU:HG	2:L:401[A]:ACO:N6A	2.29	0.48
1:A:180:LYS:O	1:B:336:ARG:NH2	2.47	0.48
1:C:126:HIS:ND1	2:C:401[A]:ACO:S1P	2.87	0.48
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.29	0.48
1:C:196:ILE:HG12	1:C:199:MET:HB2	1.96	0.48
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.47	0.48
1:A:109:ALA:HB1	1:A:164:LEU:HD11	1.96	0.48
1:C:135:GLY:HA2	1:D:302:LEU:O	2.13	0.48
1:E:286:HIS:ND1	3:E:502:HOH:O	2.35	0.47
1:H:156:ASP:OD1	2:H:401[A]:ACO:H22	2.14	0.47
2:E:401[B]:ACO:O9P	2:E:401[B]:ACO:CEP	2.61	0.47
1:F:38:ARG:HG3	2:F:401[A]:ACO:C6A	2.44	0.47
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.96	0.47
1:F:156:ASP:OD2	2:F:401[A]:ACO:HH33	2.13	0.47
1:A:225:ASP:OD2	1:A:272:ARG:NH1	2.48	0.47
1:B:85:ARG:CD	2:B:401[B]:ACO:O2A	2.63	0.47
1:F:40:SER:O	1:F:41:SER:CB	2.62	0.47
1:G:176:GLN:CD	1:H:176:GLN:HG2	2.39	0.47
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.47	0.47
1:J:196:ILE:HG12	1:J:199:MET:HB2	1.96	0.47
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.77	0.47
2:C:401[B]:ACO:O9P	2:C:401[B]:ACO:CEP	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ARG:HD3	2:B:401[B]:ACO:O2A	2.14	0.46
1:G:38:ARG:HB3	2:G:401[B]:ACO:C6A	2.45	0.46
1:J:322:ALA:O	1:J:323:ASN:C	2.57	0.46
1:A:294:SER:O	1:B:123:GLN:HG3	2.15	0.46
1:K:113:GLY:HA3	1:K:130:TYR:CE1	2.51	0.46
1:B:293:ASN:O	1:E:294:SER:HB2	2.15	0.46
1:B:80:LEU:HD22	1:B:108:TYR:CE2	2.51	0.46
1:K:9:ARG:NH2	1:K:358:TRP:HA	2.31	0.46
1:H:38:ARG:NH1	2:H:401[B]:ACO:C1B	2.79	0.46
1:C:291:PHE:O	1:C:294:SER:HB3	2.16	0.46
2:E:401[B]:ACO:OAP	2:E:401[B]:ACO:C7P	2.63	0.46
1:L:156:ASP:OD1	2:L:401[B]:ACO:S1P	2.74	0.46
1:D:46:SER:OG	3:D:501:HOH:O	2.14	0.45
1:G:69:LEU:HD13	1:G:351:ILE:CG2	2.46	0.45
1:D:322:ALA:HB3	1:D:323:ASN:HB2	1.98	0.45
1:G:196:ILE:HG12	1:G:199:MET:HB2	1.99	0.45
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.98	0.45
1:D:28:ASP:HA	1:D:53:ASN:ND2	2.30	0.45
2:E:401[A]:ACO:HH31	1:F:198:MET:HE1	1.97	0.45
1:F:38:ARG:HG3	2:F:401[A]:ACO:N1A	2.32	0.45
1:G:181:GLY:O	1:G:182:GLN:HB3	2.17	0.45
1:K:41:SER:O	1:K:42:VAL:HG23	2.16	0.45
1:A:267:ARG:HD3	3:A:515:HOH:O	2.16	0.45
2:H:401[A]:ACO:O9P	2:H:401[A]:ACO:CDP	2.64	0.45
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.52	0.45
1:G:61:LEU:HG	2:G:401[A]:ACO:N6A	2.31	0.45
1:C:16:ILE:HD12	2:C:401[A]:ACO:S1P	2.56	0.45
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.98	0.45
1:H:282:HIS:HE1	3:H:629:HOH:O	1.99	0.45
1:B:286:HIS:HE1	3:B:639:HOH:O	2.00	0.45
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.47	0.45
1:G:80:LEU:HD22	1:G:108:TYR:CE2	2.52	0.45
1:H:61:LEU:HG	2:H:401[A]:ACO:N6A	2.32	0.44
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.98	0.44
1:H:286:HIS:HE1	3:H:622:HOH:O	1.99	0.44
1:K:294:SER:O	1:L:123:GLN:HG2	2.17	0.44
2:A:401[A]:ACO:H71	2:A:401[A]:ACO:OAP	2.18	0.44
1:D:105:ARG:HH11	1:D:105:ARG:HG2	1.82	0.44
1:L:92:LEU:HD11	2:L:401[B]:ACO:O2B	2.17	0.44
1:E:1:MET:HE2	1:E:343:ARG:NH2	2.32	0.44
1:E:138:HIS:O	1:E:212:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:ILE:HG12	1:F:199:MET:HB2	2.00	0.44
1:K:60:ASP:OD1	1:K:60:ASP:C	2.61	0.44
1:H:355:LEU:O	1:H:356:THR:C	2.60	0.43
1:K:302:LEU:O	1:L:135:GLY:HA2	2.18	0.43
1:J:188:MET:HE1	2:J:401[B]:ACO:H31	1.99	0.43
1:A:181:GLY:O	1:A:182:GLN:HB3	2.18	0.43
1:I:162:MET:HB3	1:J:162:MET:HB3	2.01	0.43
1:J:19:GLY:N	1:J:20:PRO:HD2	2.33	0.43
1:K:181:GLY:O	1:K:182:GLN:HB3	2.18	0.43
1:G:54:ARG:HG2	1:G:54:ARG:HH11	1.83	0.43
1:H:286:HIS:HD2	3:H:636:HOH:O	2.02	0.43
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.53	0.43
1:J:291:PHE:O	1:J:294:SER:HB3	2.18	0.43
1:D:85:ARG:CD	2:D:401[A]:ACO:P1A	3.05	0.43
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.54	0.43
1:K:135:GLY:HA2	1:L:302:LEU:O	2.19	0.43
1:K:316:ARG:HD2	1:L:117:THR:O	2.18	0.43
1:G:79:VAL:HG22	1:G:107:ILE:HB	2.01	0.43
1:K:220:GLY:O	1:K:272:ARG:NH2	2.51	0.43
1:K:91:ARG:NH2	2:K:401[A]:ACO:O8A	2.32	0.43
1:K:323:ASN:OD1	1:K:323:ASN:N	2.51	0.43
1:C:126:HIS:CE1	2:C:401[A]:ACO:S1P	3.12	0.43
1:G:180:LYS:HB2	1:H:336:ARG:NH2	2.34	0.43
1:I:356:THR:O	1:I:359:ASP:C	2.62	0.43
1:D:106:LEU:O	1:D:181:GLY:HA3	2.19	0.42
1:E:16:ILE:HD13	2:E:401[A]:ACO:C2P	2.49	0.42
1:E:196:ILE:HG12	1:E:199:MET:HB2	2.01	0.42
1:F:85:ARG:CD	2:F:401[A]:ACO:O2A	2.66	0.42
1:G:138:HIS:HD2	3:G:539:HOH:O	2.01	0.42
1:H:241:GLU:HB2	1:H:244:PHE:CD2	2.54	0.42
1:H:349:ILE:HD11	1:H:354:VAL:CG2	2.49	0.42
1:H:69:LEU:HD13	1:H:351:ILE:HG21	2.00	0.42
1:K:38:ARG:H	1:K:38:ARG:HG2	1.71	0.42
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.54	0.42
1:G:194:VAL:O	1:G:197:GLN:HB2	2.19	0.42
1:K:109:ALA:HB1	1:K:164:LEU:HD11	2.01	0.42
1:J:60:ASP:O	1:J:66:GLY:HA3	2.20	0.42
1:B:38:ARG:HB3	2:B:401[A]:ACO:C6A	2.50	0.42
1:B:69:LEU:HD13	1:B:351:ILE:CG2	2.49	0.42
1:E:255:ASP:HB3	1:E:258:GLU:HG2	2.02	0.42
1:F:88:VAL:CG1	2:F:401[B]:ACO:H2B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:GLY:HA3	1:K:130:TYR:CZ	2.55	0.42
1:F:113:GLY:HA3	1:F:130:TYR:CZ	2.55	0.42
1:H:106:LEU:O	1:H:181:GLY:HA3	2.19	0.42
1:C:80:LEU:C	1:C:80:LEU:HD13	2.44	0.42
1:E:105:ARG:HG2	1:E:179:GLY:O	2.19	0.42
1:E:113:GLY:HA3	1:E:130:TYR:CZ	2.55	0.42
2:E:401[B]:ACO:O9P	2:E:401[B]:ACO:H141	2.19	0.42
1:I:268:TRP:N	1:I:269:PRO:CD	2.82	0.42
1:E:255:ASP:HB3	1:E:258:GLU:CG	2.49	0.42
1:E:302:LEU:O	1:F:135:GLY:HA2	2.20	0.42
1:K:16:ILE:HG13	2:K:401[A]:ACO:H22	2.02	0.42
1:H:91:ARG:NH2	2:H:401[A]:ACO:O8A	2.47	0.42
1:E:80:LEU:CD2	1:E:108:TYR:CE2	3.03	0.41
1:F:268:TRP:N	1:F:269:PRO:CD	2.83	0.41
1:I:176:GLN:NE2	1:J:176:GLN:HG2	2.35	0.41
1:A:112:THR:O	1:A:187:ALA:HA	2.20	0.41
1:D:60:ASP:OD1	1:D:62:LYS:HB2	2.20	0.41
1:D:1:MET:O	1:D:6:SER:OG	2.32	0.41
1:I:1:MET:HB2	3:I:644:HOH:O	2.19	0.41
1:G:327:GLN:NE2	1:H:197:GLN:HE21	2.19	0.41
1:F:265:ARG:NH1	3:F:514:HOH:O	2.52	0.41
1:G:138:HIS:O	1:G:212:ARG:HD3	2.20	0.41
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.56	0.41
1:D:358:TRP:O	1:D:359:ASP:C	2.62	0.41
1:L:37:ASP:O	1:L:58:THR:HA	2.21	0.41
1:L:225:ASP:OD2	1:L:272:ARG:NH1	2.54	0.41
1:A:224:TYR:HA	1:A:237:VAL:O	2.21	0.41
1:B:55:ARG:HD2	1:B:349:ILE:CD1	2.51	0.41
1:B:109:ALA:HB1	1:B:164:LEU:HD11	2.02	0.41
1:E:113:GLY:HA3	1:E:130:TYR:CE1	2.56	0.41
1:E:180:LYS:HB2	1:F:336:ARG:NH2	2.35	0.41
1:F:272:ARG:NH1	3:F:515:HOH:O	2.54	0.41
1:H:142:ARG:O	1:H:212:ARG:HD2	2.21	0.41
1:K:38:ARG:HD3	2:K:401[B]:ACO:C5A	2.50	0.41
1:K:80:LEU:HD23	1:K:108:TYR:CE2	2.55	0.41
1:A:28:ASP:HA	1:A:53:ASN:ND2	2.36	0.40
1:A:341:GLN:HA	1:A:342:PRO:HD3	1.96	0.40
1:E:109:ALA:HB1	1:E:164:LEU:HD11	2.03	0.40
1:K:106:LEU:O	1:K:181:GLY:HA3	2.20	0.40
1:L:142:ARG:O	1:L:212:ARG:HD2	2.22	0.40
1:C:36:ILE:HA	1:C:57:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG22	1:C:107:ILE:HB	2.02	0.40
1:C:138:HIS:O	1:C:212:ARG:HD3	2.21	0.40
1:D:107:ILE:HD12	1:D:171:ALA:HB1	2.04	0.40
1:B:244:PHE:HB3	1:B:295:ASP:O	2.22	0.40
1:C:18:PRO:HB3	1:C:156:ASP:O	2.21	0.40
1:E:117:THR:O	1:F:316:ARG:HD2	2.22	0.40
1:I:302:LEU:O	1:J:135:GLY:HA2	2.21	0.40
1:B:221:ALA:HA	1:B:222:PRO:HD3	1.93	0.40
1:C:109:ALA:HB1	1:C:164:LEU:HD11	2.03	0.40
1:E:91:ARG:HD3	1:G:242:PRO:HB2	2.03	0.40
1:F:113:GLY:HA3	1:F:130:TYR:CE1	2.56	0.40
2:G:401[A]:ACO:O9P	2:G:401[A]:ACO:H141	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	277/277 (100%)	274 (99%)	3 (1%)	65	56
1	B	276/277 (100%)	267 (97%)	9 (3%)	33	16
1	C	277/277 (100%)	274 (99%)	3 (1%)	65	56
1	D	276/277 (100%)	269 (98%)	7 (2%)	42	26
1	E	277/277 (100%)	267 (96%)	10 (4%)	31	14
1	F	276/277 (100%)	268 (97%)	8 (3%)	37	20
1	G	277/277 (100%)	271 (98%)	6 (2%)	45	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	276/277 (100%)	274 (99%)	2 (1%)	76	69
1	I	277/277 (100%)	272 (98%)	5 (2%)	51	38
1	J	276/277 (100%)	272 (99%)	4 (1%)	59	48
1	K	278/277 (100%)	268 (96%)	10 (4%)	31	14
1	L	276/277 (100%)	270 (98%)	6 (2%)	45	30
All	All	3319/3324 (100%)	3246 (98%)	73 (2%)	45	30

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	349	ILE
1	A	350	ASP
1	B	6	SER
1	B	41	SER
1	B	42	VAL
1	B	45	ILE
1	B	80	LEU
1	B	85	ARG
1	B	176	GLN
1	B	212	ARG
1	B	323	ASN
1	C	58	THR
1	C	91	ARG
1	C	265	ARG
1	D	6	SER
1	D	85	ARG
1	D	248	MET
1	D	294	SER
1	D	311	PRO
1	D	323	ASN
1	D	359	ASP
1	E	6	SER
1	E	42	VAL
1	E	58	THR
1	E	80	LEU
1	E	176	GLN
1	E	248	MET
1	E	258	GLU
1	E	294	SER

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Mol	Chain	Res	Type
1	E	330	PRO
1	E	351	ILE
1	F	42	VAL
1	F	45	ILE
1	F	80	LEU
1	F	85	ARG
1	F	176	GLN
1	F	277	GLU
1	F	357	ASP
1	F	359	ASP
1	G	6	SER
1	G	40	SER
1	G	76	LYS
1	G	293	ASN
1	G	350	ASP
1	G	357	ASP
1	H	177	SER
1	H	349	ILE
1	I	42	VAL
1	I	68	GLU
1	I	80	LEU
1	I	207	MET
1	I	248	MET
1	J	177	SER
1	J	212	ARG
1	J	323	ASN
1	J	359	ASP
1	K	6	SER
1	K	38	ARG
1	K	40	SER
1	K	42	VAL
1	K	58	THR
1	K	91	ARG
1	K	176	GLN
1	K	265	ARG
1	K	323	ASN
1	K	349	ILE
1	L	38	ARG
1	L	40	SER
1	L	212	ARG
1	L	258	GLU
1	L	323	ASN

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Mol	Chain	Res	Type
1	L	348	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	263	ASN
1	A	282	HIS
1	A	317	ASN
1	A	327	GLN
1	B	176	GLN
1	B	323	ASN
1	C	116	GLN
1	C	138	HIS
1	C	152	ASN
1	C	176	GLN
1	C	263	ASN
1	C	282	HIS
1	C	308	HIS
1	C	327	GLN
1	D	282	HIS
1	E	138	HIS
1	E	176	GLN
1	E	263	ASN
1	E	282	HIS
1	E	293	ASN
1	F	176	GLN
1	F	282	HIS
1	F	293	ASN
1	F	308	HIS
1	F	323	ASN
1	G	138	HIS
1	G	176	GLN
1	G	308	HIS
1	G	327	GLN
1	H	282	HIS
1	H	286	HIS
1	I	116	GLN
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	282	HIS

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Mol	Chain	Res	Type
1	I	293	ASN
1	I	327	GLN
1	J	122	GLN
1	J	134	ASN
1	J	176	GLN
1	J	282	HIS
1	J	286	HIS
1	K	138	HIS
1	K	176	GLN
1	K	327	GLN
1	L	176	GLN
1	L	293	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

24 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	ACO	F	401[A]	-	51,53,53	0.64	0	73,79,79	1.02	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACO	J	401[A]	-	51,53,53	0.74	0	73,79,79	1.15	6 (8%)
2	ACO	L	401[B]	-	51,53,53	0.76	2 (3%)	73,79,79	0.99	2 (2%)
2	ACO	I	401[B]	-	51,53,53	0.63	1 (1%)	73,79,79	0.89	3 (4%)
2	ACO	E	401[B]	-	51,53,53	0.83	3 (5%)	73,79,79	1.12	2 (2%)
2	ACO	G	401[A]	-	51,53,53	0.63	1 (1%)	73,79,79	1.22	4 (5%)
2	ACO	D	401[A]	-	51,53,53	0.70	2 (3%)	73,79,79	1.15	4 (5%)
2	ACO	K	401[A]	-	51,53,53	0.69	2 (3%)	73,79,79	0.95	2 (2%)
2	ACO	C	401[B]	-	51,53,53	0.68	1 (1%)	73,79,79	0.82	2 (2%)
2	ACO	H	401[B]	-	51,53,53	0.67	1 (1%)	73,79,79	1.20	4 (5%)
2	ACO	B	401[B]	-	51,53,53	0.68	1 (1%)	73,79,79	0.95	2 (2%)
2	ACO	A	401[A]	-	51,53,53	0.69	1 (1%)	73,79,79	1.09	4 (5%)
2	ACO	F	401[B]	-	51,53,53	0.75	1 (1%)	73,79,79	1.07	3 (4%)
2	ACO	J	401[B]	-	51,53,53	0.62	0	73,79,79	1.02	4 (5%)
2	ACO	G	401[B]	-	51,53,53	0.65	1 (1%)	73,79,79	1.07	3 (4%)
2	ACO	D	401[B]	-	51,53,53	0.52	0	73,79,79	1.08	3 (4%)
2	ACO	L	401[A]	-	51,53,53	0.73	2 (3%)	73,79,79	1.55	3 (4%)
2	ACO	E	401[A]	-	51,53,53	0.82	2 (3%)	73,79,79	1.18	4 (5%)
2	ACO	I	401[A]	-	51,53,53	0.60	0	73,79,79	1.15	6 (8%)
2	ACO	K	401[B]	-	51,53,53	0.58	0	73,79,79	1.00	3 (4%)
2	ACO	A	401[B]	-	51,53,53	0.69	1 (1%)	73,79,79	1.03	4 (5%)
2	ACO	C	401[A]	-	51,53,53	0.74	2 (3%)	73,79,79	1.27	6 (8%)
2	ACO	B	401[A]	-	51,53,53	0.73	1 (1%)	73,79,79	1.27	5 (6%)
2	ACO	H	401[A]	-	51,53,53	0.82	3 (5%)	73,79,79	1.07	2 (2%)

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	ACO	F	401[A]	-	-	4/51/67/67	0/3/3/3
2	ACO	J	401[A]	-	-	9/51/67/67	0/3/3/3
2	ACO	L	401[B]	-	-	7/51/67/67	0/3/3/3
2	ACO	I	401[B]	-	-	9/51/67/67	0/3/3/3
2	ACO	E	401[B]	-	-	15/51/67/67	0/3/3/3
2	ACO	G	401[A]	-	-	8/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	D	401[A]	-	-	8/51/67/67	0/3/3/3
2	ACO	K	401[A]	-	-	10/51/67/67	0/3/3/3
2	ACO	C	401[B]	-	-	14/51/67/67	0/3/3/3
2	ACO	H	401[B]	-	-	6/51/67/67	0/3/3/3
2	ACO	B	401[B]	-	-	9/51/67/67	0/3/3/3
2	ACO	A	401[A]	-	-	16/51/67/67	0/3/3/3
2	ACO	F	401[B]	-	-	6/51/67/67	0/3/3/3
2	ACO	J	401[B]	-	-	7/51/67/67	0/3/3/3
2	ACO	G	401[B]	-	-	5/51/67/67	0/3/3/3
2	ACO	D	401[B]	-	-	13/51/67/67	0/3/3/3
2	ACO	L	401[A]	-	-	10/51/67/67	0/3/3/3
2	ACO	E	401[A]	-	-	7/51/67/67	0/3/3/3
2	ACO	I	401[A]	-	-	4/51/67/67	0/3/3/3
2	ACO	K	401[B]	-	-	3/51/67/67	0/3/3/3
2	ACO	A	401[B]	-	-	8/51/67/67	0/3/3/3
2	ACO	C	401[A]	-	-	11/51/67/67	0/3/3/3
2	ACO	B	401[A]	-	-	5/51/67/67	0/3/3/3
2	ACO	H	401[A]	-	-	11/51/67/67	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401[A]	ACO	P2A-O3A	3.23	1.63	1.59
2	E	401[B]	ACO	P3B-O3B	3.10	1.65	1.59
2	F	401[B]	ACO	P3B-O3B	2.95	1.64	1.59
2	A	401[A]	ACO	P3B-O3B	2.90	1.64	1.59
2	E	401[A]	ACO	P1A-O3A	2.80	1.62	1.59
2	H	401[A]	ACO	P2A-O3A	2.70	1.62	1.59
2	L	401[B]	ACO	C-S1P	2.65	1.89	1.75
2	K	401[A]	ACO	P3B-O3B	2.61	1.64	1.59
2	E	401[B]	ACO	P2A-O3A	2.60	1.62	1.59
2	C	401[A]	ACO	P3B-O3B	2.58	1.64	1.59
2	L	401[A]	ACO	P2A-O3A	2.56	1.62	1.59
2	A	401[B]	ACO	P3B-O3B	2.49	1.63	1.59
2	G	401[B]	ACO	P3B-O3B	2.45	1.63	1.59
2	L	401[A]	ACO	P3B-O3B	2.43	1.63	1.59
2	I	401[B]	ACO	C-S1P	2.41	1.88	1.75
2	G	401[A]	ACO	P3B-O3B	2.39	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401[B]	ACO	P2A-O3A	2.37	1.62	1.59
2	H	401[A]	ACO	P3B-O3B	2.34	1.63	1.59
2	C	401[B]	ACO	P2A-O3A	2.29	1.62	1.59
2	D	401[A]	ACO	P2A-O3A	2.25	1.61	1.59
2	B	401[B]	ACO	P3B-O3B	2.25	1.63	1.59
2	B	401[A]	ACO	P2A-O3A	2.24	1.61	1.59
2	H	401[A]	ACO	P1A-O3A	2.19	1.61	1.59
2	H	401[B]	ACO	P2A-O3A	2.15	1.61	1.59
2	E	401[B]	ACO	P1A-O3A	2.14	1.61	1.59
2	K	401[A]	ACO	P2A-O3A	2.11	1.61	1.59
2	D	401[A]	ACO	P3B-O3B	2.02	1.63	1.59
2	C	401[A]	ACO	P2A-O3A	2.01	1.61	1.59

