wwPDB X-ray Structure Validation Summary Report (i)

Jun 4, 2025 – 07:53 pm BST

PDB ID	:	9I30 / pdb_00009i30
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with ketoprofenoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	2.08 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

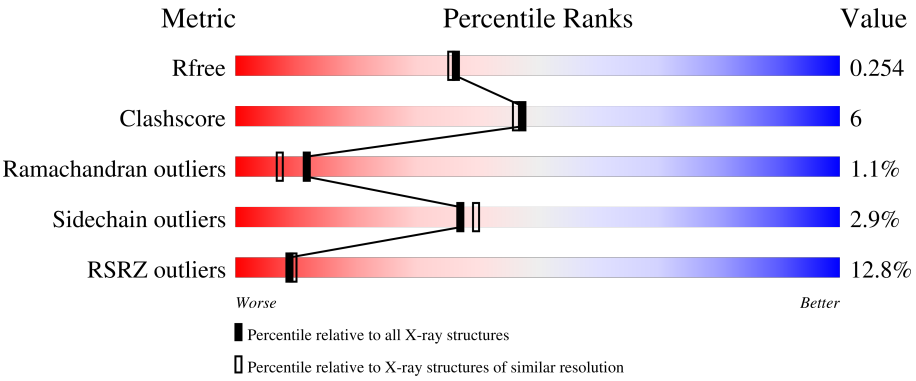
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	13% 82% 13%
1	B	364	8% 82% 15%
1	C	364	14% 83% 13%
1	D	364	12% 82% 15%
1	E	364	11% 82% 15%

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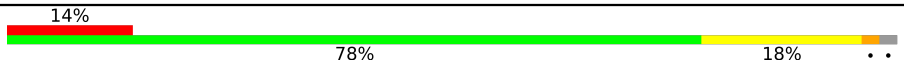
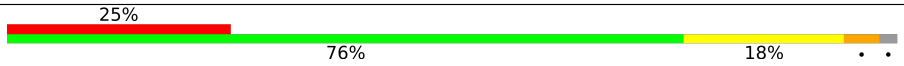
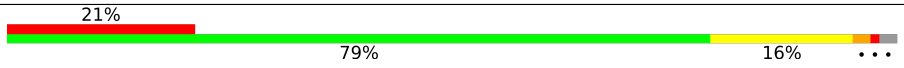
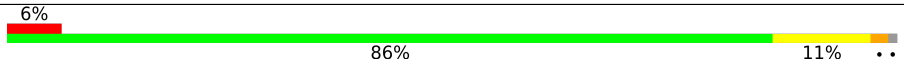
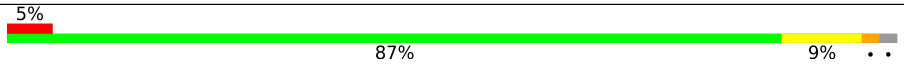
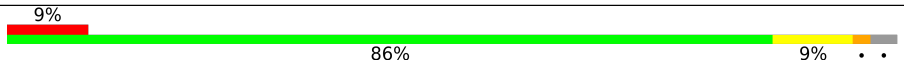
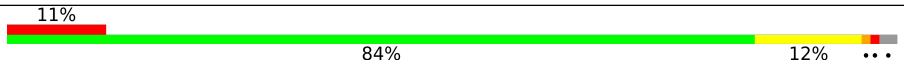
Mol	Chain	Length	Quality of chain
1	F	364	
1	G	364	
1	H	364	
1	I	364	
1	J	364	
1	K	364	
1	L	364	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 66985 atoms, of which 32336 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	354	Total	C	H	N	O	S	58	2	0
			5321	1683	2638	481	503	16			
1	B	354	Total	C	H	N	O	S	57	1	0
			5317	1683	2635	481	502	16			
1	C	357	Total	C	H	N	O	S	58	2	0
			5359	1695	2656	484	508	16			
1	D	357	Total	C	H	N	O	S	58	1	0
			5363	1697	2660	484	506	16			
1	E	355	Total	C	H	N	O	S	57	2	0
			5341	1690	2648	482	505	16			
1	F	356	Total	C	H	N	O	S	58	1	0
			5344	1691	2649	483	505	16			
1	G	355	Total	C	H	N	O	S	58	2	0
			5340	1689	2649	482	504	16			
1	H	356	Total	C	H	N	O	S	57	1	0
			5343	1691	2649	483	504	16			
1	I	359	Total	C	H	N	O	S	58	2	0
			5387	1704	2669	486	512	16			
1	J	357	Total	C	H	N	O	S	58	1	0
			5354	1694	2654	484	506	16			
1	K	354	Total	C	H	N	O	S	58	2	0
			5321	1683	2638	481	503	16			
1	L	358	Total	C	H	N	O	S	58	1	0
			5370	1699	2663	485	507	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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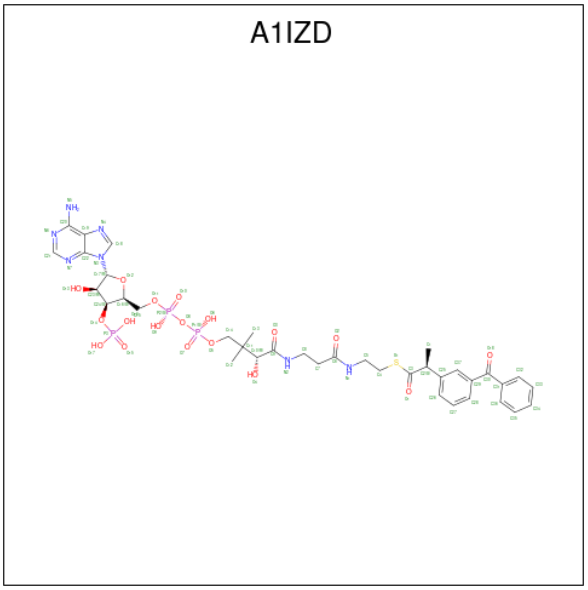
Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is (S)-ketoprofenoyl-CoA (CCD ID: A1IZD) (formula: $C_{37}H_{48}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	B	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	C	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	D	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	E	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	F	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	G	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	H	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	I	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	J	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	K	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		
2	L	1	Total	C	H	N	O	P	S	2	0
			110	37	44	7	18	3	1		

- Molecule 3 is water.