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401[A]	ACO	C2P-S1P-C	10.95	154.10	101.42
2	B	401[A]	ACO	C2P-S1P-C	7.50	137.51	101.42
2	C	401[A]	ACO	C2P-S1P-C	7.38	136.93	101.42
2	G	401[A]	ACO	C2P-S1P-C	7.34	136.74	101.42
2	E	401[B]	ACO	C2P-S1P-C	6.77	133.98	101.42
2	E	401[A]	ACO	C2P-S1P-C	6.77	133.98	101.42
2	D	401[A]	ACO	C2P-S1P-C	6.20	131.28	101.42
2	H	401[A]	ACO	C2P-S1P-C	6.19	131.19	101.42
2	F	401[B]	ACO	C2P-S1P-C	6.17	131.09	101.42
2	G	401[B]	ACO	C2P-S1P-C	5.86	129.60	101.42
2	J	401[A]	ACO	C2P-S1P-C	5.84	129.52	101.42
2	H	401[B]	ACO	C2P-S1P-C	5.80	129.33	101.42
2	A	401[A]	ACO	C2P-S1P-C	5.66	128.67	101.42
2	F	401[A]	ACO	C2P-S1P-C	5.65	128.62	101.42
2	K	401[A]	ACO	C2P-S1P-C	5.50	127.89	101.42
2	D	401[B]	ACO	C2P-S1P-C	4.96	125.28	101.42
2	K	401[B]	ACO	C2P-S1P-C	4.91	125.07	101.42
2	I	401[A]	ACO	C2P-S1P-C	4.89	124.94	101.42
2	D	401[B]	ACO	P3B-O3B-C3B	-4.88	110.41	123.43
2	B	401[B]	ACO	C2P-S1P-C	4.87	124.87	101.42
2	J	401[B]	ACO	C2P-S1P-C	4.79	124.48	101.42
2	I	401[A]	ACO	P3B-O3B-C3B	-4.75	110.76	123.43
2	L	401[B]	ACO	C2P-S1P-C	4.02	120.77	101.42
2	A	401[B]	ACO	C2P-S1P-C	3.93	120.33	101.42
2	L	401[B]	ACO	P3B-O3B-C3B	-3.67	113.64	123.43
2	H	401[B]	ACO	O3B-P3B-O7A	-3.61	96.47	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401[B]	ACO	P3B-O3B-C3B	-3.50	114.10	123.43
2	B	401[A]	ACO	O9A-P3B-O3B	-3.45	92.39	105.85
2	C	401[B]	ACO	C2P-S1P-C	3.24	117.02	101.42
2	L	401[A]	ACO	O3B-P3B-O7A	-3.22	97.85	109.33
2	H	401[B]	ACO	O9A-P3B-O3B	3.10	117.92	105.85
2	E	401[A]	ACO	O9A-P3B-O3B	-3.06	93.91	105.85
2	G	401[A]	ACO	O5A-P2A-O4A	2.94	126.14	112.44
2	G	401[A]	ACO	P3B-O3B-C3B	-2.93	115.60	123.43
2	D	401[A]	ACO	O5A-P2A-O4A	2.91	125.98	112.44
2	I	401[A]	ACO	O5A-P2A-O4A	2.90	125.95	112.44
2	C	401[A]	ACO	O9A-P3B-O3B	2.86	117.00	105.85
2	A	401[B]	ACO	CAP-C9P-N8P	2.77	121.75	116.48
2	B	401[B]	ACO	O8A-P3B-O3B	-2.75	95.12	105.85
2	F	401[A]	ACO	P3B-O3B-C3B	-2.72	116.17	123.43
2	J	401[A]	ACO	C7P-C6P-C5P	2.70	116.90	112.39
2	L	401[A]	ACO	O5A-P2A-O4A	2.70	125.00	112.44
2	B	401[A]	ACO	O3B-C3B-C2B	-2.70	102.00	111.68
2	C	401[A]	ACO	C7P-C6P-C5P	2.60	116.72	112.39
2	I	401[A]	ACO	O3A-P2A-O4A	-2.53	103.10	110.70
2	D	401[A]	ACO	C7P-C6P-C5P	2.46	116.48	112.39
2	E	401[A]	ACO	O2B-C2B-C3B	2.45	118.06	111.19
2	A	401[A]	ACO	O5A-P2A-O4A	2.40	123.59	112.44
2	I	401[B]	ACO	O5A-P2A-O4A	2.38	123.54	112.44
2	C	401[A]	ACO	O3B-P3B-O7A	-2.35	100.97	109.33
2	F	401[B]	ACO	C7P-C6P-C5P	2.33	116.28	112.39
2	I	401[A]	ACO	O2A-P1A-O3A	2.32	113.54	107.27
2	G	401[A]	ACO	C3P-N4P-C5P	2.31	127.13	122.82
2	H	401[A]	ACO	C7P-C6P-C5P	2.31	116.24	112.39
2	K	401[B]	ACO	O9A-P3B-O3B	-2.30	96.88	105.85
2	J	401[B]	ACO	O5A-P2A-O4A	2.29	123.09	112.44
2	A	401[B]	ACO	P3B-O3B-C3B	-2.29	117.32	123.43
2	A	401[B]	ACO	C2B-C1B-N9A	2.28	118.97	113.30
2	J	401[A]	ACO	O5A-P2A-O4A	2.28	123.04	112.44
2	J	401[A]	ACO	C2P-C3P-N4P	2.26	117.13	112.41
2	D	401[A]	ACO	C2B-C1B-N9A	2.21	118.80	113.30
2	F	401[B]	ACO	O5A-P2A-O4A	2.21	122.73	112.44
2	I	401[B]	ACO	P3B-O3B-C3B	-2.20	117.55	123.43
2	J	401[A]	ACO	P3B-O3B-C3B	-2.19	117.58	123.43
2	J	401[B]	ACO	O2A-P1A-O3A	2.15	113.10	107.27
2	D	401[B]	ACO	C7P-C6P-C5P	2.15	115.97	112.39
2	J	401[A]	ACO	OAP-CAP-CBP	-2.13	105.25	110.18
2	B	401[A]	ACO	O5A-P2A-O4A	2.11	122.26	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401[B]	ACO	O3B-C3B-C2B	-2.10	104.15	111.68
2	K	401[A]	ACO	P3B-O3B-C3B	-2.09	117.84	123.43
2	K	401[B]	ACO	C7P-C6P-C5P	2.08	115.86	112.39
2	A	401[A]	ACO	P3B-O3B-C3B	-2.08	117.88	123.43
2	C	401[A]	ACO	CDP-CBP-CCP	2.07	111.65	108.22
2	C	401[A]	ACO	O6A-CCP-CBP	-2.07	107.22	110.55
2	A	401[A]	ACO	CAP-C9P-N8P	2.06	120.40	116.48
2	C	401[B]	ACO	P3B-O3B-C3B	-2.05	117.96	123.43
2	I	401[B]	ACO	O3A-P2A-O4A	-2.05	104.54	110.70
2	B	401[A]	ACO	C6P-C5P-N4P	2.05	120.07	116.34
2	E	401[B]	ACO	O5P-C5P-C6P	-2.03	118.34	122.02
2	I	401[A]	ACO	OAP-CAP-CBP	-2.03	105.48	110.18
2	H	401[B]	ACO	O2A-P1A-O3A	2.02	112.73	107.27
2	E	401[A]	ACO	P3B-O3B-C3B	-2.01	118.05	123.43
2	G	401[B]	ACO	O5A-P2A-O4A	2.01	121.81	112.44

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	ACO	C9P-CAP-CBP-CCP
2	A	401[A]	ACO	C9P-CAP-CBP-CEP
2	A	401[A]	ACO	CAP-C9P-N8P-C7P
2	A	401[A]	ACO	O9P-C9P-N8P-C7P
2	A	401[A]	ACO	C5P-C6P-C7P-N8P
2	A	401[A]	ACO	C3P-C2P-S1P-C
2	A	401[B]	ACO	CAP-C9P-N8P-C7P
2	A	401[B]	ACO	O9P-C9P-N8P-C7P
2	A	401[B]	ACO	S1P-C2P-C3P-N4P
2	A	401[B]	ACO	O-C-S1P-C2P
2	A	401[B]	ACO	CH3-C-S1P-C2P
2	B	401[A]	ACO	C5B-O5B-P1A-O1A
2	B	401[B]	ACO	C5B-O5B-P1A-O1A
2	B	401[B]	ACO	CAP-C9P-N8P-C7P
2	B	401[B]	ACO	O9P-C9P-N8P-C7P
2	B	401[B]	ACO	C5P-C6P-C7P-N8P
2	C	401[A]	ACO	S1P-C2P-C3P-N4P
2	C	401[A]	ACO	C3P-C2P-S1P-C
2	C	401[A]	ACO	O-C-S1P-C2P
2	C	401[A]	ACO	CH3-C-S1P-C2P
2	C	401[B]	ACO	C9P-CAP-CBP-CCP
2	C	401[B]	ACO	C9P-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
2	C	401[B]	ACO	C9P-CAP-CBP-CEP
2	D	401[A]	ACO	C5B-O5B-P1A-O1A
2	D	401[A]	ACO	C5B-O5B-P1A-O3A
2	D	401[A]	ACO	C3P-C2P-S1P-C
2	D	401[B]	ACO	C3B-C4B-C5B-O5B
2	D	401[B]	ACO	CDP-CBP-CCP-O6A
2	D	401[B]	ACO	CEP-CBP-CCP-O6A
2	D	401[B]	ACO	CAP-CBP-CCP-O6A
2	D	401[B]	ACO	C2P-C3P-N4P-C5P
2	D	401[B]	ACO	S1P-C2P-C3P-N4P
2	D	401[B]	ACO	C3P-C2P-S1P-C
2	E	401[A]	ACO	CAP-C9P-N8P-C7P
2	E	401[A]	ACO	O9P-C9P-N8P-C7P
2	E	401[A]	ACO	O-C-S1P-C2P
2	E	401[A]	ACO	CH3-C-S1P-C2P
2	E	401[B]	ACO	C9P-CAP-CBP-CCP
2	E	401[B]	ACO	C9P-CAP-CBP-CDP
2	E	401[B]	ACO	C9P-CAP-CBP-CEP
2	E	401[B]	ACO	CAP-C9P-N8P-C7P
2	E	401[B]	ACO	O9P-C9P-N8P-C7P
2	E	401[B]	ACO	C5P-C6P-C7P-N8P
2	E	401[B]	ACO	S1P-C2P-C3P-N4P
2	E	401[B]	ACO	O-C-S1P-C2P
2	E	401[B]	ACO	CH3-C-S1P-C2P
2	F	401[A]	ACO	C3P-C2P-S1P-C
2	F	401[B]	ACO	C5B-O5B-P1A-O1A
2	F	401[B]	ACO	C5P-C6P-C7P-N8P
2	G	401[A]	ACO	C5B-O5B-P1A-O1A
2	G	401[A]	ACO	C5B-O5B-P1A-O3A
2	G	401[A]	ACO	C5P-C6P-C7P-N8P
2	G	401[A]	ACO	C2P-C3P-N4P-C5P
2	G	401[B]	ACO	P1A-O3A-P2A-O6A
2	G	401[B]	ACO	C3P-C2P-S1P-C
2	H	401[A]	ACO	S1P-C2P-C3P-N4P
2	H	401[A]	ACO	C3P-C2P-S1P-C
2	H	401[A]	ACO	O-C-S1P-C2P
2	H	401[A]	ACO	CH3-C-S1P-C2P
2	H	401[B]	ACO	O-C-S1P-C2P
2	H	401[B]	ACO	CH3-C-S1P-C2P
2	I	401[A]	ACO	C3P-C2P-S1P-C
2	I	401[B]	ACO	CCP-O6A-P2A-O4A
2	I	401[B]	ACO	O-C-S1P-C2P

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Mol	Chain	Res	Type	Atoms
2	I	401[B]	ACO	CH3-C-S1P-C2P
2	J	401[A]	ACO	C5B-O5B-P1A-O1A
2	J	401[A]	ACO	C5B-O5B-P1A-O3A
2	J	401[A]	ACO	C3P-C2P-S1P-C
2	J	401[B]	ACO	S1P-C2P-C3P-N4P
2	J	401[B]	ACO	C3P-C2P-S1P-C
2	K	401[A]	ACO	C3P-C2P-S1P-C
2	K	401[B]	ACO	C3P-C2P-S1P-C
2	L	401[A]	ACO	C5B-O5B-P1A-O2A
2	L	401[A]	ACO	C3P-C2P-S1P-C
2	L	401[A]	ACO	O-C-S1P-C2P
2	L	401[A]	ACO	CH3-C-S1P-C2P
2	L	401[B]	ACO	S1P-C2P-C3P-N4P
2	L	401[B]	ACO	O-C-S1P-C2P
2	L	401[B]	ACO	CH3-C-S1P-C2P
2	D	401[B]	ACO	O5P-C5P-N4P-C3P
2	J	401[B]	ACO	O5P-C5P-N4P-C3P
2	D	401[B]	ACO	C6P-C5P-N4P-C3P
2	H	401[A]	ACO	C6P-C5P-N4P-C3P
2	J	401[B]	ACO	C6P-C5P-N4P-C3P
2	C	401[A]	ACO	O5P-C5P-N4P-C3P
2	H	401[A]	ACO	O5P-C5P-N4P-C3P
2	A	401[A]	ACO	O5P-C5P-N4P-C3P
2	C	401[A]	ACO	C6P-C5P-N4P-C3P
2	H	401[B]	ACO	C6P-C7P-N8P-C9P
2	D	401[B]	ACO	O4B-C4B-C5B-O5B
2	D	401[A]	ACO	O5P-C5P-N4P-C3P
2	A	401[A]	ACO	C6P-C5P-N4P-C3P
2	L	401[A]	ACO	O4B-C4B-C5B-O5B
2	D	401[A]	ACO	C6P-C5P-N4P-C3P
2	J	401[A]	ACO	O5P-C5P-N4P-C3P
2	E	401[A]	ACO	C5P-C6P-C7P-N8P
2	K	401[B]	ACO	C5P-C6P-C7P-N8P
2	L	401[B]	ACO	C2B-C3B-O3B-P3B
2	C	401[B]	ACO	OAP-CAP-CBP-CEP
2	E	401[B]	ACO	OAP-CAP-CBP-CEP
2	D	401[B]	ACO	P2A-O3A-P1A-O1A
2	A	401[A]	ACO	O9P-C9P-CAP-CBP
2	K	401[A]	ACO	O5P-C5P-N4P-C3P
2	L	401[B]	ACO	C6P-C7P-N8P-C9P
2	A	401[B]	ACO	P1A-O3A-P2A-O6A
2	D	401[B]	ACO	P2A-O3A-P1A-O5B

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Mol	Chain	Res	Type	Atoms
2	C	401[A]	ACO	C6P-C7P-N8P-C9P
2	I	401[A]	ACO	O5P-C5P-N4P-C3P
2	B	401[B]	ACO	C9P-CAP-CBP-CEP
2	L	401[A]	ACO	C3B-C4B-C5B-O5B
2	C	401[B]	ACO	P2A-O3A-P1A-O2A
2	E	401[B]	ACO	P2A-O3A-P1A-O2A
2	I	401[A]	ACO	P2A-O3A-P1A-O2A
2	J	401[A]	ACO	C6P-C7P-N8P-C9P
2	J	401[A]	ACO	C6P-C5P-N4P-C3P
2	A	401[A]	ACO	CEP-CBP-CCP-O6A
2	B	401[B]	ACO	CDP-CBP-CCP-O6A
2	B	401[B]	ACO	CEP-CBP-CCP-O6A
2	C	401[B]	ACO	CDP-CBP-CCP-O6A
2	H	401[A]	ACO	CDP-CBP-CCP-O6A
2	A	401[A]	ACO	C3B-O3B-P3B-O7A
2	A	401[B]	ACO	C3P-C2P-S1P-C
2	H	401[B]	ACO	C3B-O3B-P3B-O7A
2	H	401[B]	ACO	C3P-C2P-S1P-C
2	I	401[B]	ACO	C3B-O3B-P3B-O7A
2	K	401[A]	ACO	C6P-C7P-N8P-C9P
2	H	401[A]	ACO	CAP-CBP-CCP-O6A
2	C	401[B]	ACO	C5B-O5B-P1A-O1A
2	C	401[B]	ACO	CCP-O6A-P2A-O4A
2	C	401[B]	ACO	OAP-CAP-CBP-CCP
2	E	401[B]	ACO	OAP-CAP-CBP-CCP
2	F	401[B]	ACO	C5B-O5B-P1A-O3A
2	I	401[B]	ACO	C5B-O5B-P1A-O1A
2	K	401[A]	ACO	C5B-O5B-P1A-O1A
2	L	401[A]	ACO	C5B-O5B-P1A-O1A
2	L	401[A]	ACO	C5B-O5B-P1A-O3A
2	C	401[B]	ACO	OAP-CAP-CBP-CDP
2	B	401[A]	ACO	P2A-O3A-P1A-O2A
2	E	401[A]	ACO	P2A-O3A-P1A-O2A
2	F	401[A]	ACO	P2A-O3A-P1A-O1A
2	F	401[A]	ACO	P2A-O3A-P1A-O2A
2	G	401[A]	ACO	P2A-O3A-P1A-O2A
2	J	401[A]	ACO	P2A-O3A-P1A-O2A
2	J	401[B]	ACO	P2A-O3A-P1A-O2A
2	K	401[A]	ACO	P2A-O3A-P1A-O2A
2	K	401[B]	ACO	P2A-O3A-P1A-O2A
2	D	401[B]	ACO	C3B-O3B-P3B-O8A
2	J	401[A]	ACO	C3B-O3B-P3B-O9A

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Mol	Chain	Res	Type	Atoms
2	G	401[A]	ACO	S1P-C2P-C3P-N4P
2	A	401[A]	ACO	N8P-C9P-CAP-CBP
2	L	401[B]	ACO	C4B-C3B-O3B-P3B
2	K	401[A]	ACO	C6P-C5P-N4P-C3P
2	B	401[A]	ACO	O4B-C4B-C5B-O5B
2	G	401[A]	ACO	O4B-C4B-C5B-O5B
2	J	401[A]	ACO	O4B-C4B-C5B-O5B
2	C	401[A]	ACO	C3B-O3B-P3B-O7A
2	G	401[A]	ACO	C3B-O3B-P3B-O7A
2	K	401[A]	ACO	C3B-O3B-P3B-O7A
2	B	401[B]	ACO	P2A-O3A-P1A-O2A
2	C	401[A]	ACO	P2A-O3A-P1A-O2A
2	G	401[B]	ACO	P2A-O3A-P1A-O1A
2	I	401[B]	ACO	P2A-O3A-P1A-O2A
2	L	401[A]	ACO	P1A-O3A-P2A-O5A
2	L	401[A]	ACO	C5P-C6P-C7P-N8P
2	D	401[A]	ACO	O4B-C4B-C5B-O5B
2	C	401[B]	ACO	CH3-C-S1P-C2P
2	A	401[A]	ACO	C9P-CAP-CBP-CDP
2	A	401[A]	ACO	O4B-C4B-C5B-O5B
2	F	401[A]	ACO	O4B-C4B-C5B-O5B
2	E	401[B]	ACO	OAP-CAP-CBP-CDP
2	A	401[B]	ACO	P2A-O3A-P1A-O2A
2	B	401[A]	ACO	P2A-O3A-P1A-O1A
2	C	401[B]	ACO	P2A-O3A-P1A-O1A
2	D	401[A]	ACO	P2A-O3A-P1A-O1A
2	E	401[B]	ACO	P2A-O3A-P1A-O1A
2	F	401[B]	ACO	P2A-O3A-P1A-O2A
2	G	401[B]	ACO	P2A-O3A-P1A-O2A
2	I	401[A]	ACO	P2A-O3A-P1A-O1A
2	J	401[B]	ACO	P2A-O3A-P1A-O1A
2	K	401[A]	ACO	P2A-O3A-P1A-O1A
2	B	401[B]	ACO	O9P-C9P-CAP-CBP
2	E	401[A]	ACO	O9P-C9P-CAP-CBP
2	C	401[B]	ACO	O4B-C4B-C5B-O5B
2	E	401[B]	ACO	O4B-C4B-C5B-O5B
2	F	401[B]	ACO	O4B-C4B-C5B-O5B
2	B	401[A]	ACO	C3B-O3B-P3B-O8A
2	C	401[A]	ACO	C3B-O3B-P3B-O9A
2	I	401[B]	ACO	C3B-O3B-P3B-O9A
2	K	401[A]	ACO	C3B-O3B-P3B-O9A
2	A	401[A]	ACO	CDP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	C	401[B]	ACO	CEP-CBP-CCP-O6A
2	H	401[A]	ACO	CEP-CBP-CCP-O6A
2	D	401[A]	ACO	C5P-C6P-C7P-N8P
2	I	401[B]	ACO	C5P-C6P-C7P-N8P
2	G	401[B]	ACO	C3B-O3B-P3B-O7A
2	H	401[A]	ACO	C3B-O3B-P3B-O7A
2	J	401[B]	ACO	C3B-O3B-P3B-O7A
2	A	401[A]	ACO	P2A-O3A-P1A-O2A
2	C	401[A]	ACO	P2A-O3A-P1A-O1A
2	F	401[B]	ACO	P2A-O3A-P1A-O1A
2	H	401[A]	ACO	P2A-O3A-P1A-O2A
2	H	401[B]	ACO	P2A-O3A-P1A-O2A
2	I	401[B]	ACO	P2A-O3A-P1A-O1A
2	L	401[B]	ACO	P2A-O3A-P1A-O2A
2	K	401[A]	ACO	O4B-C4B-C5B-O5B

There are no ring outliers.

23 monomers are involved in 96 short contacts:

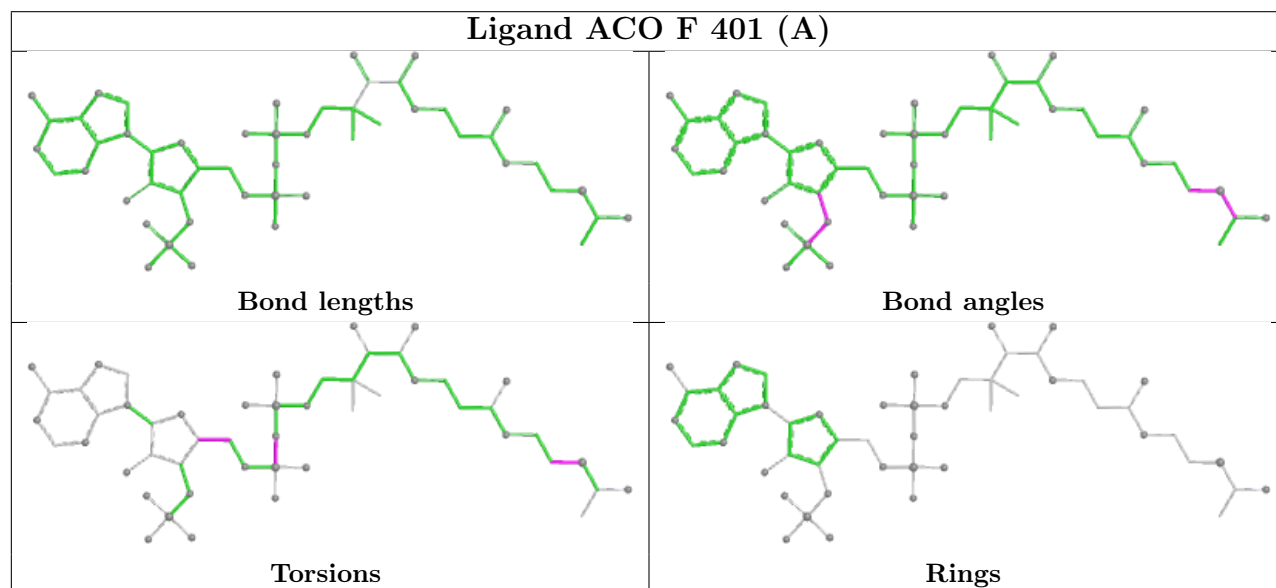
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401[A]	ACO	8	0
2	J	401[A]	ACO	1	0
2	L	401[B]	ACO	4	0
2	I	401[B]	ACO	1	0
2	E	401[B]	ACO	5	0
2	G	401[A]	ACO	3	0
2	D	401[A]	ACO	4	0
2	K	401[A]	ACO	5	0
2	C	401[B]	ACO	4	0
2	H	401[B]	ACO	4	0
2	B	401[B]	ACO	10	0
2	A	401[A]	ACO	4	0
2	F	401[B]	ACO	7	0
2	J	401[B]	ACO	1	0
2	G	401[B]	ACO	1	0
2	D	401[B]	ACO	1	0
2	L	401[A]	ACO	2	0
2	E	401[A]	ACO	8	0
2	K	401[B]	ACO	3	0
2	A	401[B]	ACO	5	0
2	C	401[A]	ACO	4	0
2	B	401[A]	ACO	5	0

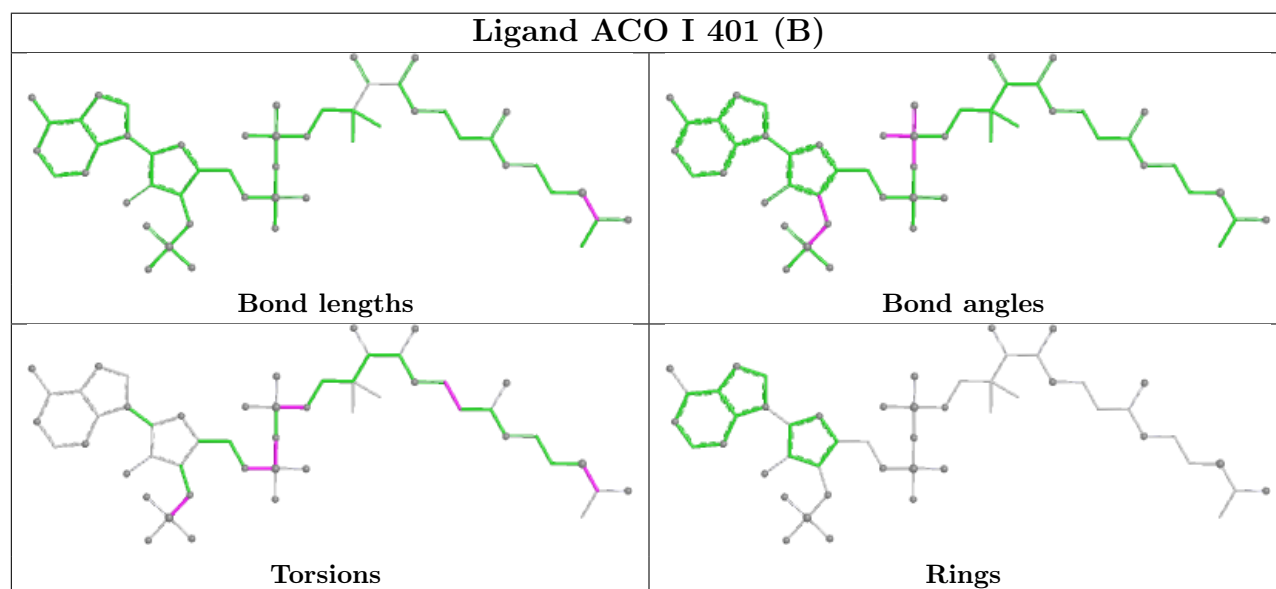
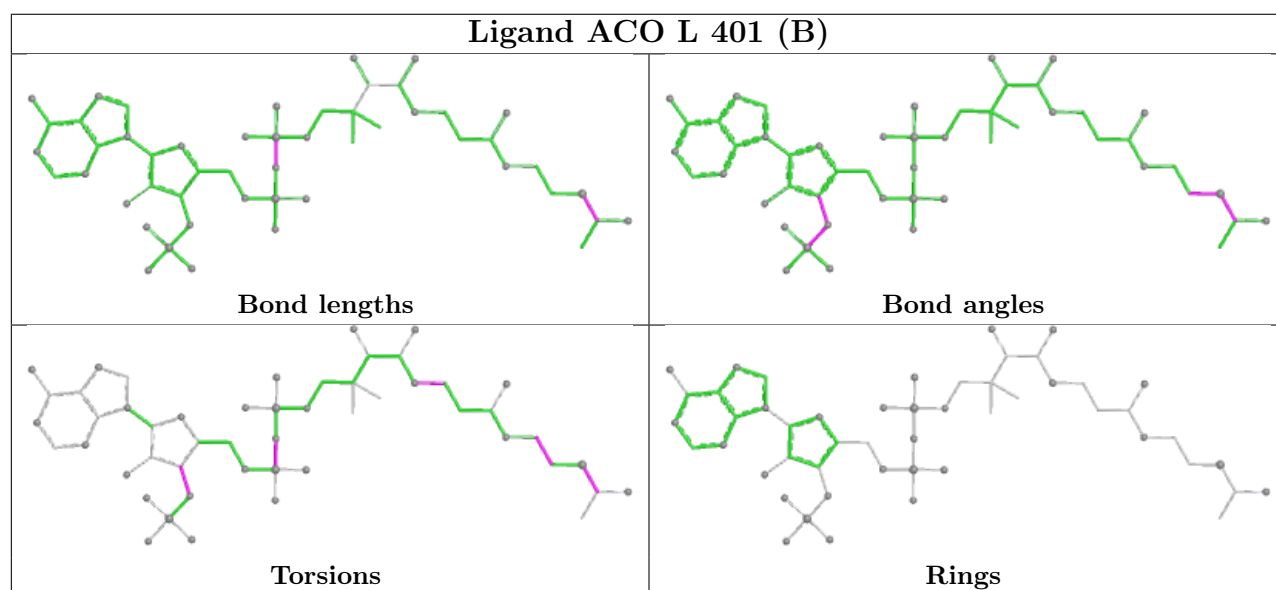
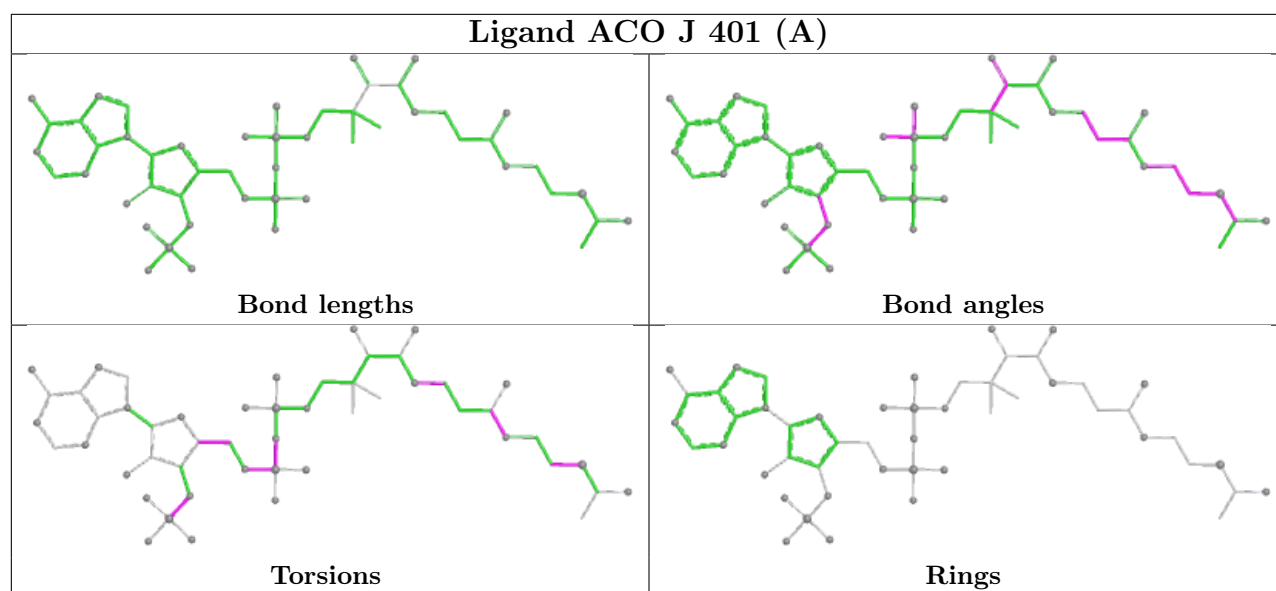
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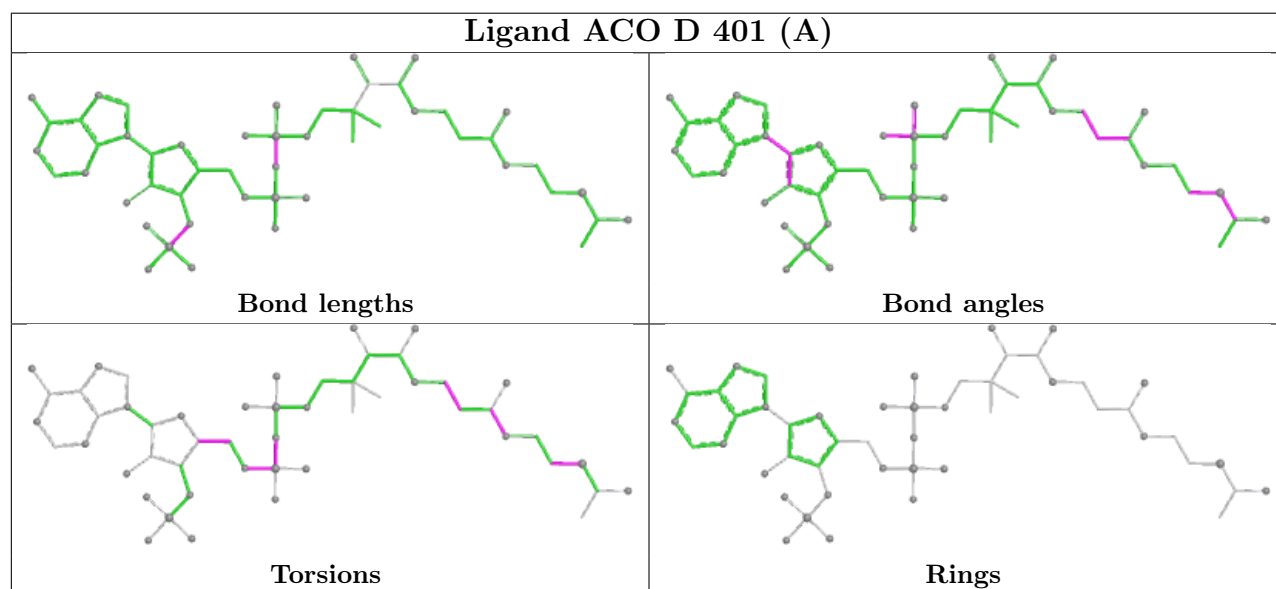
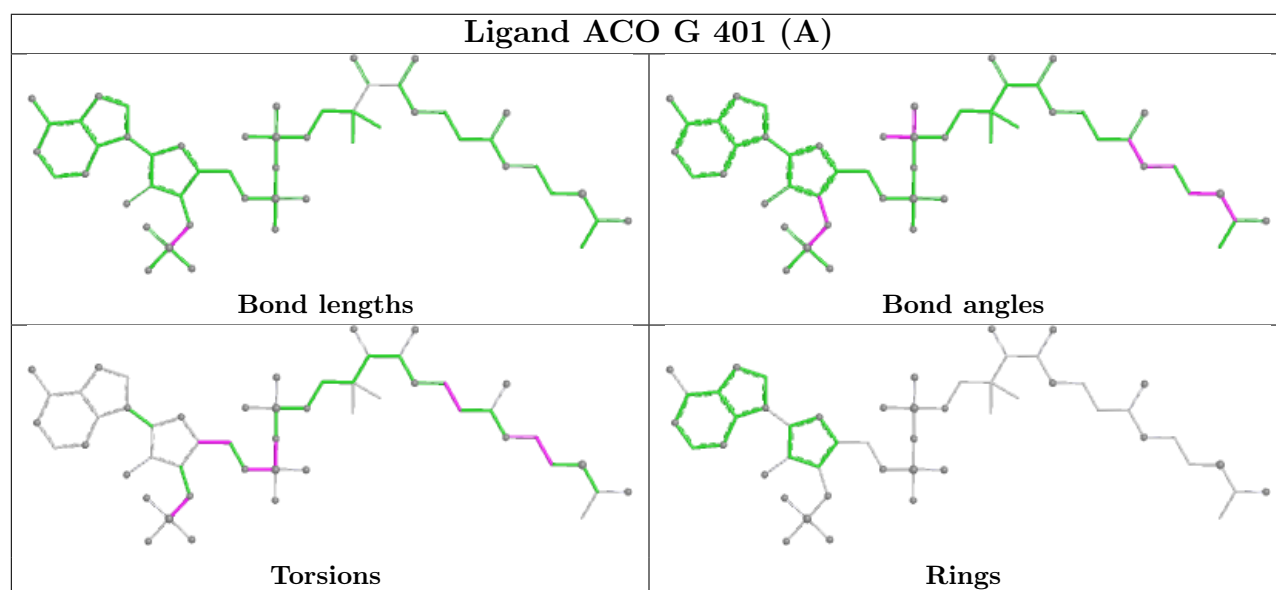
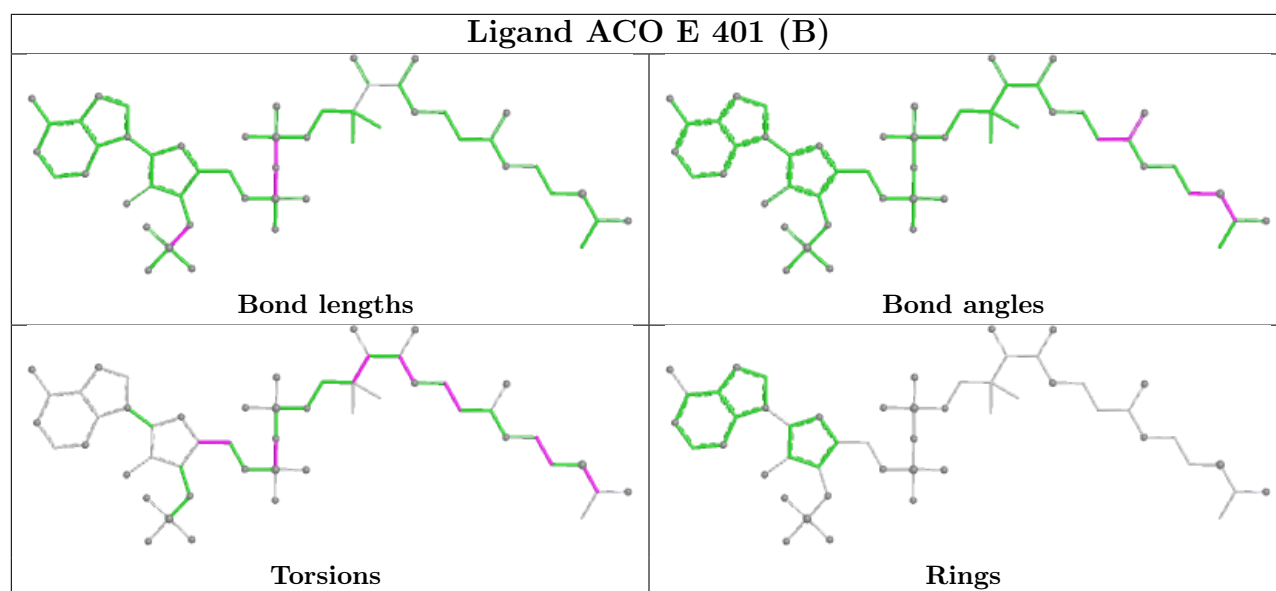
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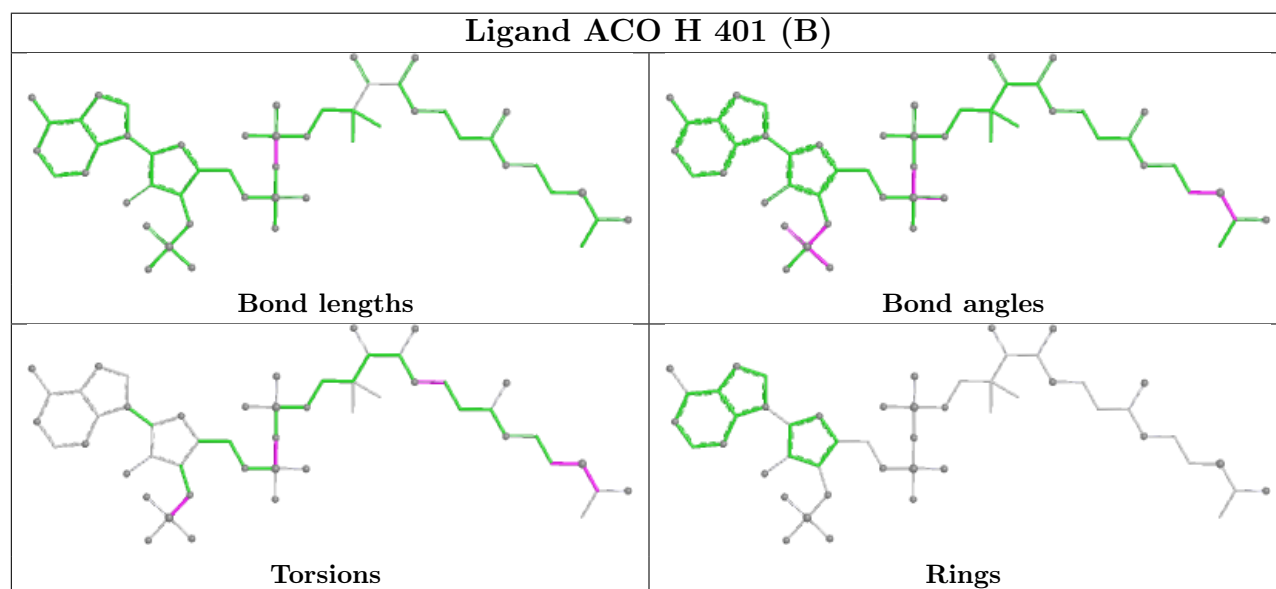
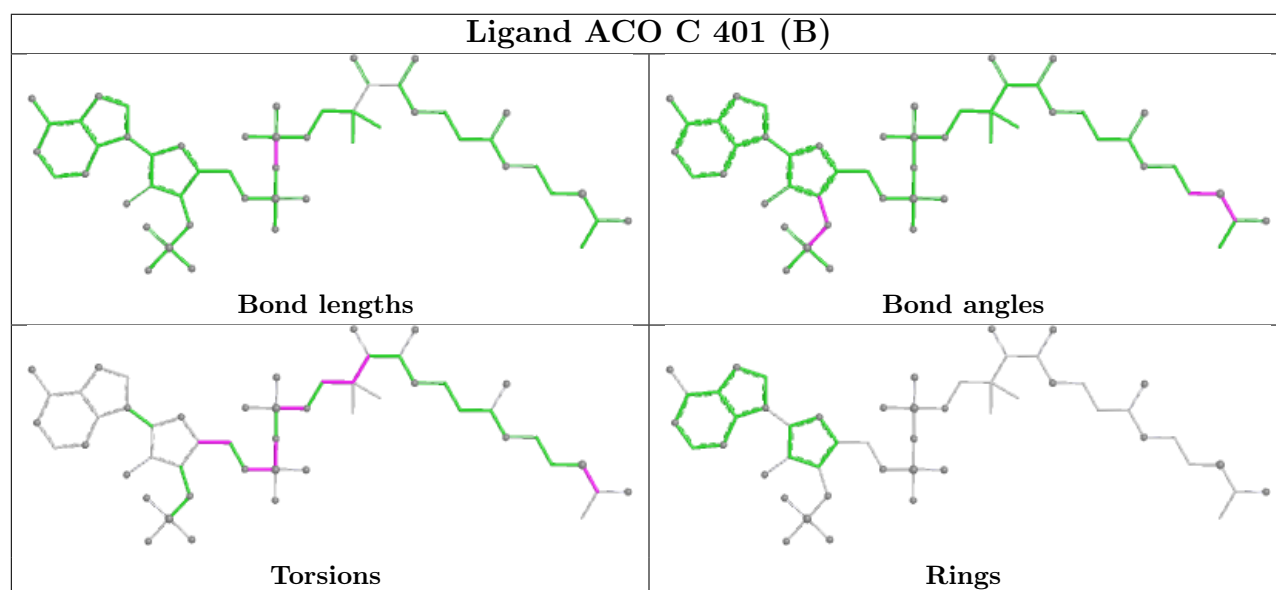
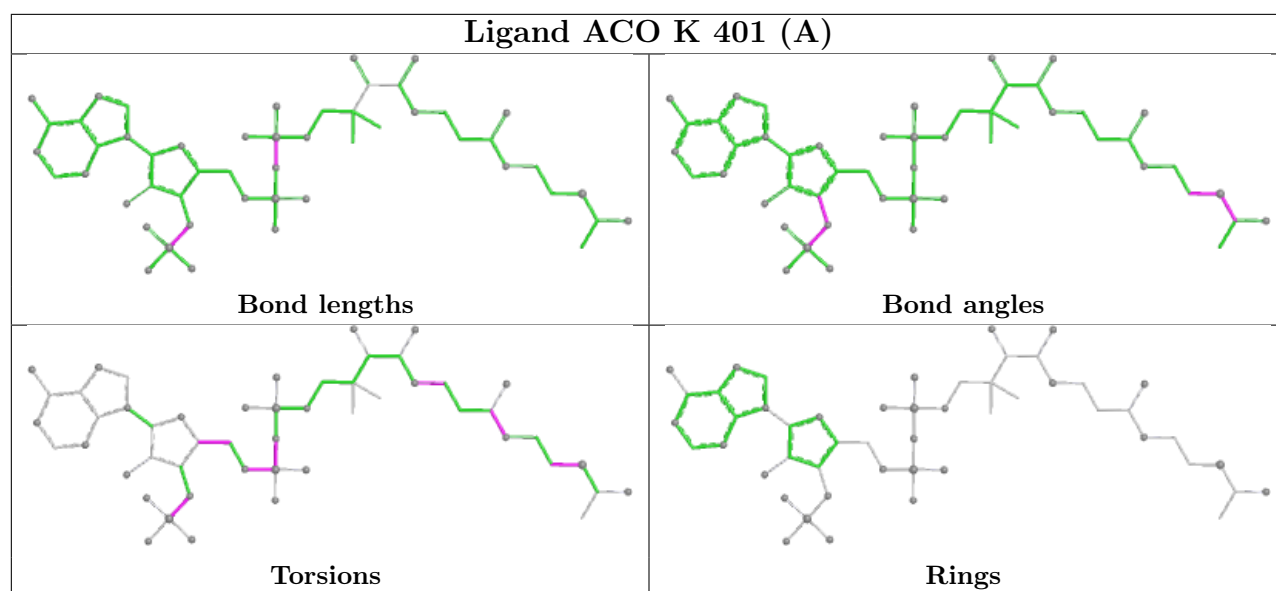
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401[A]	ACO	6	0