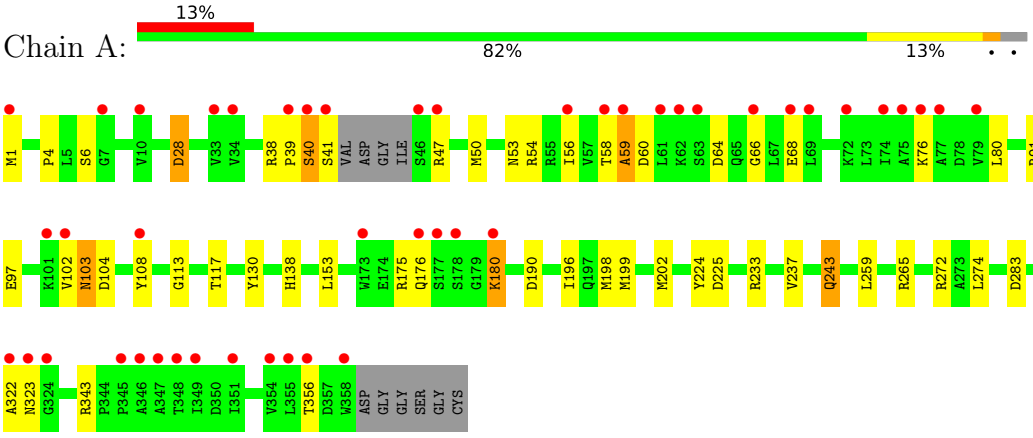
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	115	Total	O	0	0
			115	115		
3	C	131	Total	O	0	0
			131	131		
3	D	135	Total	O	0	0
			135	135		
3	E	114	Total	O	0	0
			114	114		
3	F	122	Total	O	0	0
			122	122		
3	G	117	Total	O	0	0
			117	117		
3	H	109	Total	O	0	0
			109	109		
3	I	135	Total	O	0	0
			135	135		
3	J	139	Total	O	0	0
			139	139		
3	K	136	Total	O	0	0
			136	136		
3	L	130	Total	O	0	0
			130	130		

3 Residue-property plots (i)

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

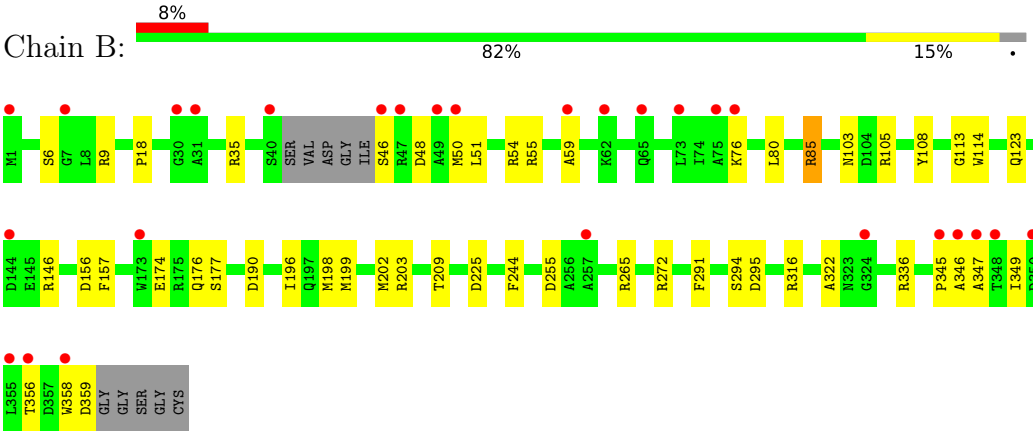
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



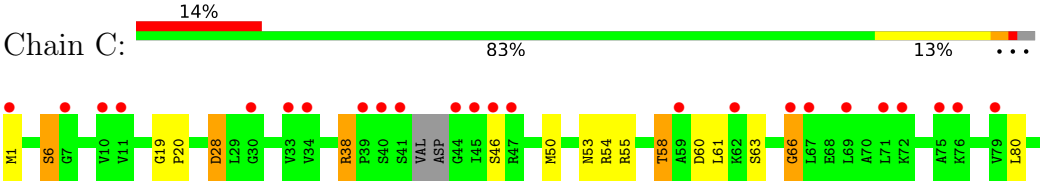
• Molecule 1: Alpha-methylacyl-CoA racemase

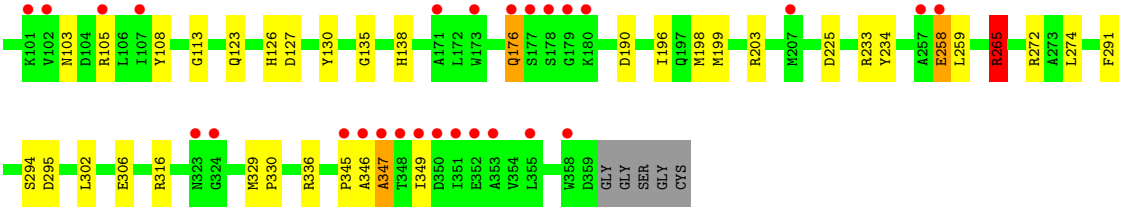
Chain B:



• Molecule 1: Alpha-methylacyl-CoA racemase

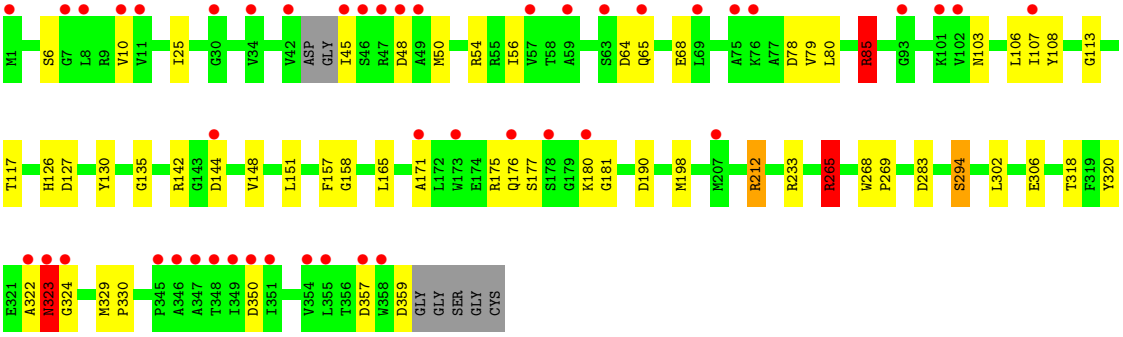
Chain C:





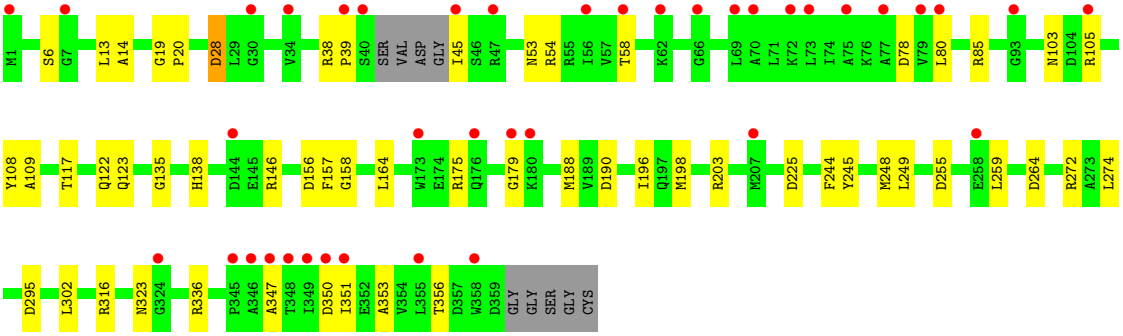
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain D:



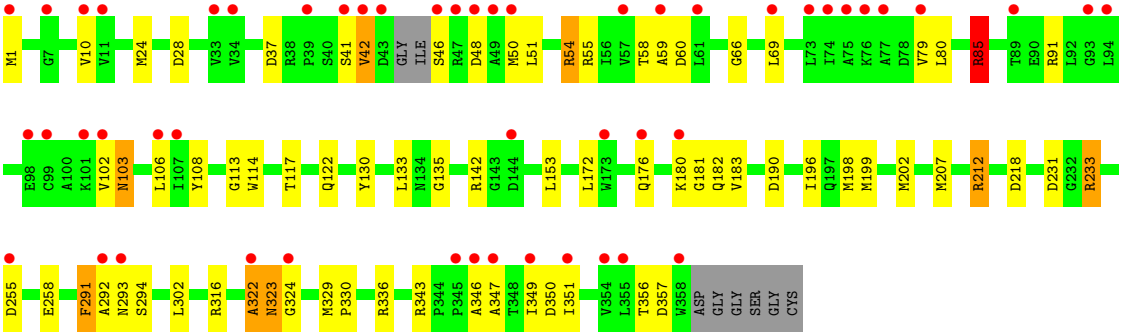
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain E:



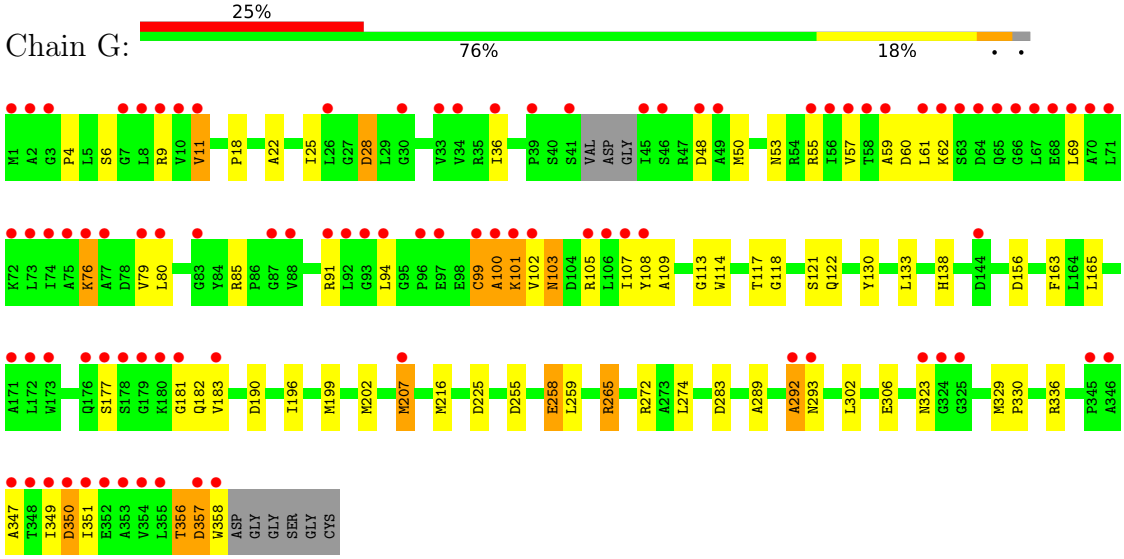
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain F:



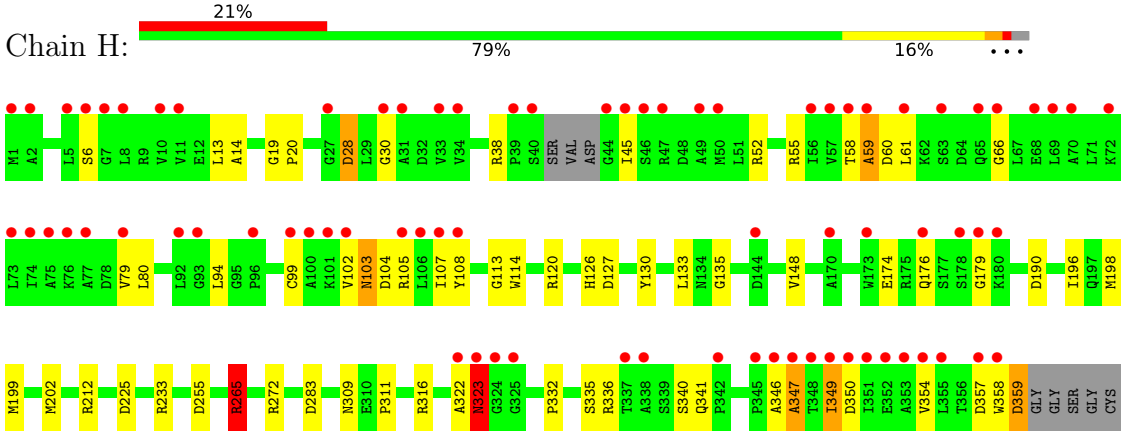
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain G:



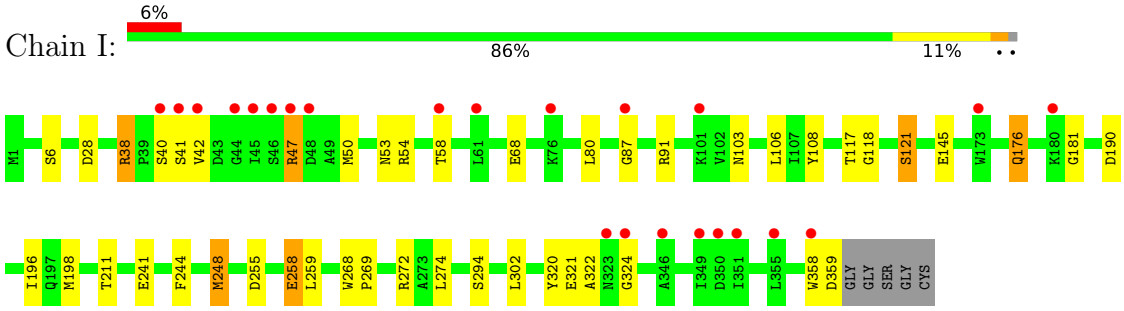
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain H:



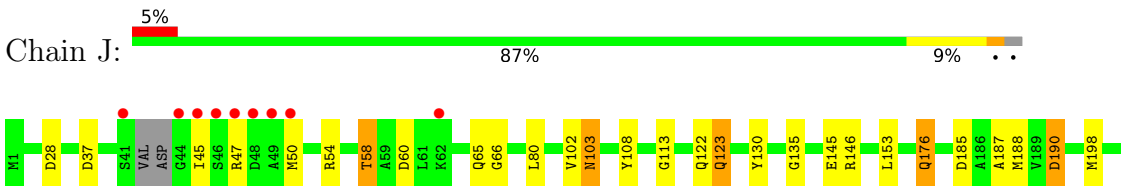
• Molecule 1: Alpha-methylacyl-CoA racemase

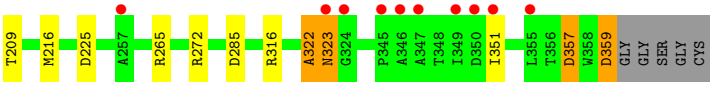
Chain I:



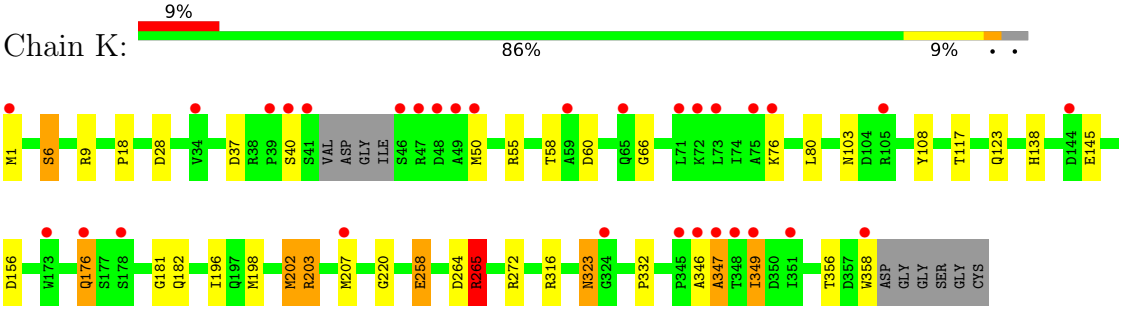
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain J:

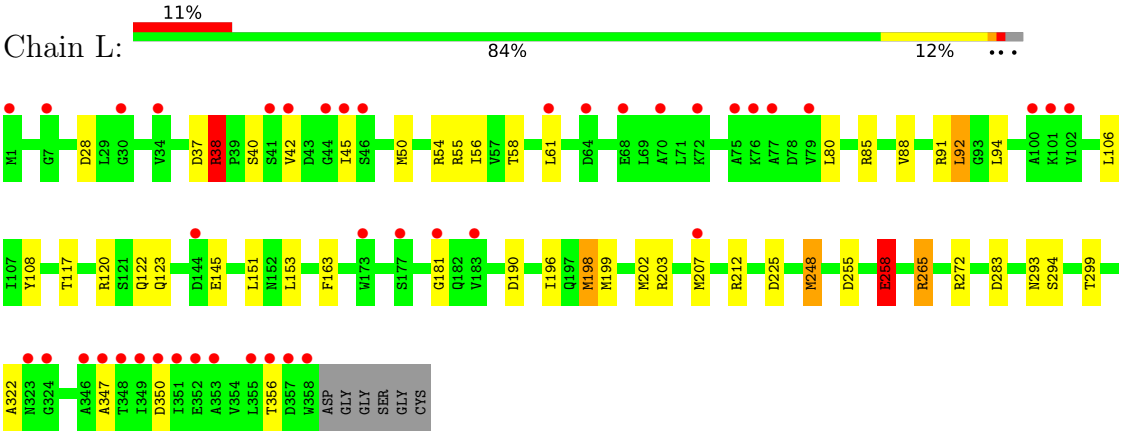




• Molecule 1: Alpha-methylacyl-CoA racemase



• Molecule 1: Alpha-methylacyl-CoA racemase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	276.69Å 276.69Å 390.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.75 – 2.08 225.75 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.75-2.08) 99.9 (225.75-2.08)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.216 , 0.251 0.218 , 0.254	Depositor DCC
R_{free} test set	22415 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 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	66985	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1IZD