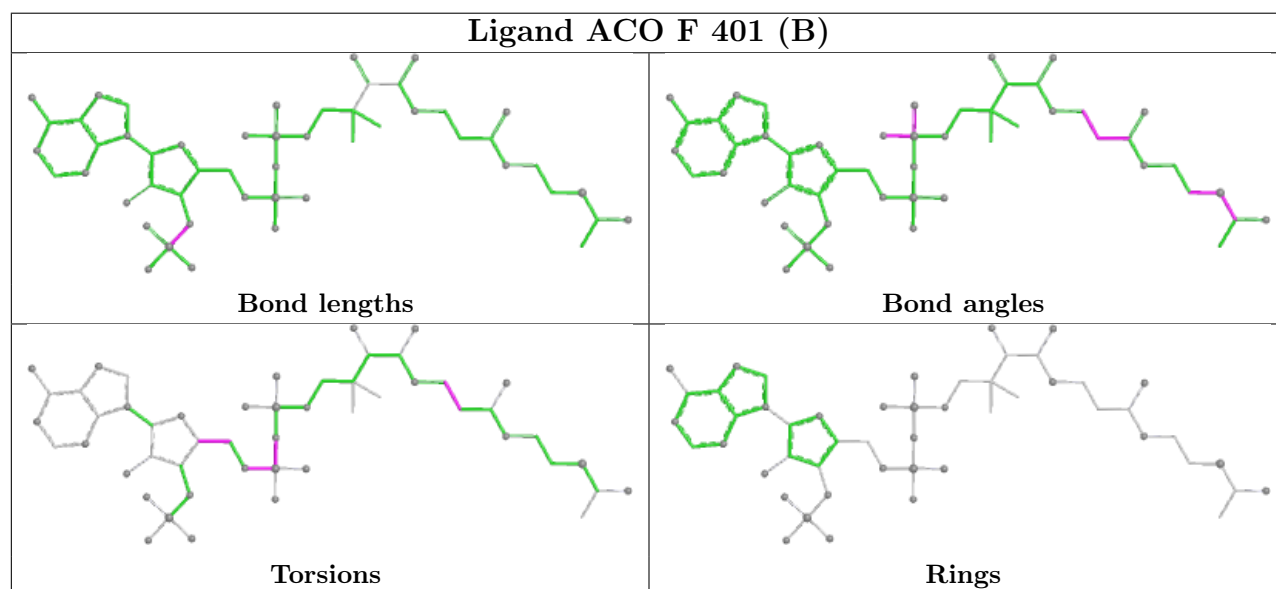
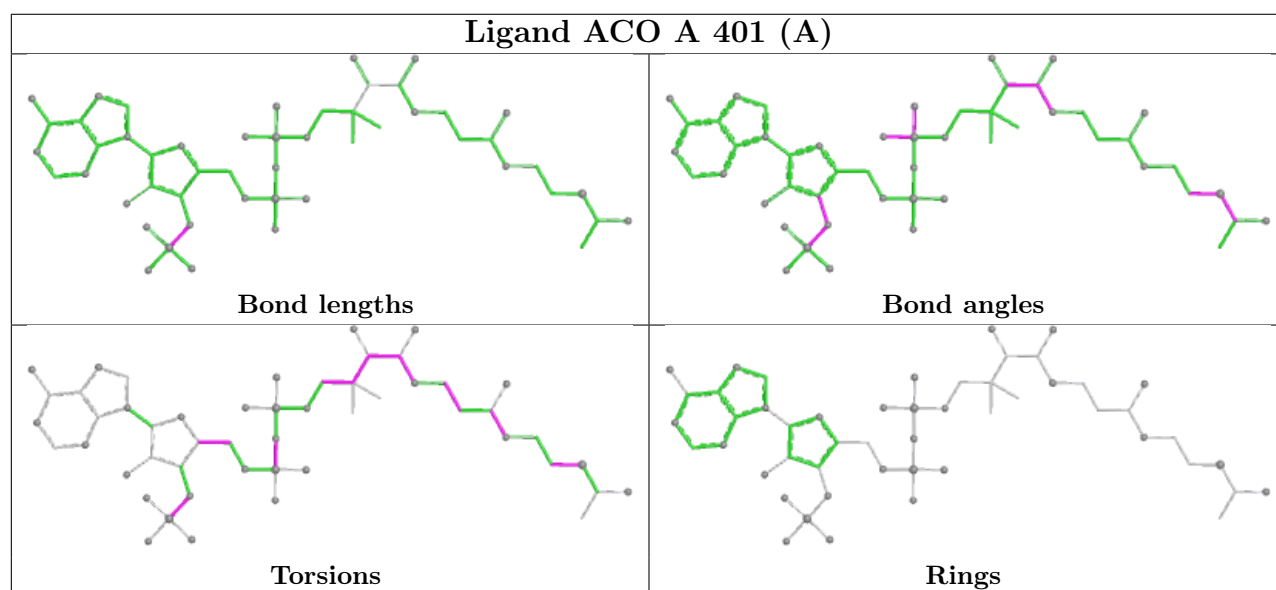
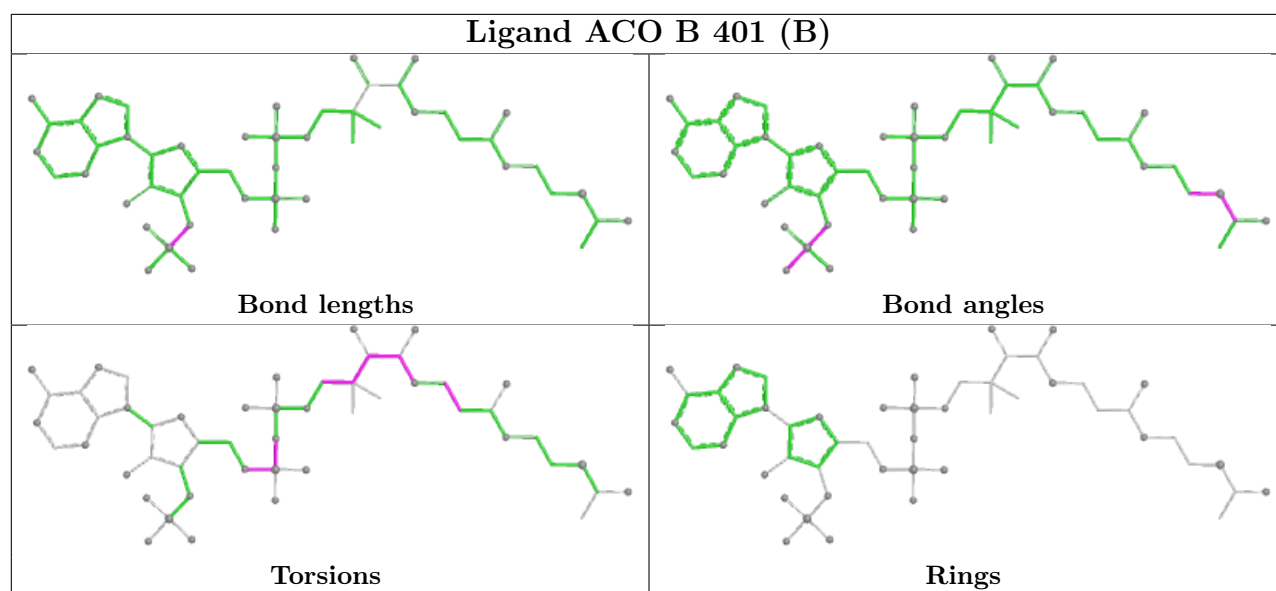
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

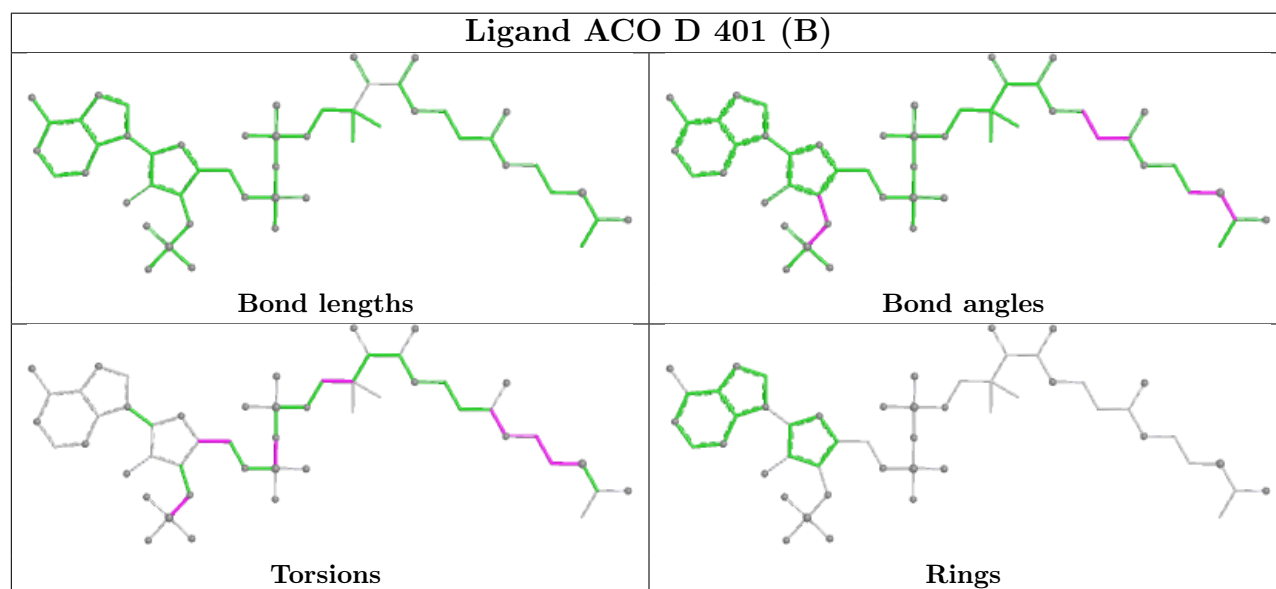
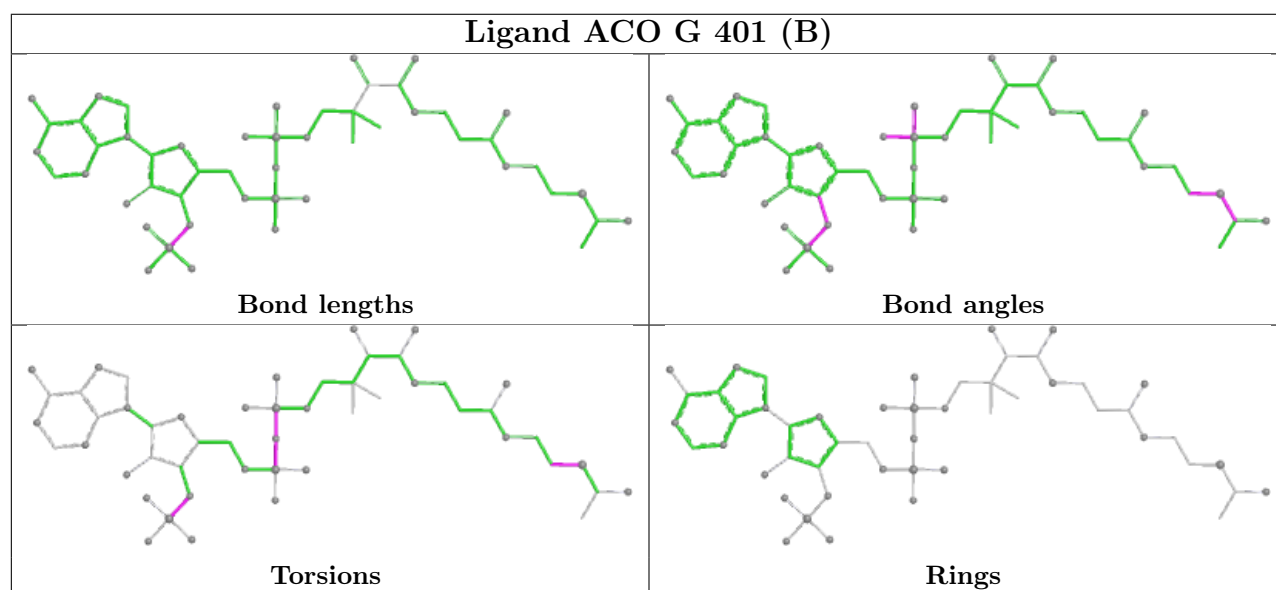
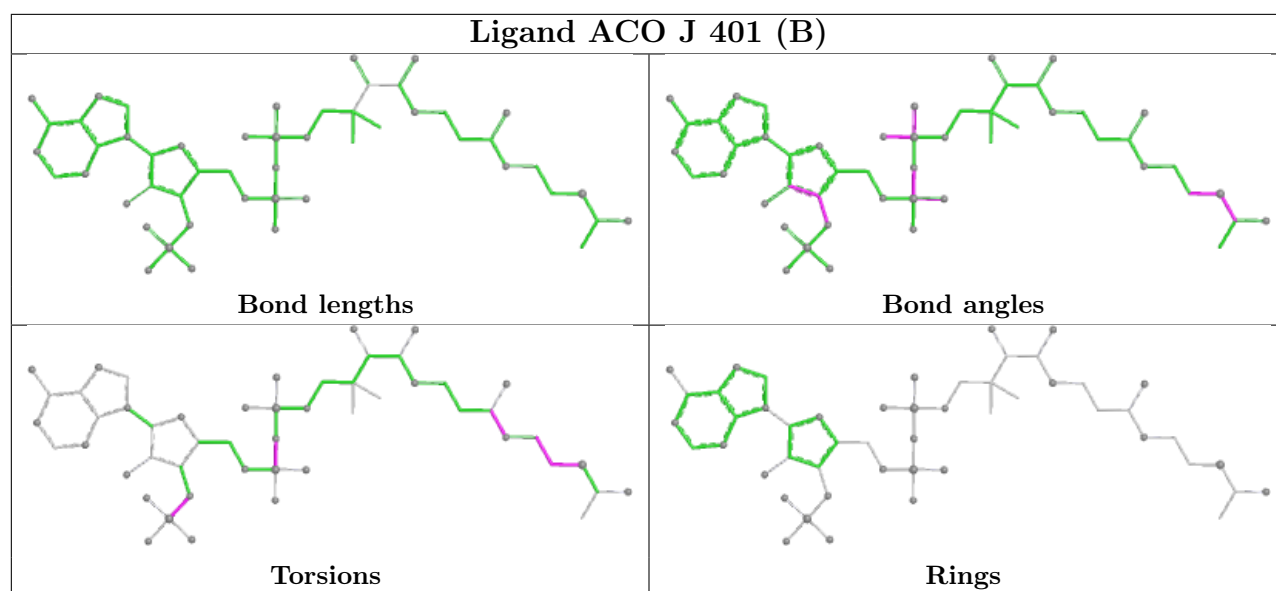