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	0.64	0/2755	1.12	5/3746 (0.1%)
1	B	0.64	0/2748	1.13	5/3737 (0.1%)
1	C	0.63	0/2775	1.19	14/3773 (0.4%)
1	D	0.65	0/2769	1.21	13/3766 (0.3%)
1	E	0.64	0/2765	1.13	8/3760 (0.2%)
1	F	0.63	0/2761	1.14	8/3755 (0.2%)
1	G	0.62	0/2763	1.18	10/3757 (0.3%)
1	H	0.63	0/2760	1.16	9/3753 (0.2%)
1	I	0.63	0/2791	1.13	7/3797 (0.2%)
1	J	0.64	0/2766	1.19	12/3761 (0.3%)
1	K	0.64	0/2755	1.14	7/3746 (0.2%)
1	L	0.66	0/2774	1.17	11/3774 (0.3%)
All	All	0.64	0/33182	1.16	109/45125 (0.2%)

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	5
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	2
1	F	0	5
1	G	0	1
1	H	0	4
1	J	0	1
1	K	0	1
1	L	0	6

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

There are no bond length outliers.

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	123	GLN	CB-CA-C	11.03	127.82	109.84
1	I	255	ASP	CB-CA-C	9.50	125.58	110.19
1	C	203	ARG	N-CA-CB	9.39	124.83	110.28
1	L	123	GLN	N-CA-CB	-9.32	95.50	109.95
1	C	91	ARG	CB-CA-C	-9.26	95.99	110.81

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	54	ARG	Peptide
1	A	91	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2683	2638	2626	34	0
1	B	2682	2635	2627	33	0
1	C	2703	2656	2644	39	0
1	D	2703	2660	2652	29	0
1	E	2693	2648	2636	25	0
1	F	2695	2649	2641	43	0
1	G	2691	2649	2637	48	0
1	H	2694	2649	2641	40	0
1	I	2718	2669	2658	25	0
1	J	2700	2654	2646	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2683	2638	2626	27	0
1	L	2707	2663	2656	22	0
2	A	66	44	0	2	0
2	B	66	44	0	3	0
2	C	66	44	0	2	0
2	D	66	44	0	3	0
2	E	66	44	0	4	0
2	F	66	44	0	4	0
2	G	66	44	0	1	0
2	H	66	44	0	3	0
2	I	66	44	0	1	0
2	J	66	44	0	2	0
2	K	66	44	0	2	0
2	L	66	44	0	3	0
3	A	122	0	0	1	0
3	B	115	0	0	2	0
3	C	131	0	0	3	0
3	D	135	0	0	0	0
3	E	114	0	0	1	0
3	F	122	0	0	2	0
3	G	117	0	0	3	0
3	H	109	0	0	0	0
3	I	135	0	0	4	0
3	J	139	0	0	2	0
3	K	136	0	0	2	0
3	L	130	0	0	1	0
All	All	34649	32336	31690	358	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 6.

The worst 5 of 358 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ARG:HD3	2:F:401:A1IZD:O10	1.83	0.78
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.66	0.77
1:G:80:LEU:HD23	1:G:108:TYR:CE1	2.21	0.75
1:G:80:LEU:CD2	1:G:108:TYR:CE1	2.71	0.73
1:C:91:ARG:NH1	1:C:91:ARG:HG3	2.04	0.73

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	352/364 (97%)	325 (92%)	23 (6%)	4 (1%)	12 7
1	B	351/364 (96%)	334 (95%)	14 (4%)	3 (1%)	14 10
1	C	355/364 (98%)	338 (95%)	14 (4%)	3 (1%)	16 12
1	D	354/364 (97%)	334 (94%)	18 (5%)	2 (1%)	22 18
1	E	353/364 (97%)	333 (94%)	17 (5%)	3 (1%)	16 12
1	F	353/364 (97%)	327 (93%)	19 (5%)	7 (2%)	6 2
1	G	353/364 (97%)	325 (92%)	19 (5%)	9 (2%)	4 1
1	H	353/364 (97%)	328 (93%)	21 (6%)	4 (1%)	12 7
1	I	359/364 (99%)	341 (95%)	16 (4%)	2 (1%)	22 18
1	J	354/364 (97%)	338 (96%)	14 (4%)	2 (1%)	22 18
1	K	352/364 (97%)	329 (94%)	19 (5%)	4 (1%)	12 7
1	L	357/364 (98%)	336 (94%)	18 (5%)	3 (1%)	16 12
All	All	4246/4368 (97%)	3988 (94%)	212 (5%)	46 (1%)	12 7

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	103	ASN
1	B	103	ASN
1	B	347	ALA
1	C	347	ALA

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	273/277 (99%)	265 (97%)	8 (3%)	37	40
1	B	272/277 (98%)	266 (98%)	6 (2%)	47	51
1	C	275/277 (99%)	268 (98%)	7 (2%)	42	46
1	D	275/277 (99%)	266 (97%)	9 (3%)	33	34
1	E	274/277 (99%)	268 (98%)	6 (2%)	47	51
1	F	274/277 (99%)	269 (98%)	5 (2%)	54	59
1	G	274/277 (99%)	266 (97%)	8 (3%)	37	40
1	H	273/277 (99%)	265 (97%)	8 (3%)	37	40
1	I	277/277 (100%)	267 (96%)	10 (4%)	30	31
1	J	274/277 (99%)	267 (97%)	7 (3%)	41	44
1	K	273/277 (99%)	264 (97%)	9 (3%)	33	34
1	L	275/277 (99%)	263 (96%)	12 (4%)	24	23
All	All	3289/3324 (99%)	3194 (97%)	95 (3%)	37	40

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	6	SER
1	J	351	ILE
1	I	41	SER
1	I	176	GLN
1	K	40	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	286	HIS
1	J	134	ASN
1	H	327	GLN
1	I	263	ASN
1	J	282	HIS

5.3.3 RNA

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)

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	A1IZD	I	401	-	62,70,70	0.93	3 (4%)	80,103,103	1.32	10 (12%)
2	A1IZD	D	401	-	62,70,70	0.98	4 (6%)	80,103,103	1.18	6 (7%)
2	A1IZD	A	401	-	62,70,70	0.89	5 (8%)	80,103,103	1.34	13 (16%)
2	A1IZD	L	401	-	62,70,70	0.88	3 (4%)	80,103,103	1.26	9 (11%)
2	A1IZD	G	401	-	62,70,70	0.87	3 (4%)	80,103,103	1.51	11 (13%)
2	A1IZD	B	401	-	62,70,70	0.98	4 (6%)	80,103,103	1.27	10 (12%)
2	A1IZD	H	401	-	62,70,70	1.16	3 (4%)	80,103,103	1.24	9 (11%)
2	A1IZD	E	401	-	62,70,70	1.02	4 (6%)	80,103,103	1.26	8 (10%)
2	A1IZD	J	401	-	62,70,70	0.82	1 (1%)	80,103,103	1.32	7 (8%)
2	A1IZD	F	401	-	62,70,70	0.93	5 (8%)	80,103,103	1.61	12 (15%)
2	A1IZD	C	401	-	62,70,70	0.86	3 (4%)	80,103,103	1.45	10 (12%)
2	A1IZD	K	401	-	62,70,70	0.85	3 (4%)	80,103,103	1.35	10 (12%)

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	A1IZD	I	401	-	-	10/63/83/83	0/5/5/5
2	A1IZD	D	401	-	-	8/63/83/83	0/5/5/5
2	A1IZD	A	401	-	-	14/63/83/83	0/5/5/5
2	A1IZD	L	401	-	-	14/63/83/83	0/5/5/5
2	A1IZD	G	401	-	-	20/63/83/83	0/5/5/5
2	A1IZD	B	401	-	-	9/63/83/83	0/5/5/5
2	A1IZD	H	401	-	-	9/63/83/83	0/5/5/5
2	A1IZD	E	401	-	-	16/63/83/83	0/5/5/5
2	A1IZD	J	401	-	-	14/63/83/83	0/5/5/5
2	A1IZD	F	401	-	-	8/63/83/83	0/5/5/5
2	A1IZD	C	401	-	-	12/63/83/83	0/5/5/5
2	A1IZD	K	401	-	-	10/63/83/83	0/5/5/5

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	A1IZD	C2-C3	5.90	1.58	1.53
2	E	401	A1IZD	C2-C3	4.06	1.56	1.53
2	D	401	A1IZD	C2-C3	3.88	1.56	1.53
2	B	401	A1IZD	C2-C3	3.50	1.56	1.53
2	I	401	A1IZD	O1-C3	3.47	1.25	1.20

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	A1IZD	C2-C3-S1	6.45	118.81	111.81
2	F	401	A1IZD	O1-C3-C2	-5.72	114.92	124.12
2	D	401	A1IZD	C23-C24-C16	-5.27	93.88	103.22
2	C	401	A1IZD	O1-C3-S1	5.17	130.76	123.80
2	C	401	A1IZD	O1-C3-C2	-5.06	115.99	124.12

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1IZD	C9-C10-C11-C14
2	A	401	A1IZD	C9-C10-C11-C12
2	A	401	A1IZD	C9-C10-C11-C13
2	A	401	A1IZD	C6-C7-C8-N2
2	A	401	A1IZD	C14-O5-P1-O8

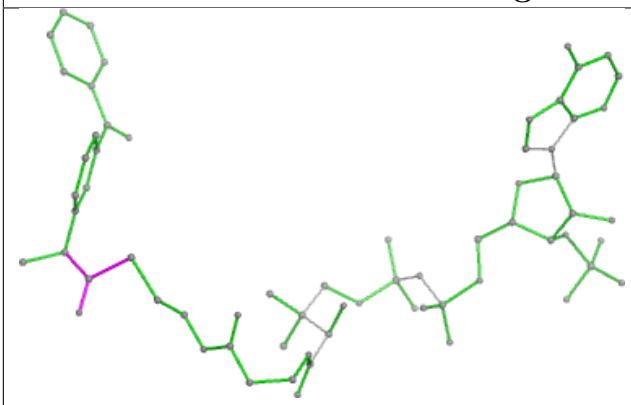
There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	A1IZD	1	0
2	D	401	A1IZD	3	0
2	A	401	A1IZD	2	0
2	L	401	A1IZD	3	0
2	G	401	A1IZD	1	0
2	B	401	A1IZD	3	0
2	H	401	A1IZD	3	0
2	E	401	A1IZD	4	0
2	J	401	A1IZD	2	0
2	F	401	A1IZD	4	0
2	C	401	A1IZD	2	0
2	K	401	A1IZD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 A1IZD I 401



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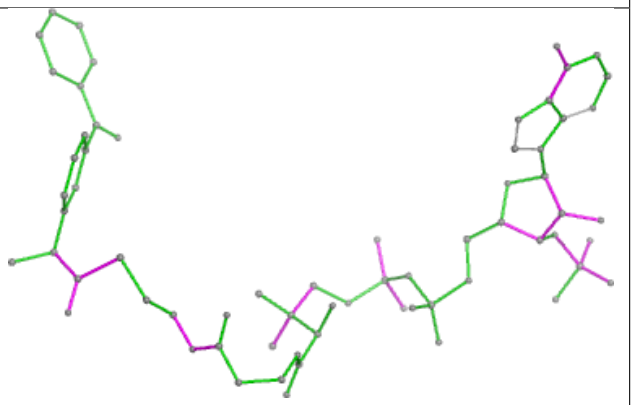

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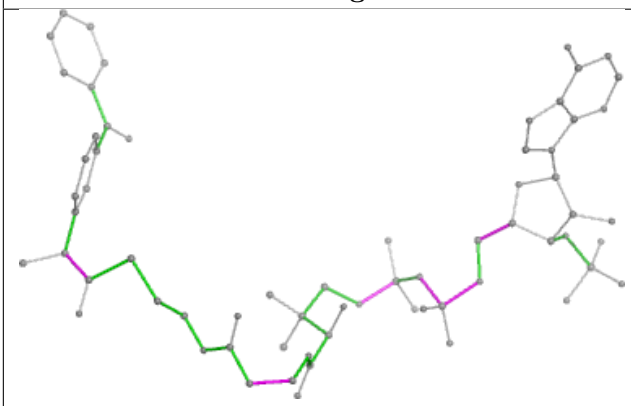