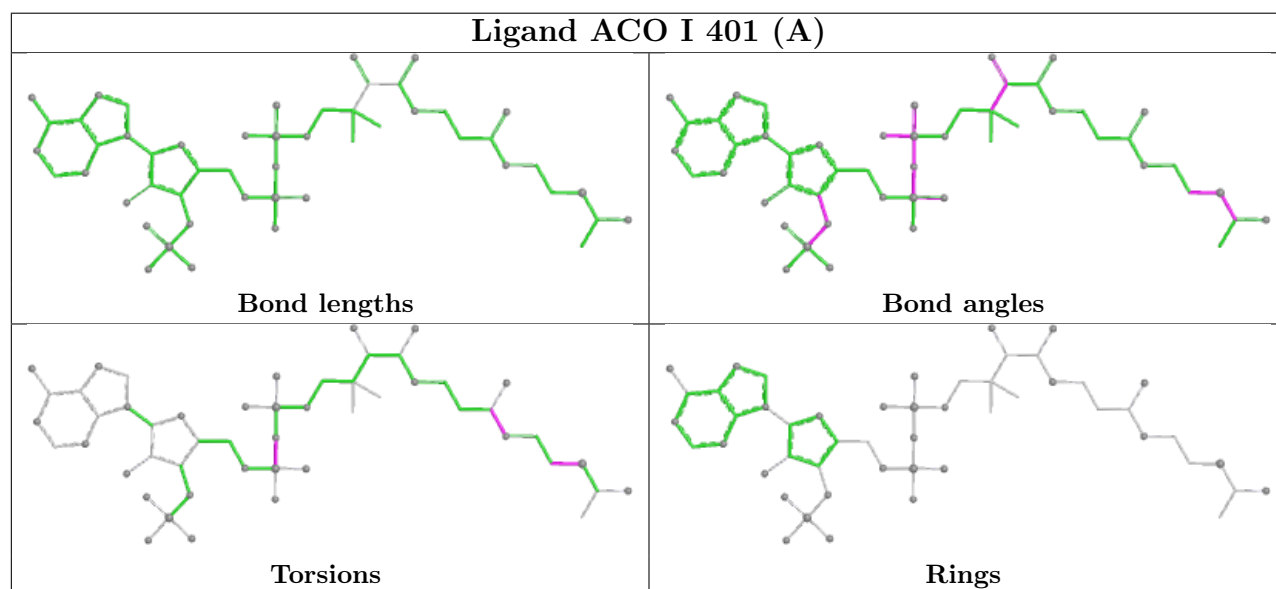
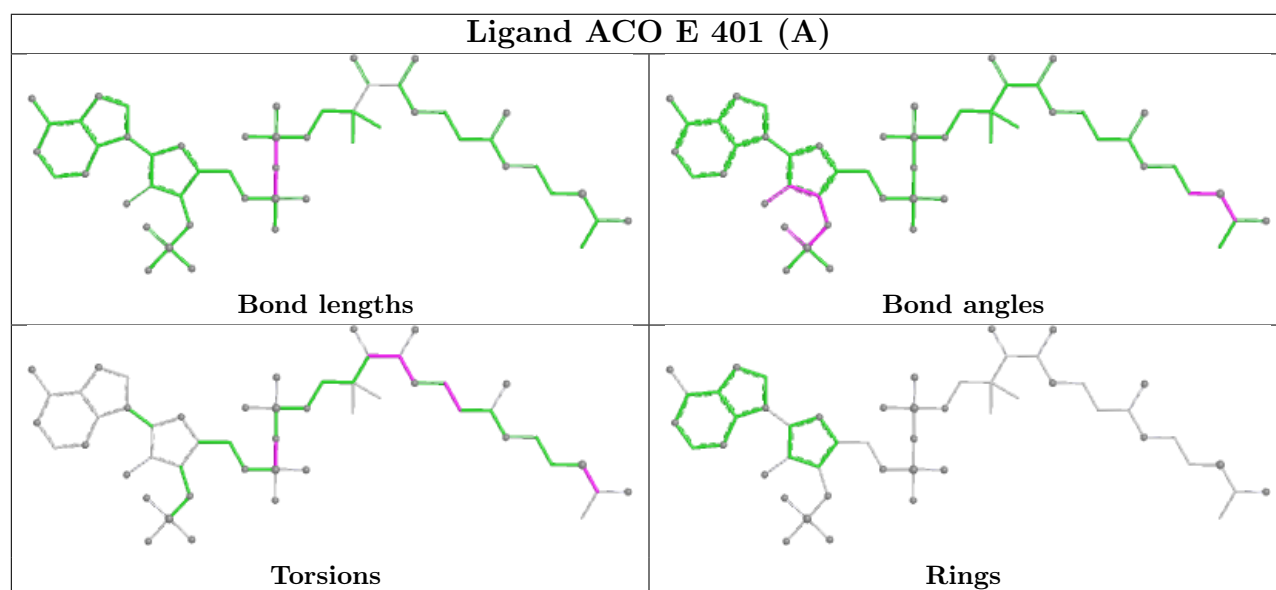
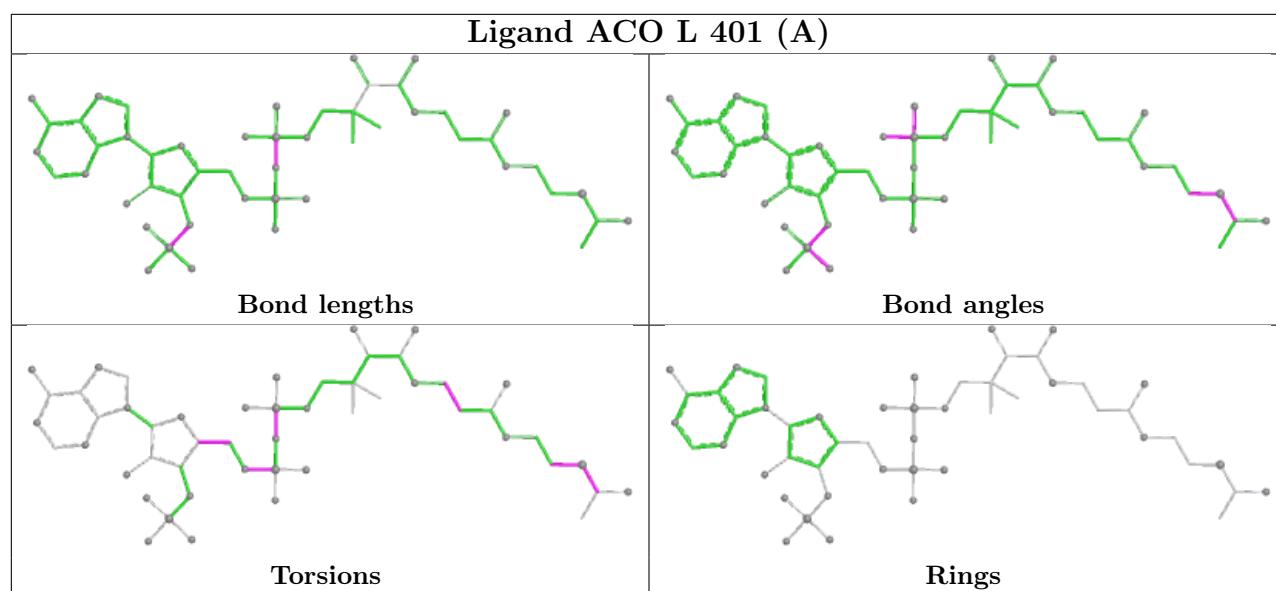


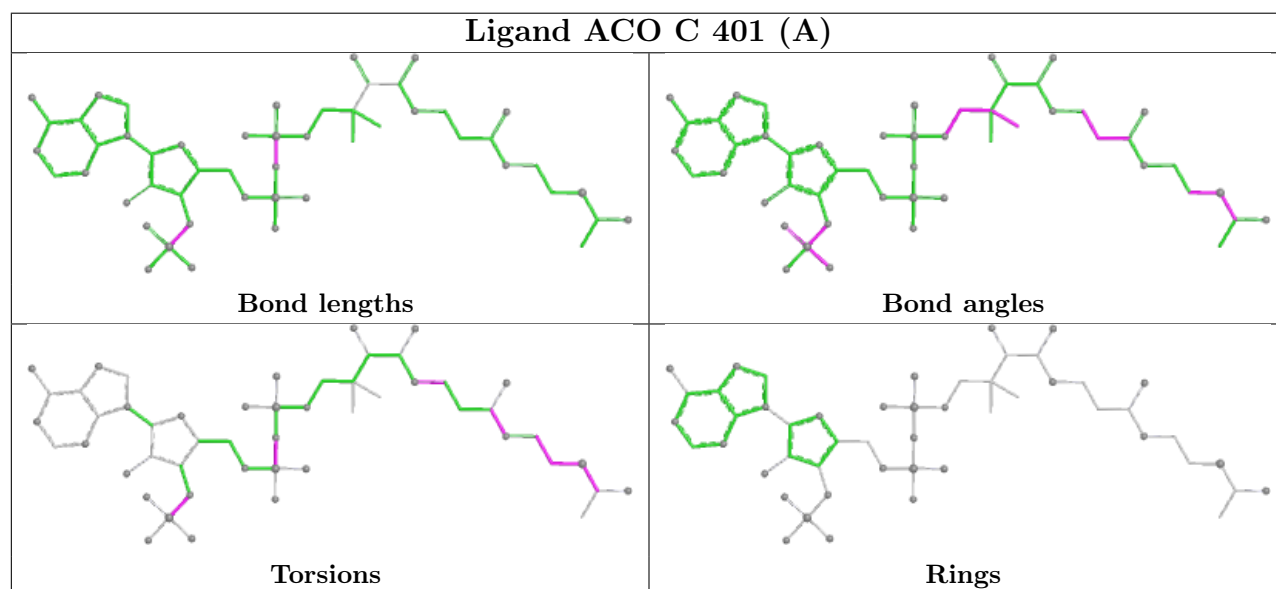
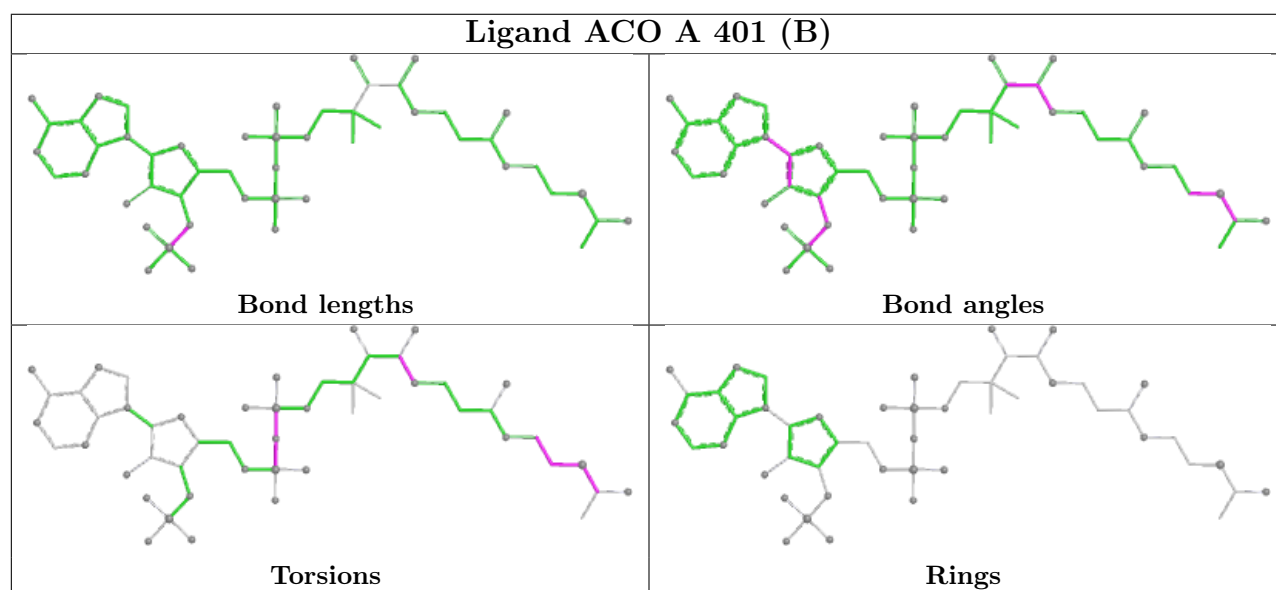
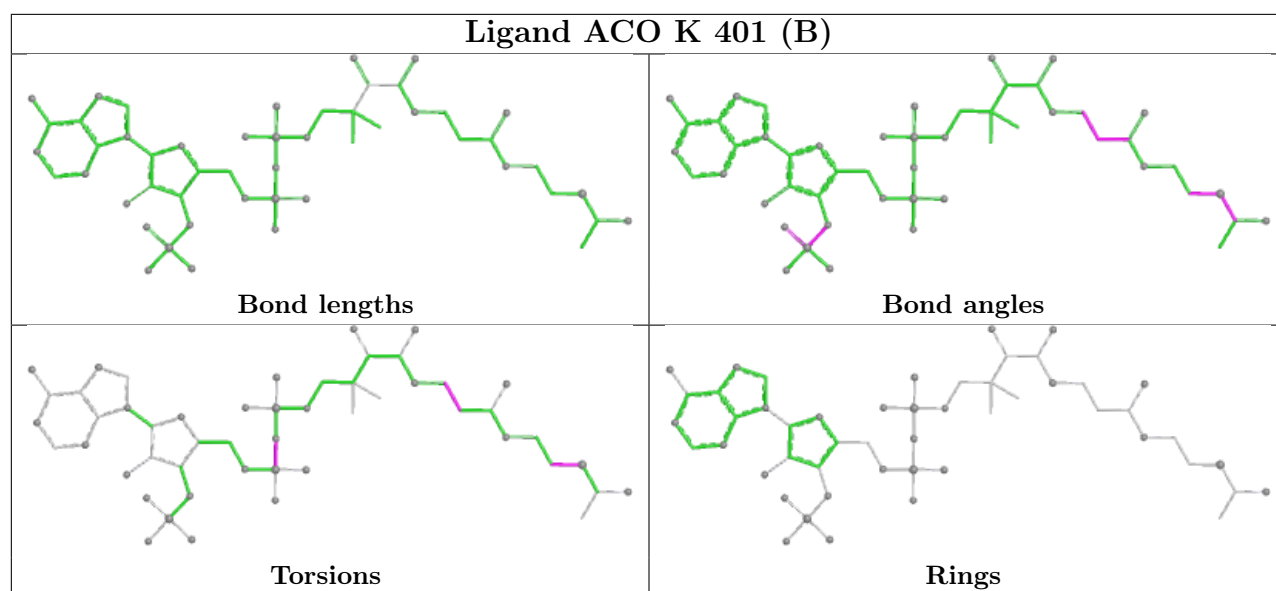


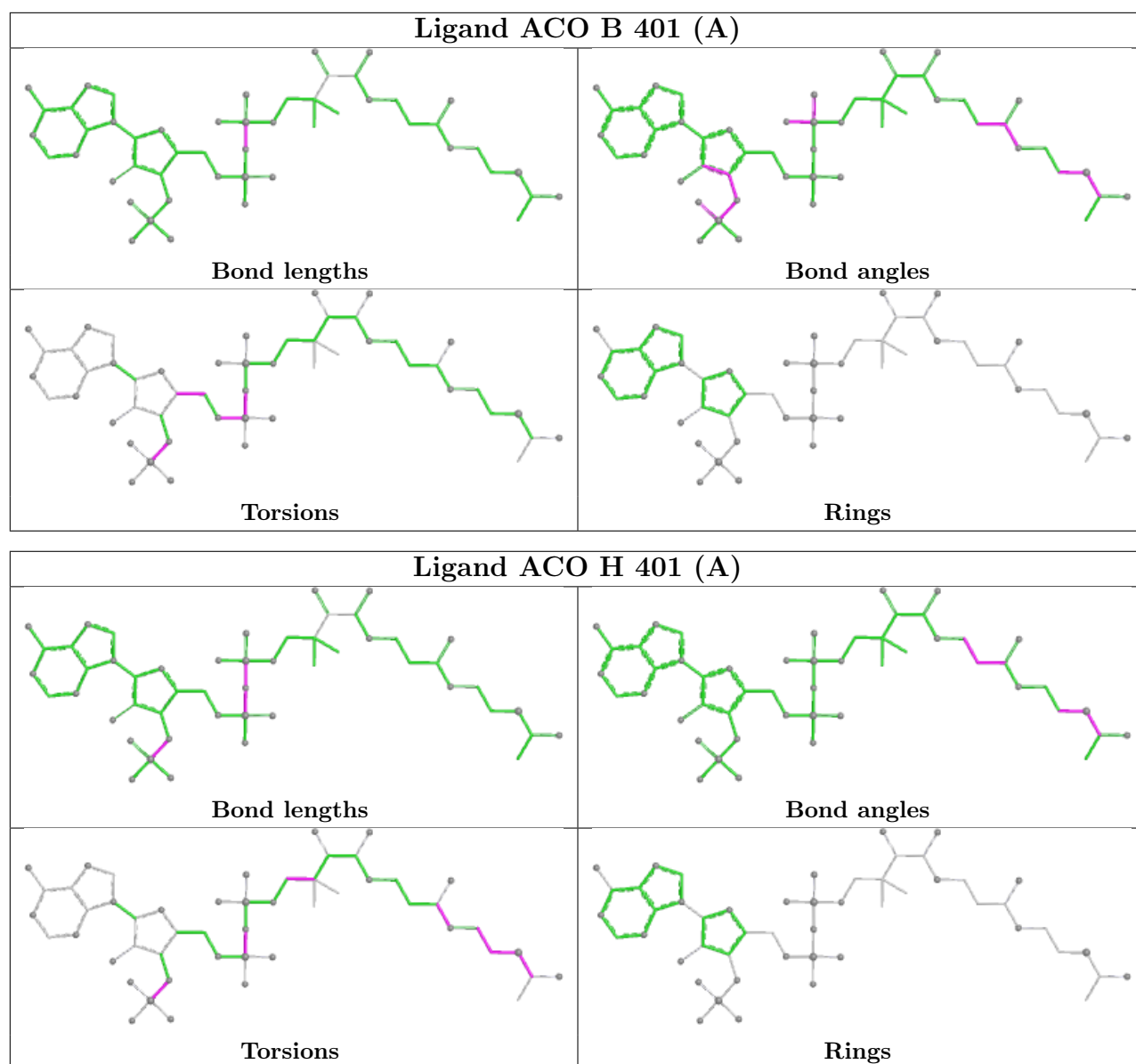












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/364 (98%)	0.94	73 (20%) 3 3	24, 36, 75, 108	2 (0%)
1	B	359/364 (98%)	0.80	49 (13%) 7 7	22, 37, 73, 110	1 (0%)
1	C	359/364 (98%)	0.92	65 (18%) 3 4	22, 37, 73, 111	2 (0%)
1	D	359/364 (98%)	0.98	74 (20%) 2 2	23, 38, 69, 101	1 (0%)
1	E	359/364 (98%)	0.81	55 (15%) 5 5	23, 37, 68, 104	2 (0%)
1	F	359/364 (98%)	0.96	75 (20%) 2 2	23, 38, 72, 119	1 (0%)
1	G	359/364 (98%)	1.15	90 (25%) 1 1	23, 39, 77, 114	2 (0%)
1	H	359/364 (98%)	0.96	76 (21%) 2 2	23, 38, 75, 106	1 (0%)
1	I	359/364 (98%)	0.74	40 (11%) 10 12	23, 35, 64, 99	2 (0%)
1	J	359/364 (98%)	0.63	32 (8%) 15 17	23, 35, 66, 113	1 (0%)
1	K	360/364 (98%)	0.78	59 (16%) 4 5	18, 36, 70, 106	3 (0%)
1	L	359/364 (98%)	0.79	54 (15%) 5 5	23, 37, 67, 101	1 (0%)
All	All	4309/4368 (98%)	0.87	742 (17%) 4 4	18, 37, 72, 119	19 (0%)