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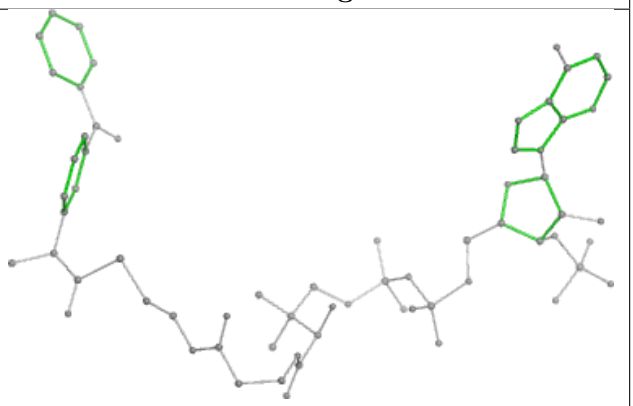
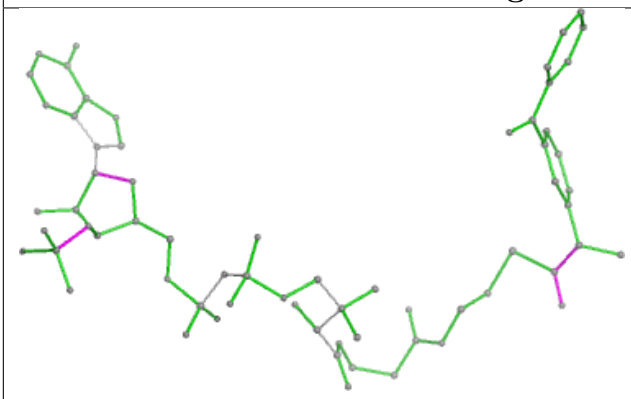


Rings

Ligand A1IZD D 401



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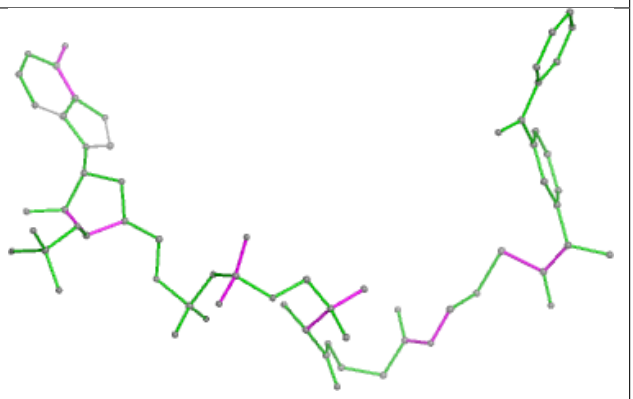

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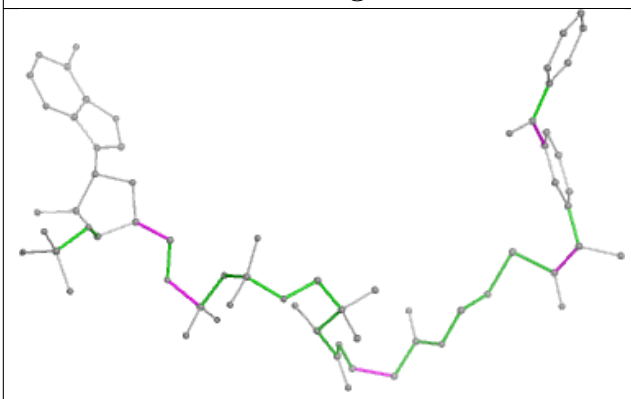

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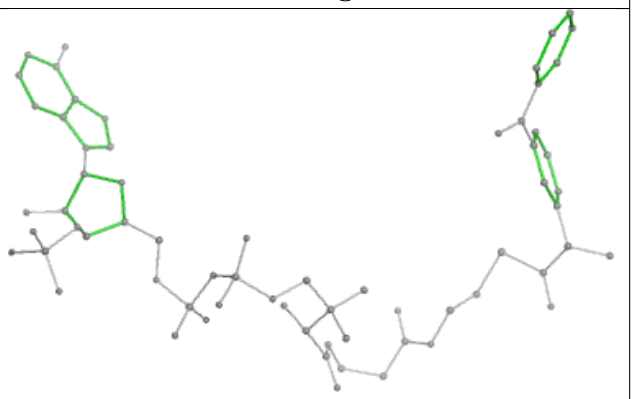
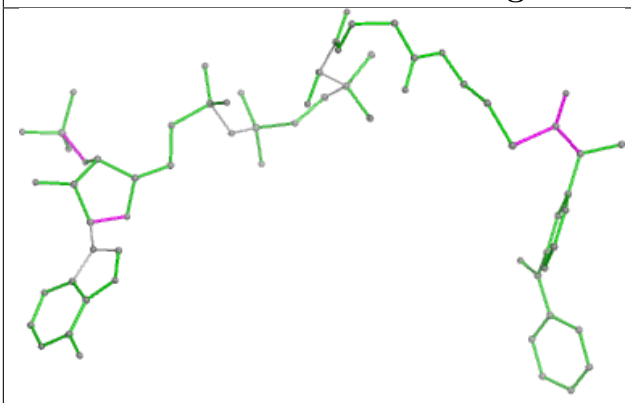


Rings

Ligand A1IZD A 401



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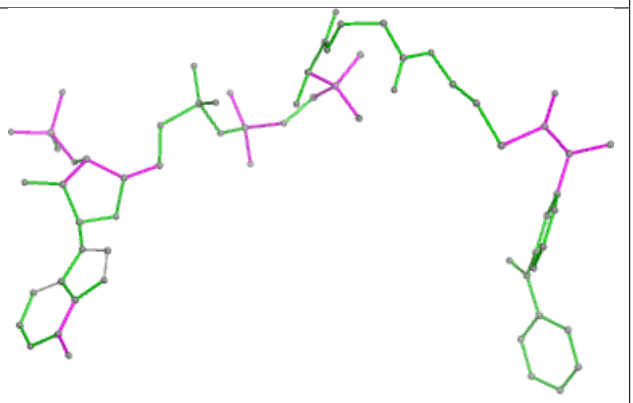