All (742) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	VAL	7.1
1	C	42	VAL	6.9
1	B	45	ILE	6.7
1	G	351	ILE	5.7
1	E	324	GLY	5.6
1	B	42	VAL	5.5
1	C	351	ILE	5.4
1	F	351	ILE	5.4
1	A	346	ALA	5.4
1	G	324	GLY	5.2
1	A	42	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	5.1
1	H	42	VAL	5.1
1	K	360	GLY	5.0
1	C	349	ILE	5.0
1	J	351	ILE	5.0
1	A	351	ILE	4.9
1	E	349	ILE	4.9
1	G	45	ILE	4.9
1	B	351	ILE	4.9
1	D	346	ALA	4.9
1	G	355	LEU	4.8
1	D	323	ASN	4.8
1	B	346	ALA	4.8
1	G	358	TRP	4.8
1	F	292	ALA	4.8
1	G	59	ALA	4.8
1	D	351	ILE	4.8
1	A	324	GLY	4.8
1	K	42	VAL	4.7
1	H	351	ILE	4.7
1	E	42	VAL	4.6
1	G	346	ALA	4.6
1	J	346	ALA	4.6
1	F	323	ASN	4.5
1	I	351	ILE	4.5
1	K	349	ILE	4.5
1	H	346	ALA	4.5
1	H	45	ILE	4.5
1	C	347	ALA	4.5
1	G	292	ALA	4.5
1	H	34	VAL	4.4
1	I	349	ILE	4.4
1	F	346	ALA	4.4
1	G	347	ALA	4.4
1	H	349	ILE	4.4
1	K	45	ILE	4.4
1	G	102	VAL	4.3
1	A	358	TRP	4.3
1	H	324	GLY	4.3
1	I	42	VAL	4.3
1	L	323	ASN	4.3
1	C	45	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	45	ILE	4.3
1	C	346	ALA	4.2
1	C	180	LYS	4.2
1	A	69	LEU	4.2
1	G	10	VAL	4.1
1	G	42	VAL	4.1
1	C	207	MET	4.1
1	C	358	TRP	4.1
1	A	58	THR	4.1
1	A	323	ASN	4.1
1	A	355	LEU	4.1
1	G	101	LYS	4.1
1	H	323	ASN	4.1
1	F	358	TRP	4.1
1	G	11	VAL	4.1
1	J	45	ILE	4.1
1	C	353	ALA	4.0
1	I	323	ASN	4.0
1	K	324	GLY	4.0
1	E	207	MET	4.0
1	L	351	ILE	4.0
1	L	346	ALA	3.9
1	G	69	LEU	3.9
1	D	102	VAL	3.9
1	H	173	TRP	3.9
1	G	34	VAL	3.9
1	C	75	ALA	3.8
1	J	207	MET	3.8
1	C	76	LYS	3.8
1	G	33	VAL	3.8
1	E	144	ASP	3.7
1	A	45	ILE	3.7
1	G	349	ILE	3.7
1	K	351	ILE	3.7
1	F	324	GLY	3.7
1	B	323	ASN	3.7
1	I	47	ARG	3.7
1	A	173	TRP	3.7
1	A	356	THR	3.7
1	B	358	TRP	3.7
1	H	358	TRP	3.7
1	H	355	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	173	TRP	3.6
1	E	351	ILE	3.6
1	E	323	ASN	3.6
1	G	293	ASN	3.6
1	D	7	GLY	3.6
1	D	324	GLY	3.6
1	G	176	GLN	3.6
1	G	41	SER	3.6
1	E	355	LEU	3.6
1	G	67	LEU	3.6
1	G	56	ILE	3.5
1	A	102	VAL	3.5
1	G	354	VAL	3.5
1	C	323	ASN	3.5
1	H	47	ARG	3.5
1	D	349	ILE	3.5
1	D	322	ALA	3.5
1	D	355	LEU	3.5
1	H	322	ALA	3.5
1	J	353	ALA	3.5
1	K	75	ALA	3.5
1	C	30	GLY	3.5
1	B	349	ILE	3.5
1	G	79	VAL	3.5
1	G	1	MET	3.5
1	B	347	ALA	3.5
1	D	92	LEU	3.5
1	B	43	ASP	3.5
1	B	1	MET	3.4
1	F	354	VAL	3.4
1	F	347	ALA	3.4
1	D	45	ILE	3.4
1	F	326	TRP	3.4
1	L	42	VAL	3.4
1	G	75	ALA	3.4
1	K	180	LYS	3.4
1	H	144	ASP	3.4
1	J	144	ASP	3.4
1	E	176	GLN	3.4
1	C	173	TRP	3.4
1	D	59	ALA	3.4
1	E	75	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	8	LEU	3.4
1	I	69	LEU	3.4
1	A	76	LYS	3.3
1	L	44	GLY	3.3
1	G	107	ILE	3.3
1	A	354	VAL	3.3
1	J	42	VAL	3.3
1	D	358	TRP	3.3
1	A	180	LYS	3.3
1	J	323	ASN	3.3
1	A	75	ALA	3.3
1	H	59	ALA	3.3
1	H	80	LEU	3.3
1	D	348	THR	3.3
1	L	173	TRP	3.3
1	A	47	ARG	3.3
1	K	44	GLY	3.3
1	B	41	SER	3.3
1	G	57	VAL	3.3
1	K	346	ALA	3.3
1	F	176	GLN	3.3
1	A	71	LEU	3.3
1	E	58	THR	3.3
1	F	259	LEU	3.2
1	A	40	SER	3.2
1	I	324	GLY	3.2
1	G	72	LYS	3.2
1	I	173	TRP	3.2
1	A	34	VAL	3.2
1	G	8	LEU	3.2
1	L	80	LEU	3.2
1	B	324	GLY	3.2
1	C	324	GLY	3.2
1	G	7	GLY	3.2
1	G	181	GLY	3.2
1	H	76	LYS	3.2
1	E	257	ALA	3.2
1	K	347	ALA	3.2
1	C	354	VAL	3.2
1	D	69	LEU	3.2
1	G	71	LEU	3.2
1	K	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	69	LEU	3.2
1	C	176	GLN	3.2
1	H	7	GLY	3.2
1	E	47	ARG	3.2
1	G	99	CYS	3.2
1	H	354	VAL	3.1
1	D	93	GLY	3.1
1	G	66	GLY	3.1
1	A	348	THR	3.1
1	A	59	ALA	3.1
1	D	347	ALA	3.1
1	E	346	ALA	3.1
1	E	353	ALA	3.1
1	B	44	GLY	3.1
1	E	66	GLY	3.1
1	F	44	GLY	3.1
1	J	359	ASP	3.1
1	C	47	ARG	3.1
1	C	105	ARG	3.1
1	B	75	ALA	3.1
1	I	41	SER	3.1
1	H	16	ILE	3.1
1	G	352	GLU	3.1
1	D	173	TRP	3.1
1	F	57	VAL	3.1
1	K	350	ASP	3.1
1	L	350	ASP	3.1
1	H	207	MET	3.1
1	A	289	ALA	3.1
1	J	347	ALA	3.1
1	L	75	ALA	3.1
1	A	72	LYS	3.0
1	H	73	LEU	3.0
1	G	173	TRP	3.0
1	I	358	TRP	3.0
1	G	345	PRO	3.0
1	E	347	ALA	3.0
1	I	144	ASP	3.0
1	I	45	ILE	3.0
1	A	67	LEU	3.0
1	D	207	MET	3.0
1	F	71	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	105	ARG	3.0
1	H	57	VAL	3.0
1	E	173	TRP	3.0
1	B	348	THR	3.0
1	C	66	GLY	3.0
1	D	44	GLY	3.0
1	A	322	ALA	3.0
1	D	353	ALA	3.0
1	E	322	ALA	3.0
1	J	75	ALA	3.0
1	F	47	ARG	3.0
1	F	349	ILE	3.0
1	H	74	ILE	3.0
1	C	69	LEU	3.0
1	D	354	VAL	3.0
1	K	144	ASP	3.0
1	K	176	GLN	3.0
1	K	358	TRP	3.0
1	H	345	PRO	3.0
1	I	1	MET	3.0
1	I	207	MET	3.0
1	D	75	ALA	3.0
1	D	107	ILE	3.0
1	E	45	ILE	3.0
1	J	349	ILE	3.0
1	F	355	LEU	2.9
1	K	355	LEU	2.9
1	L	92	LEU	2.9
1	B	350	ASP	2.9
1	F	144	ASP	2.9
1	B	30	GLY	2.9
1	E	1	MET	2.9
1	A	347	ALA	2.9
1	B	59	ALA	2.9
1	F	59	ALA	2.9
1	G	70	ALA	2.9
1	H	353	ALA	2.9
1	I	346	ALA	2.9
1	L	349	ILE	2.9
1	A	73	LEU	2.9
1	B	76	LYS	2.9
1	I	44	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	323	ASN	2.9
1	G	353	ALA	2.9
1	H	2	ALA	2.9
1	J	59	ALA	2.9
1	K	353	ALA	2.9
1	B	46	SER	2.9
1	D	56	ILE	2.9
1	F	357	ASP	2.9
1	C	67	LEU	2.9
1	G	73	LEU	2.9
1	H	69	LEU	2.9
1	K	73	LEU	2.9
1	K	11	VAL	2.9
1	D	2	ALA	2.9
1	H	359	ASP	2.9
1	J	326	TRP	2.9
1	K	359	ASP	2.9
1	L	355	LEU	2.9
1	E	93	GLY	2.9
1	H	348	THR	2.8
1	A	101	LYS	2.8
1	F	180	LYS	2.8
1	G	105	ARG	2.8
1	C	171	ALA	2.8
1	G	322	ALA	2.8
1	K	100	ALA	2.8
1	L	353	ALA	2.8
1	B	359	ASP	2.8
1	E	358	TRP	2.8
1	J	173	TRP	2.8
1	F	93	GLY	2.8
1	D	34	VAL	2.8
1	G	76	LYS	2.8
1	D	357	ASP	2.8
1	A	63	SER	2.8
1	A	100	ALA	2.8
1	B	289	ALA	2.8
1	F	75	ALA	2.8
1	G	44	GLY	2.8
1	A	56	ILE	2.8
1	G	36	ILE	2.8
1	H	106	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	355	LEU	2.8
1	K	74	ILE	2.8
1	G	58	THR	2.8
1	A	290	VAL	2.8
1	B	354	VAL	2.8
1	C	43	ASP	2.8
1	B	207	MET	2.8
1	H	178	SER	2.8
1	G	100	ALA	2.8
1	A	30	GLY	2.8
1	A	66	GLY	2.8
1	F	101	LYS	2.8
1	C	71	LEU	2.8
1	K	10	VAL	2.8
1	B	65	GLN	2.7
1	F	72	LYS	2.7
1	G	30	GLY	2.7
1	H	44	GLY	2.7
1	A	1	MET	2.7
1	A	74	ILE	2.7
1	A	345	PRO	2.7
1	H	1	MET	2.7
1	L	1	MET	2.7
1	L	354	VAL	2.7
1	L	358	TRP	2.7
1	F	76	LYS	2.7
1	G	77	ALA	2.7
1	H	66	GLY	2.7
1	C	359	ASP	2.7
1	F	69	LEU	2.7
1	G	178	SER	2.7
1	F	33	VAL	2.7
1	L	102	VAL	2.7
1	A	326	TRP	2.7
1	B	77	ALA	2.7
1	B	353	ALA	2.7
1	C	59	ALA	2.7
1	H	347	ALA	2.7
1	D	26	LEU	2.7
1	H	5	LEU	2.7
1	E	16	ILE	2.7
1	G	62	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	180	LYS	2.7
1	E	79	VAL	2.7
1	F	325	GLY	2.6
1	H	49	ALA	2.6
1	H	350	ASP	2.6
1	H	326	TRP	2.6
1	F	9	ARG	2.6
1	I	176	GLN	2.6
1	C	356	THR	2.6
1	K	58	THR	2.6
1	A	177	SER	2.6
1	G	177	SER	2.6
1	K	71	LEU	2.6
1	E	10	VAL	2.6
1	F	79	VAL	2.6
1	I	102	VAL	2.6
1	L	207	MET	2.6
1	B	47	ARG	2.6
1	G	350	ASP	2.6
1	H	72	LYS	2.6
1	K	348	THR	2.6
1	H	63	SER	2.6
1	I	326	TRP	2.6
1	J	358	TRP	2.6
1	B	355	LEU	2.6
1	I	80	LEU	2.6
1	I	92	LEU	2.6
1	E	56	ILE	2.6
1	G	74	ILE	2.6
1	H	107	ILE	2.6
1	D	1	MET	2.6
1	F	38	ARG	2.6
1	G	207	MET	2.6
1	J	324	GLY	2.6
1	C	79	VAL	2.6
1	F	34	VAL	2.6
1	E	348	THR	2.6
1	L	348	THR	2.6
1	C	39	PRO	2.6
1	G	326	TRP	2.6
1	B	73	LEU	2.6
1	C	355	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	67	LEU	2.6
1	G	26	LEU	2.6
1	C	1	MET	2.6
1	H	176	GLN	2.6
1	E	104	ASP	2.6
1	F	81	ILE	2.6
1	F	66	GLY	2.6
1	J	72	LYS	2.6
1	B	257	ALA	2.6
1	E	77	ALA	2.6
1	G	183	VAL	2.6
1	J	102	VAL	2.6
1	C	108	TYR	2.5
1	D	47	ARG	2.5
1	H	71	LEU	2.5
1	B	173	TRP	2.5
1	K	173	TRP	2.5
1	B	62	LYS	2.5
1	E	7	GLY	2.5
1	I	101	LYS	2.5
1	K	76	LYS	2.5
1	A	77	ALA	2.5
1	G	49	ALA	2.5
1	H	31	ALA	2.5
1	E	105	ARG	2.5
1	L	357	ASP	2.5
1	I	62	LYS	2.5
1	A	61	LEU	2.5
1	F	274	LEU	2.5
1	J	73	LEU	2.5
1	E	59	ALA	2.5
1	E	204	ALA	2.5
1	F	49	ALA	2.5
1	G	2	ALA	2.5
1	A	11	VAL	2.5
1	C	102	VAL	2.5
1	K	102	VAL	2.5
1	G	96	PRO	2.5
1	A	43	ASP	2.5
1	B	144	ASP	2.5
1	J	43	ASP	2.5
1	C	101	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	2.5
1	D	106	LEU	2.5
1	E	67	LEU	2.5
1	H	30	GLY	2.5
1	A	41	SER	2.5
1	B	40	SER	2.5
1	F	11	VAL	2.5
1	F	43	ASP	2.5
1	I	354	VAL	2.5
1	L	34	VAL	2.5
1	A	39	PRO	2.5
1	J	39	PRO	2.5
1	A	288	GLY	2.4
1	F	293	ASN	2.4
1	C	178	SER	2.4
1	K	40	SER	2.4
1	F	356	THR	2.4
1	G	348	THR	2.4
1	I	353	ALA	2.4
1	L	72	LYS	2.4
1	D	359	ASP	2.4
1	D	326	TRP	2.4
1	A	96	PRO	2.4
1	H	102	VAL	2.4
1	K	39	PRO	2.4
1	A	93	GLY	2.4
1	C	7	GLY	2.4
1	G	93	GLY	2.4
1	D	71	LEU	2.4
1	F	1	MET	2.4
1	F	73	LEU	2.4
1	J	71	LEU	2.4
1	K	207	MET	2.4
1	L	41	SER	2.4
1	L	36	ILE	2.4
1	C	322	ALA	2.4
1	H	75	ALA	2.4
1	B	105	ARG	2.4
1	D	105	ARG	2.4
1	B	345	PRO	2.4
1	L	183	VAL	2.4
1	C	44	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	178	SER	2.4
1	D	80	LEU	2.4
1	E	69	LEU	2.4
1	E	259	LEU	2.4
1	I	61	LEU	2.4
1	K	94	LEU	2.4
1	L	76	LYS	2.4
1	F	48	ASP	2.4
1	L	144	ASP	2.4
1	G	47	ARG	2.4
1	H	58	THR	2.4
1	L	47	ARG	2.4
1	C	338	ALA	2.4
1	D	171	ALA	2.4
1	H	204	ALA	2.4
1	C	93	GLY	2.4
1	F	27	GLY	2.4
1	H	179	GLY	2.4
1	H	183	VAL	2.4
1	K	34	VAL	2.4
1	K	354	VAL	2.4
1	L	79	VAL	2.4
1	L	88	VAL	2.4
1	A	207	MET	2.4
1	K	178	SER	2.4
1	L	46	SER	2.4
1	K	72	LYS	2.4
1	F	106	LEU	2.3
1	G	172	LEU	2.3
1	I	94	LEU	2.3
1	D	108	TYR	2.3
1	A	277	GLU	2.3
1	A	65	GLN	2.3
1	C	65	GLN	2.3
1	C	74	ILE	2.3
1	D	16	ILE	2.3
1	D	36	ILE	2.3
1	K	59	ALA	2.3
1	D	345	PRO	2.3
1	A	7	GLY	2.3
1	D	101	LYS	2.3
1	C	10	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	10	VAL	2.3
1	D	42	VAL	2.3
1	D	57	VAL	2.3
1	F	41	SER	2.3
1	G	43	ASP	2.3
1	G	91	ARG	2.3
1	I	350	ASP	2.3
1	L	43	ASP	2.3
1	A	99	CYS	2.3
1	F	80	LEU	2.3
1	H	172	LEU	2.3
1	L	71	LEU	2.3
1	G	356	THR	2.3
1	H	337	THR	2.3
1	A	353	ALA	2.3
1	G	289	ALA	2.3
1	H	56	ILE	2.3
1	D	180	LYS	2.3
1	E	76	LYS	2.3
1	K	93	GLY	2.3
1	A	178	SER	2.3
1	A	105	ARG	2.3
1	A	350	ASP	2.3
1	B	11	VAL	2.3
1	G	357	ASP	2.3
1	H	10	VAL	2.3
1	H	79	VAL	2.3
1	L	11	VAL	2.3
1	D	258	GLU	2.3
1	H	352	GLU	2.3
1	F	65	GLN	2.3
1	A	94	LEU	2.3
1	D	8	LEU	2.3
1	D	73	LEU	2.3
1	G	94	LEU	2.3
1	I	259	LEU	2.3
1	J	355	LEU	2.3
1	C	345	PRO	2.3
1	D	49	ALA	2.3
1	D	70	ALA	2.3
1	H	338	ALA	2.3
1	B	7	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	56	ILE	2.3
1	H	27	GLY	2.3
1	L	45	ILE	2.3
1	D	178	SER	2.3
1	C	350	ASP	2.3
1	F	68	GLU	2.3
1	D	11	VAL	2.3
1	F	102	VAL	2.3
1	D	58	THR	2.3
1	D	61	LEU	2.3
1	D	76	LYS	2.3
1	G	80	LEU	2.3
1	C	91	ARG	2.2
1	G	9	ARG	2.2
1	L	326	TRP	2.2
1	D	31	ALA	2.2
1	F	100	ALA	2.2
1	G	63	SER	2.2
1	C	104	ASP	2.2
1	B	102	VAL	2.2
1	H	180	LYS	2.2
1	F	348	THR	2.2
1	J	47	ARG	2.2
1	K	47	ARG	2.2
1	L	58	THR	2.2
1	E	73	LEU	2.2
1	K	80	LEU	2.2
1	A	6	SER	2.2
1	C	179	GLY	2.2
1	F	7	GLY	2.2
1	F	46	SER	2.2
1	H	65	GLN	2.2
1	J	261	PRO	2.2
1	K	41	SER	2.2
1	I	75	ALA	2.2
1	K	77	ALA	2.2
1	K	322	ALA	2.2
1	L	2	ALA	2.2
1	K	326	TRP	2.2
1	D	74	ILE	2.2
1	L	107	ILE	2.2
1	B	180	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	33	VAL	2.2
1	D	88	VAL	2.2
1	H	33	VAL	2.2
1	J	57	VAL	2.2
1	K	57	VAL	2.2
1	A	68	GLU	2.2
1	J	356	THR	2.2
1	B	51	LEU	2.2
1	C	80	LEU	2.2
1	D	94	LEU	2.2
1	G	288	GLY	2.2
1	I	43	ASP	2.2
1	K	63	SER	2.2
1	K	357	ASP	2.2
1	L	6	SER	2.2
1	F	261	PRO	2.2
1	I	2	ALA	2.2
1	L	347	ALA	2.2
1	F	74	ILE	2.2
1	I	36	ILE	2.2
1	A	91	ARG	2.2
1	H	38	ARG	2.2
1	C	34	VAL	2.2
1	E	33	VAL	2.2
1	F	255	ASP	2.2
1	C	40	SER	2.2
1	C	99	CYS	2.2
1	C	106	LEU	2.2
1	J	69	LEU	2.2
1	L	181	GLY	2.2
1	E	289	ALA	2.2
1	F	70	ALA	2.2
1	G	109	ALA	2.2
1	L	100	ALA	2.2
1	L	322	ALA	2.2
1	B	38	ARG	2.2
1	B	56	ILE	2.1
1	E	356	THR	2.1
1	G	64	ASP	2.1
1	F	10	VAL	2.1
1	I	10	VAL	2.1
1	D	177	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	2.1
1	E	179	GLY	2.1
1	G	179	GLY	2.1
1	G	325	GLY	2.1
1	L	7	GLY	2.1
1	L	30	GLY	2.1
1	D	67	LEU	2.1
1	E	80	LEU	2.1
1	F	254	LEU	2.1
1	G	5	LEU	2.1
1	G	106	LEU	2.1
1	H	96	PRO	2.1
1	L	106	LEU	2.1
1	E	101	LYS	2.1
1	F	62	LYS	2.1
1	A	292	ALA	2.1
1	F	256	ALA	2.1
1	G	65	GLN	2.1
1	K	65	GLN	2.1
1	C	107	ILE	2.1
1	D	32	ASP	2.1
1	D	48	ASP	2.1
1	D	144	ASP	2.1
1	I	255	ASP	2.1
1	C	177	SER	2.1
1	C	326	TRP	2.1
1	A	38	ARG	2.1
1	C	181	GLY	2.1
1	D	30	GLY	2.1
1	D	79	VAL	2.1
1	E	91	ARG	2.1
1	J	352	GLU	2.1
1	K	67	LEU	2.1
1	A	2	ALA	2.1
1	E	171	ALA	2.1
1	F	2	ALA	2.1
1	F	353	ALA	2.1
1	D	350	ASP	2.1
1	E	74	ILE	2.1
1	G	32	ASP	2.1
1	H	43	ASP	2.1
1	L	74	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	40	SER	2.1
1	H	6	SER	2.1
1	G	97	GLU	2.1
1	B	93	GLY	2.1
1	B	325	GLY	2.1
1	K	66	GLY	2.1
1	F	207	MET	2.1
1	A	183	VAL	2.1
1	C	33	VAL	2.1
1	D	183	VAL	2.1
1	K	79	VAL	2.1
1	K	323	ASN	2.1
1	E	65	GLN	2.1
1	A	172	LEU	2.1
1	B	69	LEU	2.1
1	C	73	LEU	2.1
1	E	94	LEU	2.1
1	C	257	ALA	2.1
1	D	100	ALA	2.1
1	E	70	ALA	2.1
1	F	171	ALA	2.1
1	F	257	ALA	2.1
1	G	171	ALA	2.1
1	E	359	ASP	2.1
1	H	357	ASP	2.1
1	A	9	ARG	2.1
1	H	91	ARG	2.1
1	G	40	SER	2.0
1	L	16	ILE	2.0
1	H	108	TYR	2.0
1	C	58	THR	2.0
1	J	1	MET	2.0
1	H	3	GLY	2.0
1	H	325	GLY	2.0
1	I	87	GLY	2.0
1	J	206	GLY	2.0
1	K	181	GLY	2.0
1	A	10	VAL	2.0
1	B	34	VAL	2.0
1	C	57	VAL	2.0
1	K	345	PRO	2.0
1	L	10	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	57	VAL	2.0
1	C	51	LEU	2.0
1	H	92	LEU	2.0
1	I	67	LEU	2.0
1	K	172	LEU	2.0
1	I	257	ALA	2.0
1	F	350	ASP	2.0
1	K	43	ASP	2.0
1	K	105	ARG	2.0
1	I	68	GLU	2.0
1	E	72	LYS	2.0
1	A	46	SER	2.0
1	L	40	SER	2.0
1	B	36	ILE	2.0
1	L	356	THR	2.0
1	D	320	TYR	2.0
1	F	260	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACO	F	401[A]	51/51	0.83	0.16	26,40,50,65	51
2	ACO	F	401[B]	51/51	0.83	0.16	31,42,49,56	51
2	ACO	H	401[A]	51/51	0.84	0.19	33,50,70,74	51
2	ACO	H	401[B]	51/51	0.84	0.19	36,45,62,64	51
2	ACO	E	401[A]	51/51	0.86	0.18	35,50,76,81	51
2	ACO	E	401[B]	51/51	0.86	0.18	31,54,88,92	51

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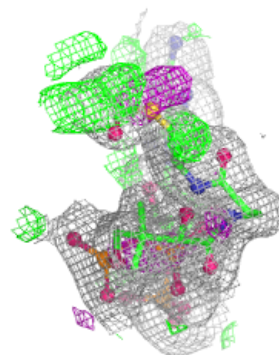
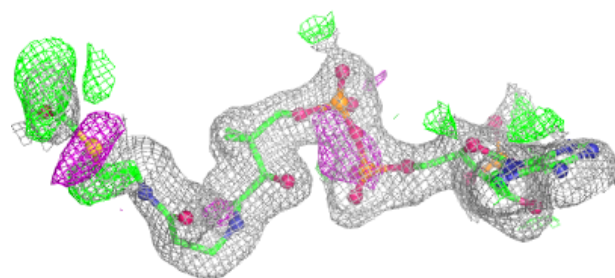
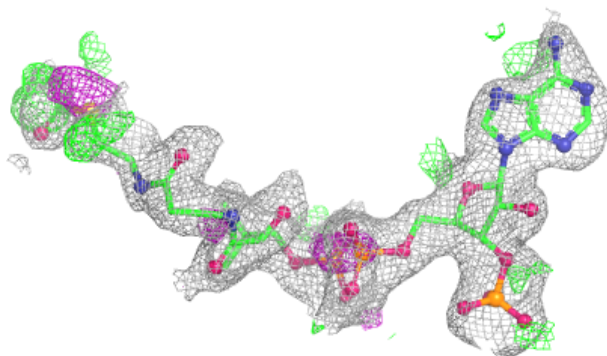
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACO	A	401[A]	51/51	0.87	0.17	21,46,76,78	51
2	ACO	A	401[B]	51/51	0.87	0.17	31,45,62,78	51
2	ACO	G	401[A]	51/51	0.89	0.14	35,46,60,66	51
2	ACO	G	401[B]	51/51	0.89	0.14	30,43,63,66	51
2	ACO	C	401[A]	51/51	0.89	0.13	30,42,51,58	51
2	ACO	C	401[B]	51/51	0.89	0.13	26,51,59,65	51
2	ACO	J	401[A]	51/51	0.89	0.12	23,37,43,50	51
2	ACO	J	401[B]	51/51	0.89	0.12	25,40,53,63	51
2	ACO	B	401[A]	51/51	0.90	0.12	19,39,49,56	51
2	ACO	B	401[B]	51/51	0.90	0.12	33,46,66,75	51
2	ACO	L	401[A]	51/51	0.90	0.12	27,39,45,48	51
2	ACO	L	401[B]	51/51	0.90	0.12	31,41,50,60	51
2	ACO	K	401[A]	51/51	0.91	0.13	32,42,51,55	51
2	ACO	K	401[B]	51/51	0.91	0.13	29,39,53,66	51
2	ACO	I	401[A]	51/51	0.91	0.12	27,40,49,54	51
2	ACO	I	401[B]	51/51	0.91	0.12	26,42,53,58	51
2	ACO	D	401[A]	51/51	0.94	0.11	20,34,54,59	51
2	ACO	D	401[B]	51/51	0.94	0.11	35,54,68,80	51

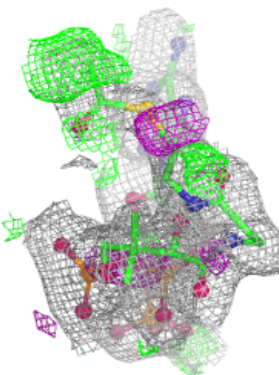
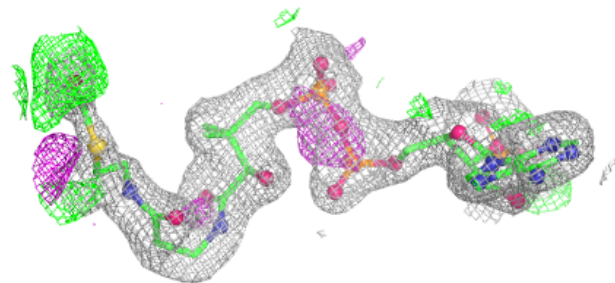
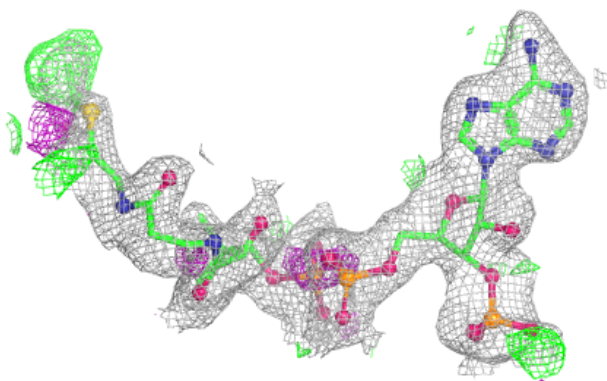
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO F 401 (A):

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

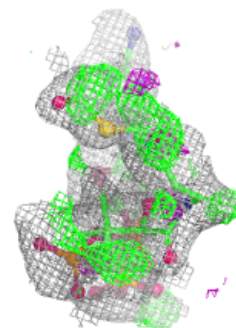
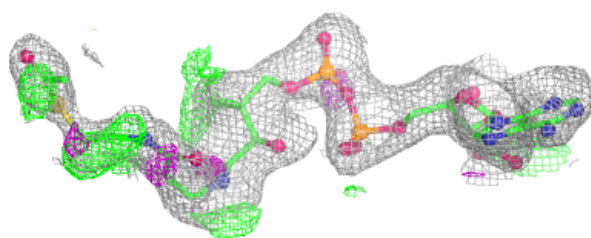
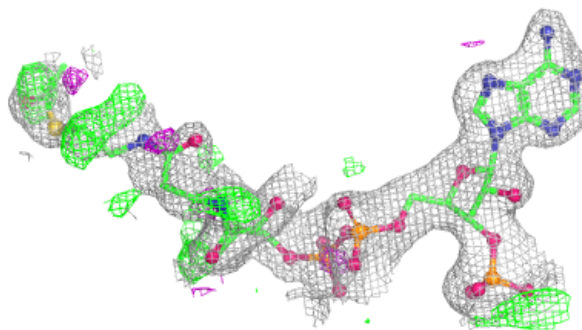
**Electron density around ACO F 401 (B):**

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

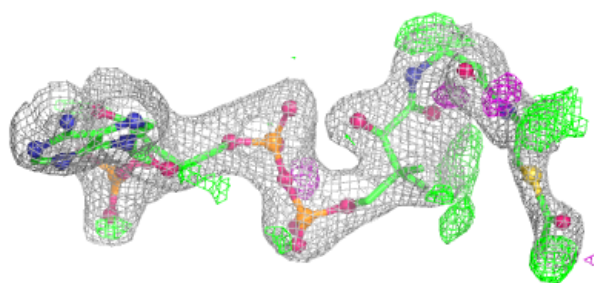
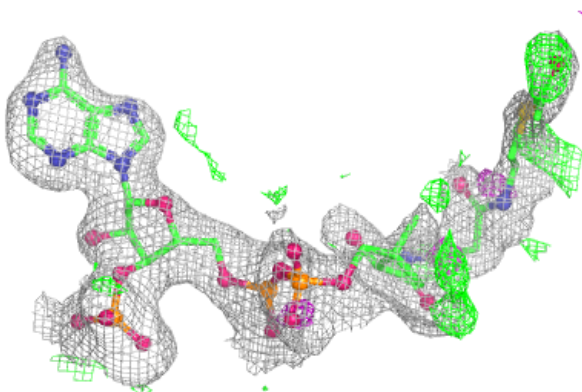


Electron density around ACO H 401 (A):

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

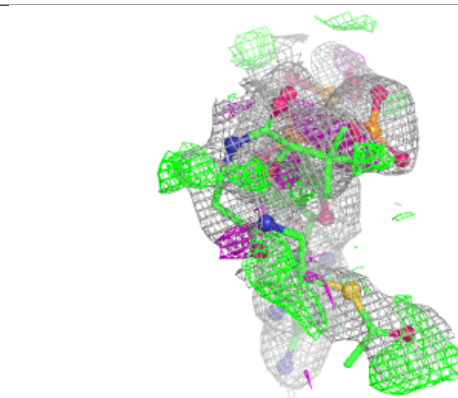
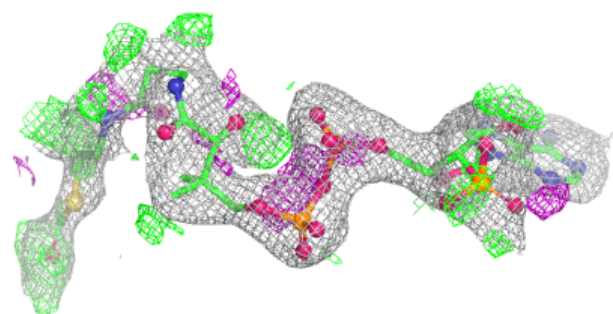
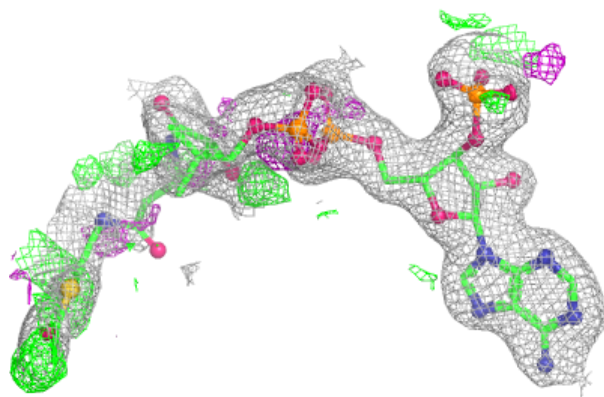
**Electron density around ACO H 401 (B):**

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

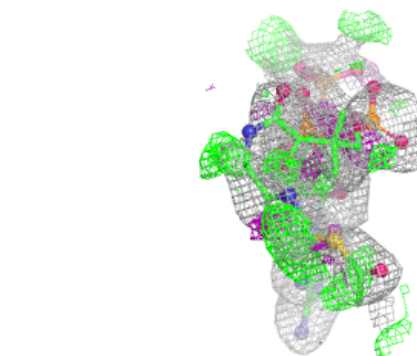
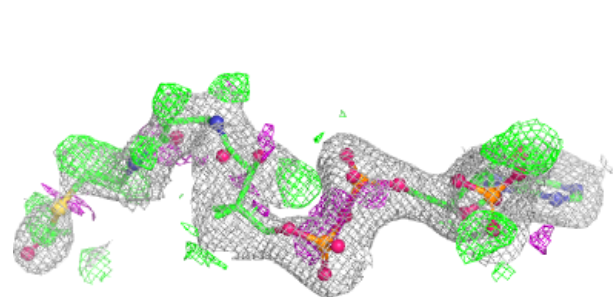
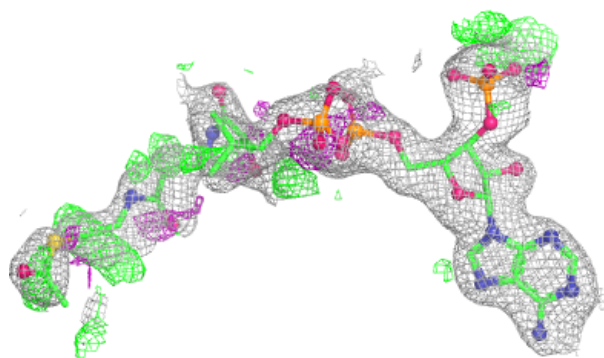


Electron density around ACO E 401 (A):

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

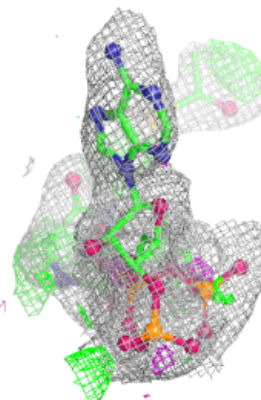
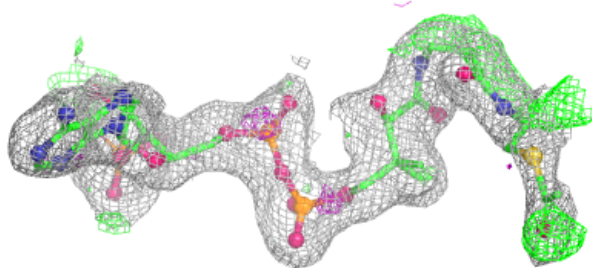
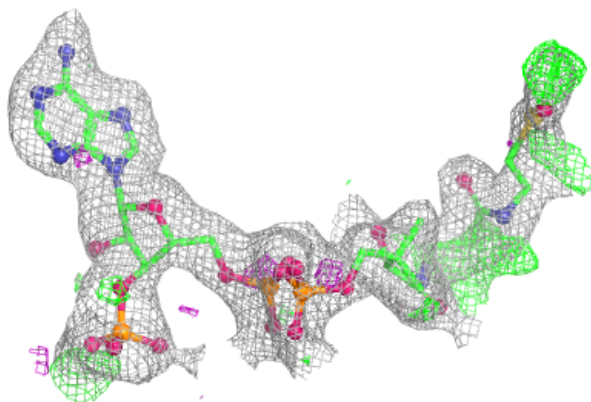
**Electron density around ACO E 401 (B):**

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

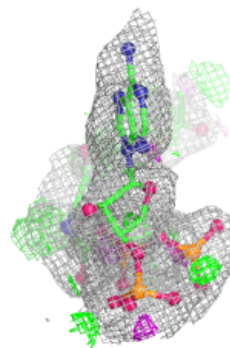
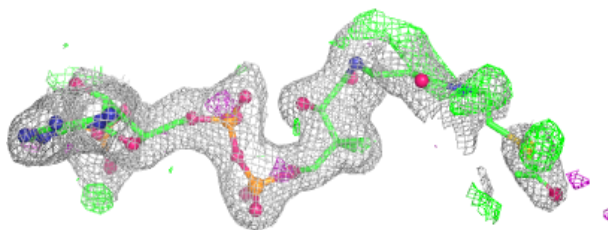
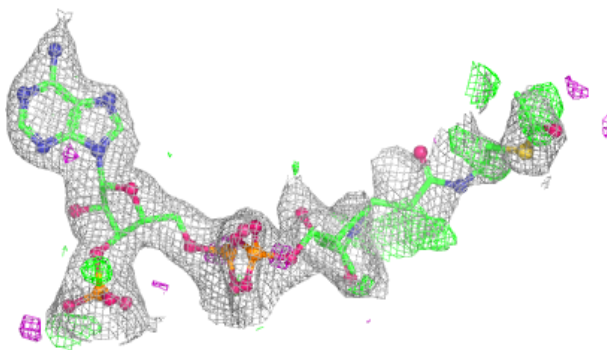


Electron density around ACO A 401 (A):

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

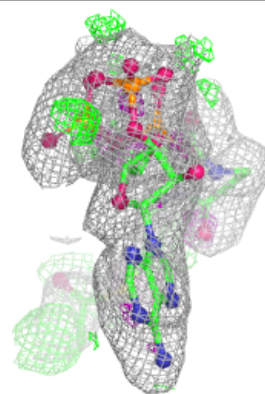
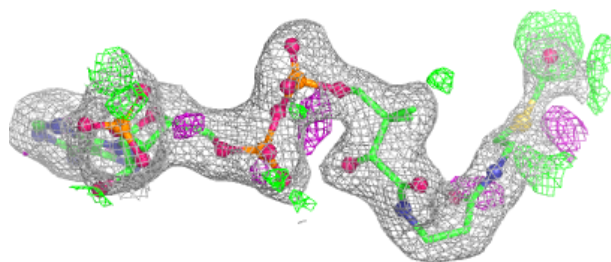
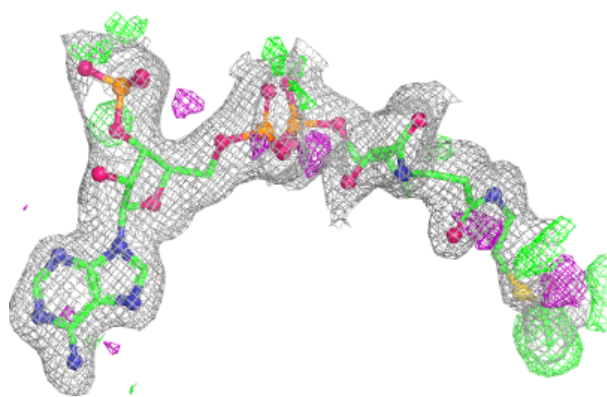
**Electron density around ACO A 401 (B):**

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

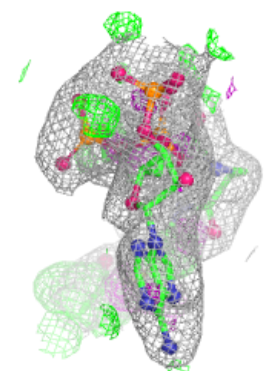
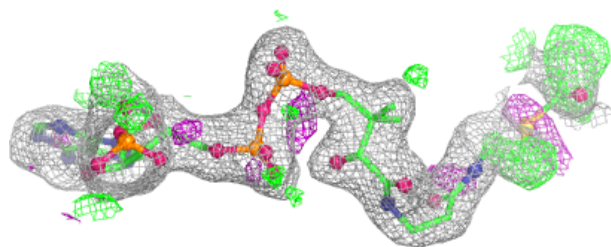
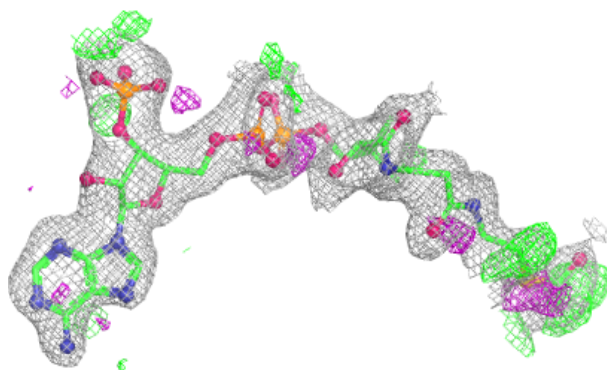


Electron density around ACO G 401 (A):

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

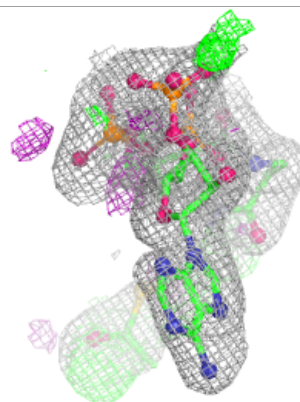
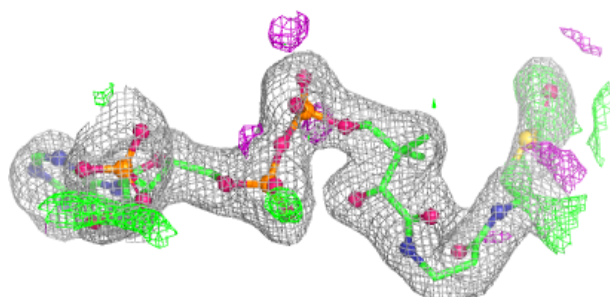
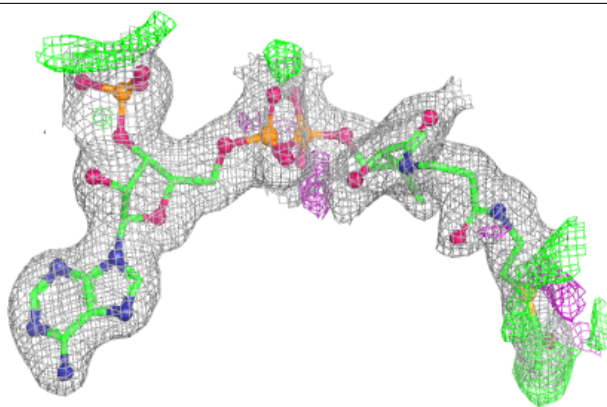
**Electron density around ACO G 401 (B):**

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

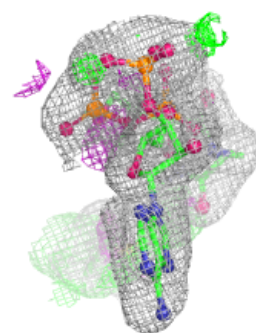
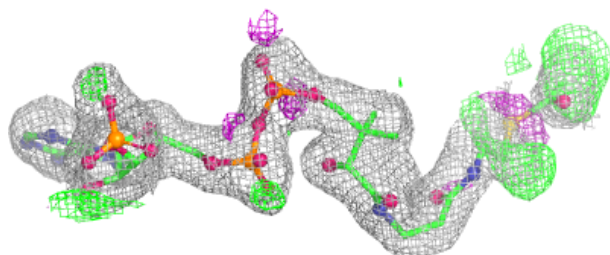
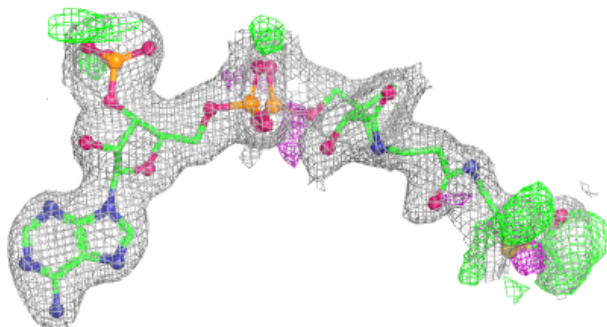


Electron density around ACO C 401 (A):

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

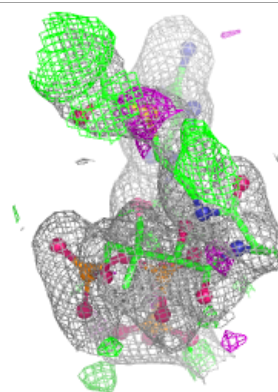
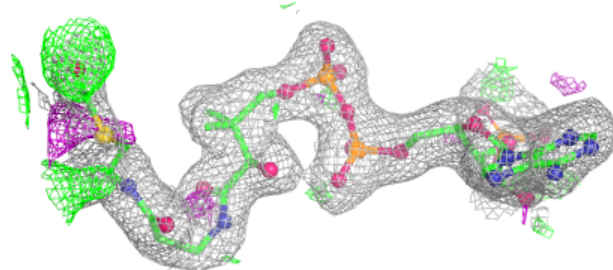
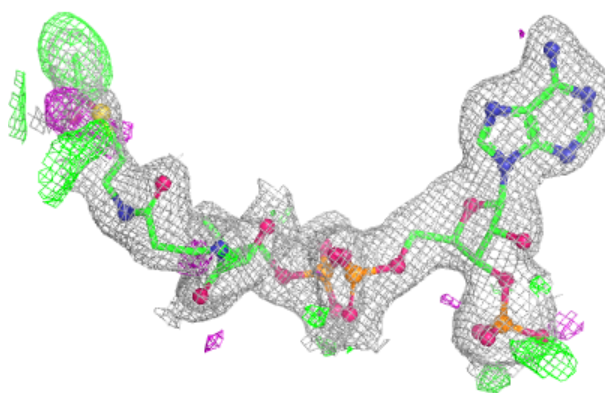
**Electron density around ACO C 401 (B):**

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

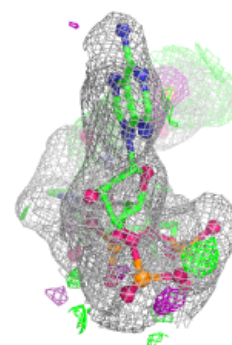
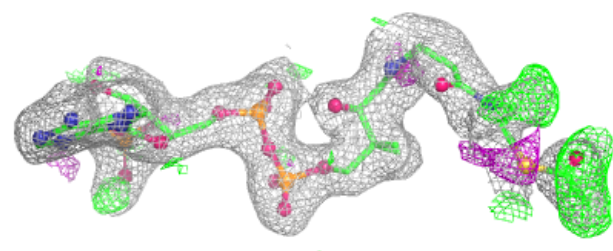
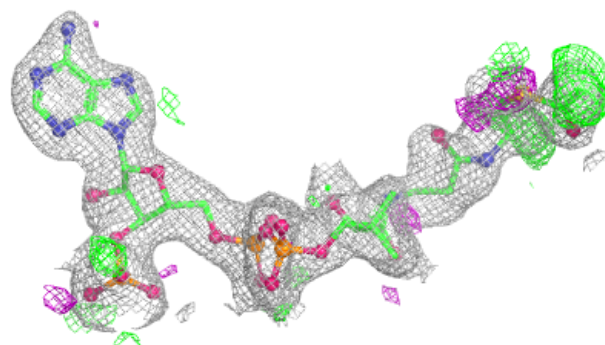


Electron density around ACO J 401 (A):

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

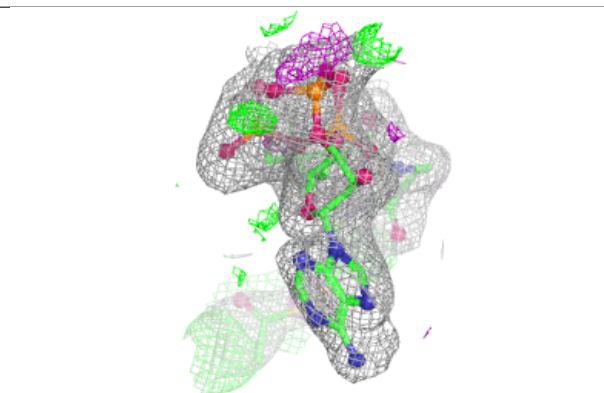
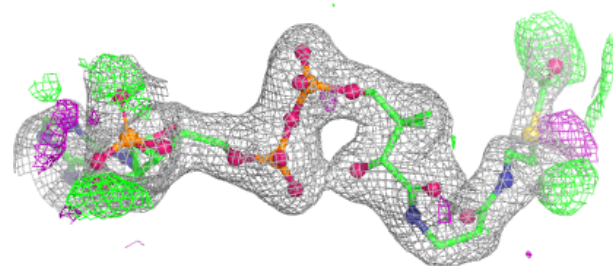
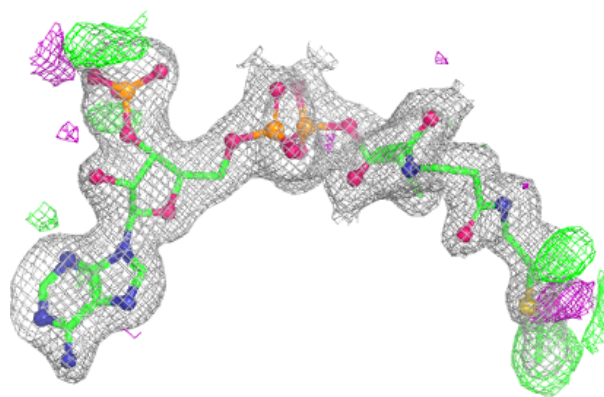
**Electron density around ACO J 401 (B):**

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

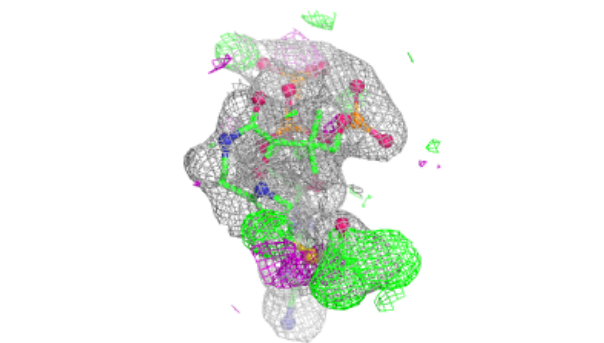
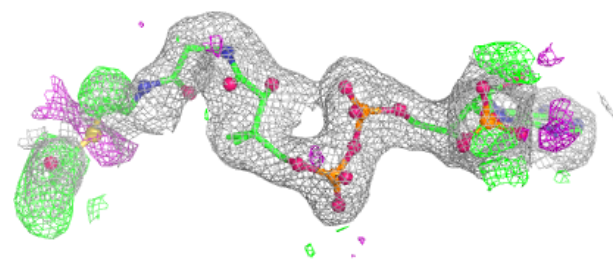
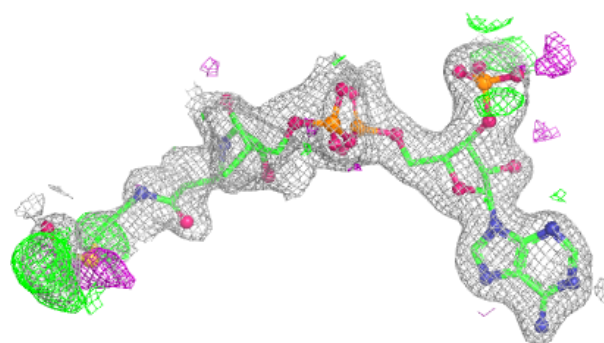


Electron density around ACO B 401 (A):

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

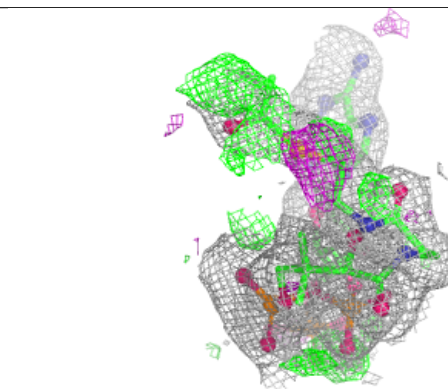
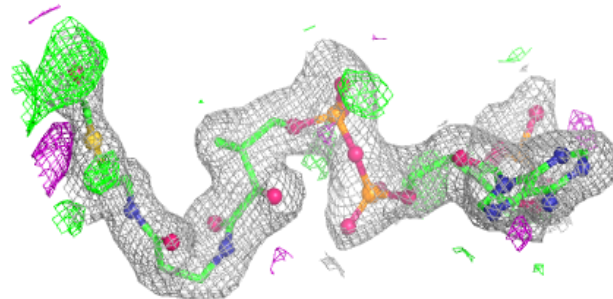
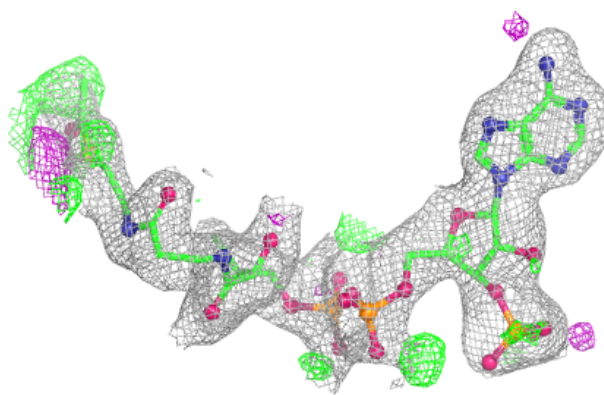
**Electron density around ACO B 401 (B):**

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

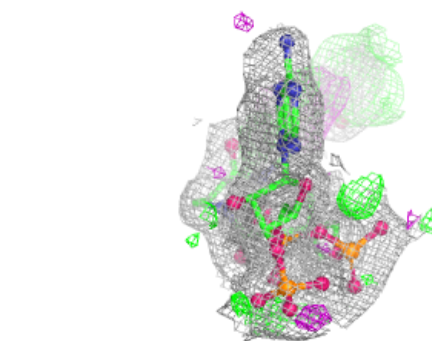
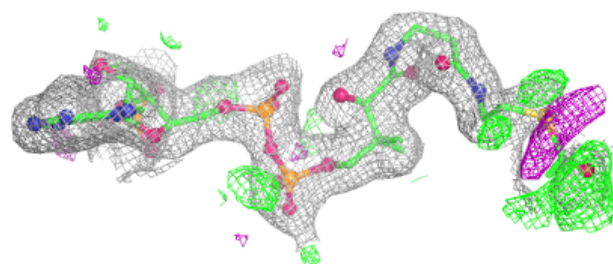
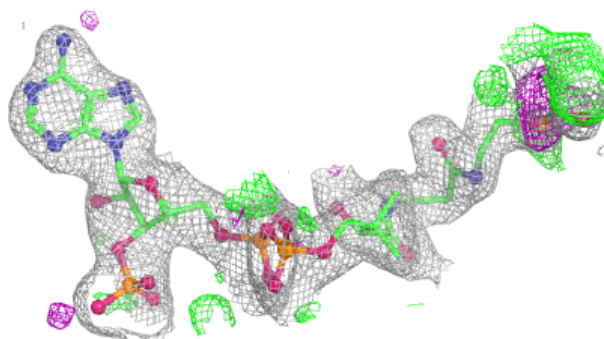


Electron density around ACO L 401 (A):

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

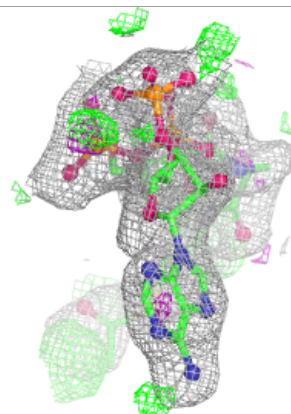
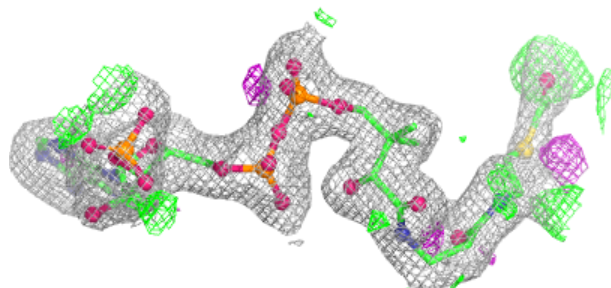
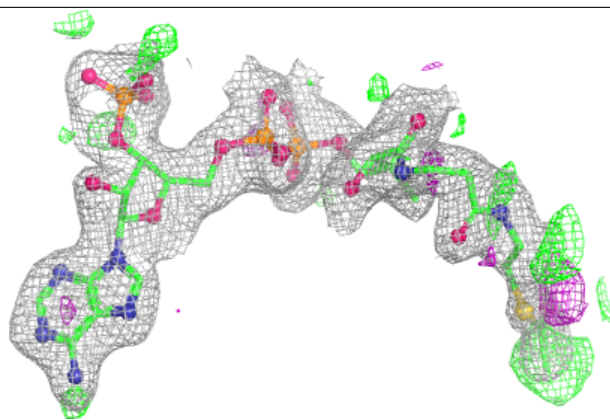
**Electron density around ACO L 401 (B):**

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

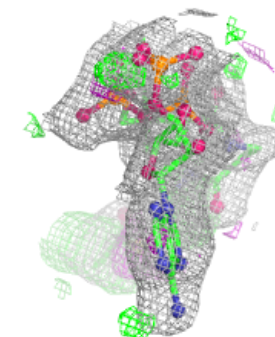
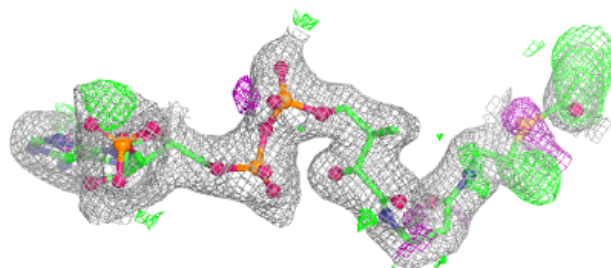
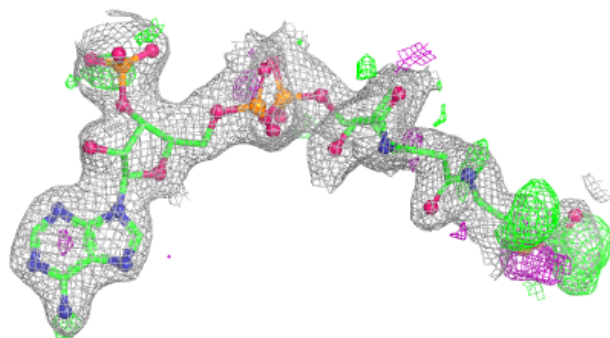


Electron density around ACO K 401 (A):

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

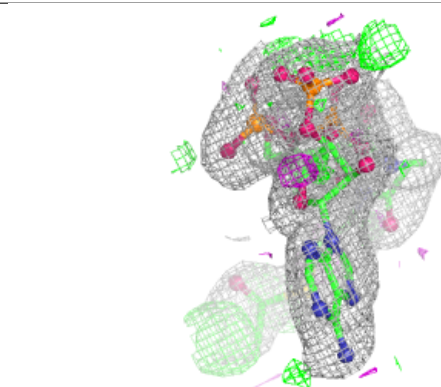
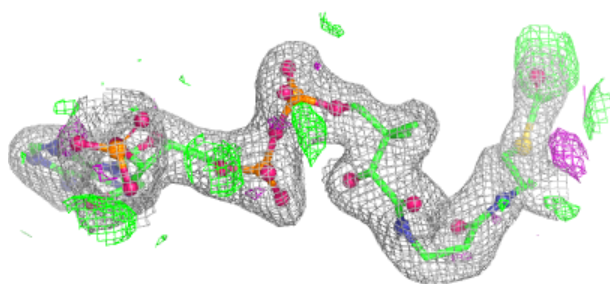
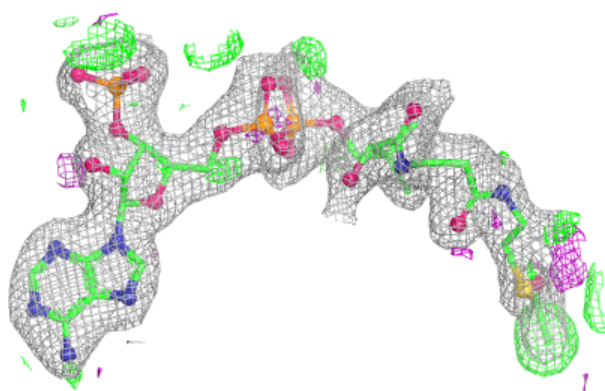
**Electron density around ACO K 401 (B):**

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

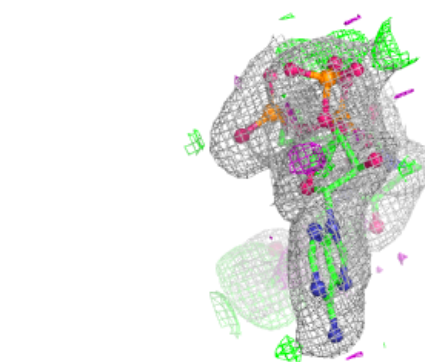
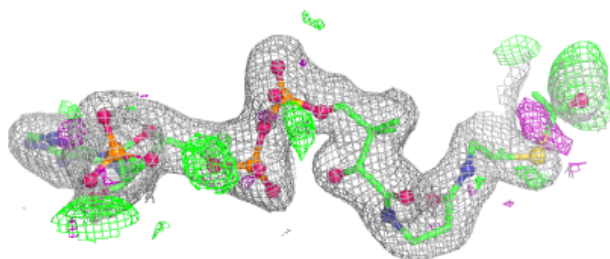
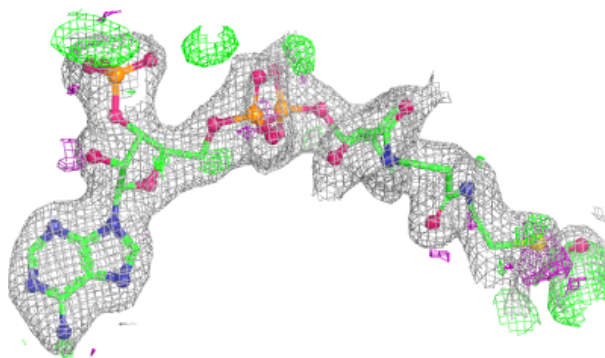


Electron density around ACO I 401 (A):

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

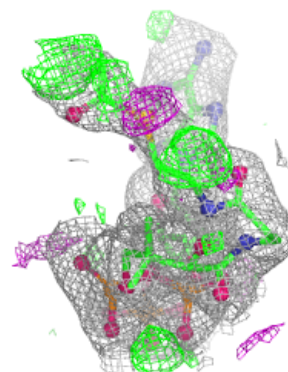
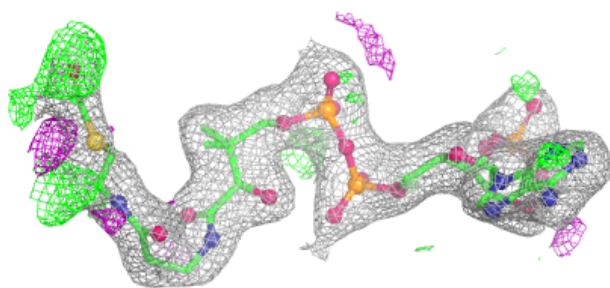
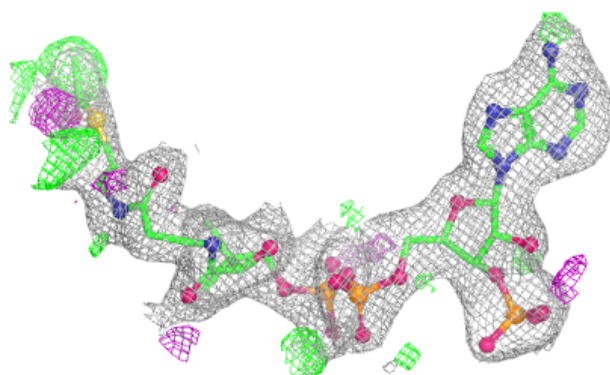
**Electron density around ACO I 401 (B):**

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

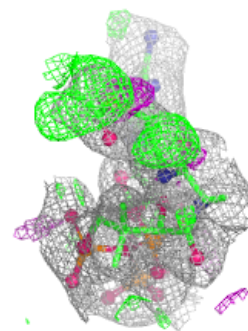
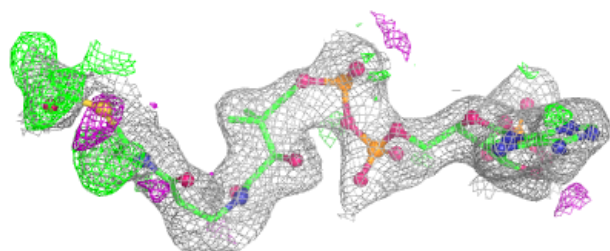
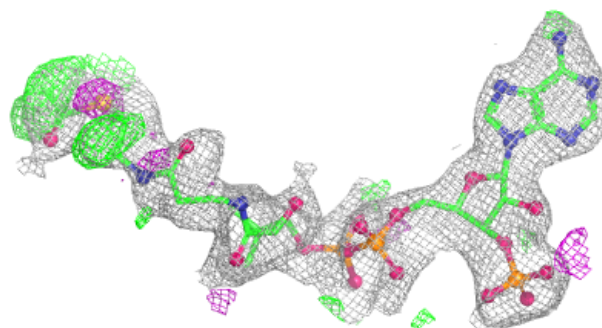


Electron density around ACO D 401 (A):

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

**Electron density around ACO D 401 (B):**

$2mF_o-DF_c$ (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.