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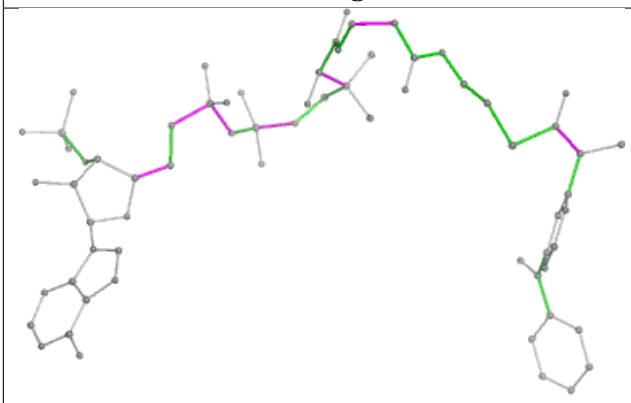

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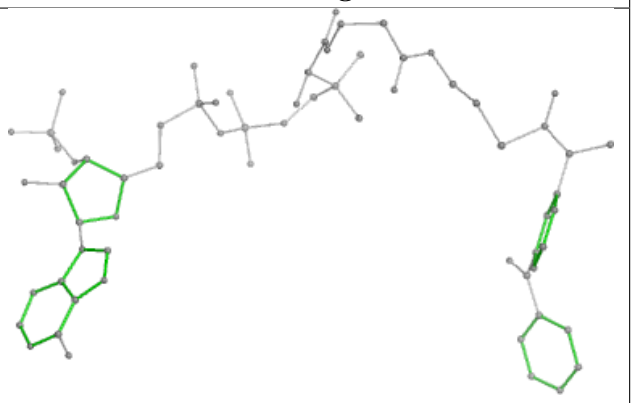
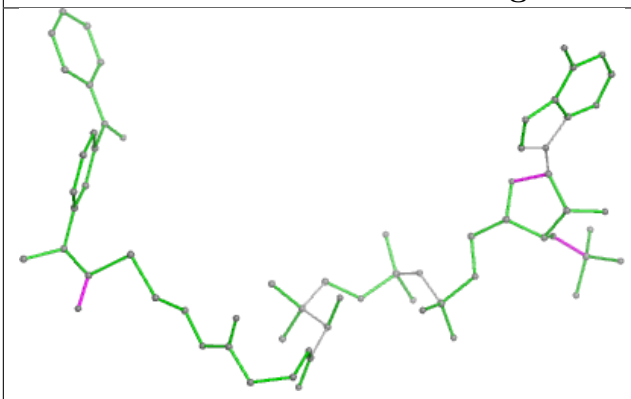


Rings

Ligand A1IZD L 401



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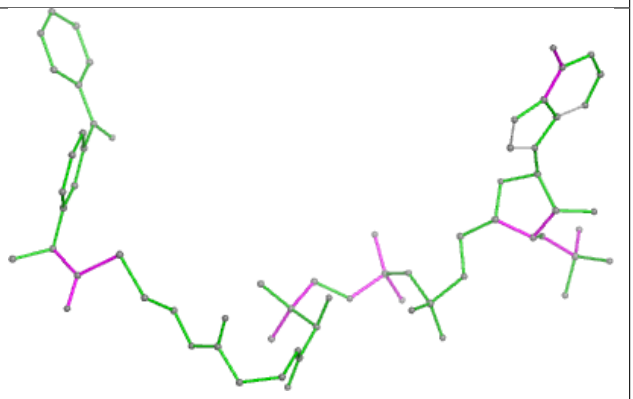

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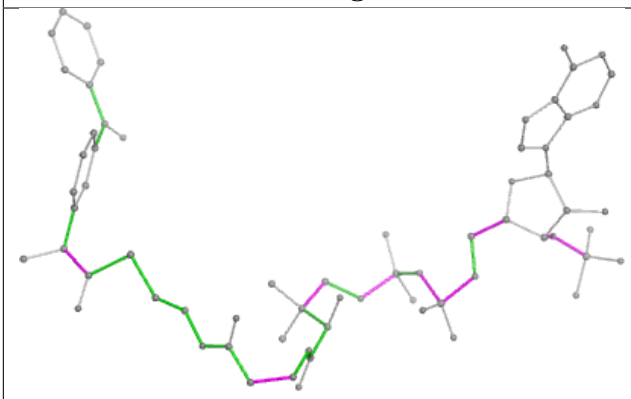

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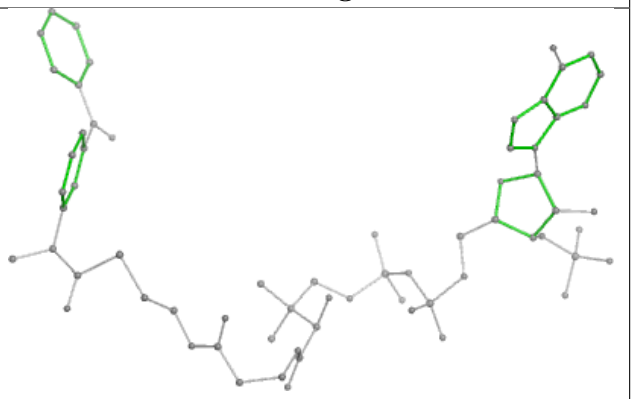
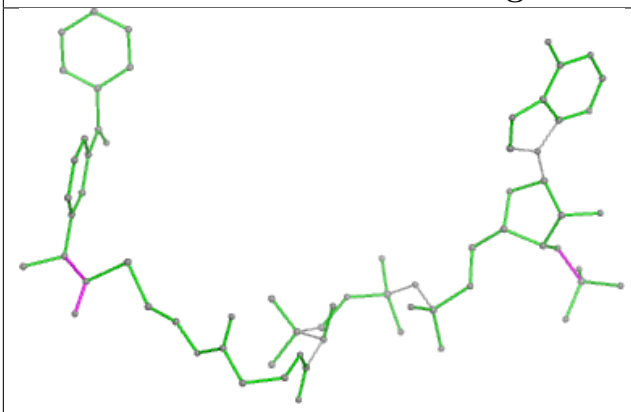
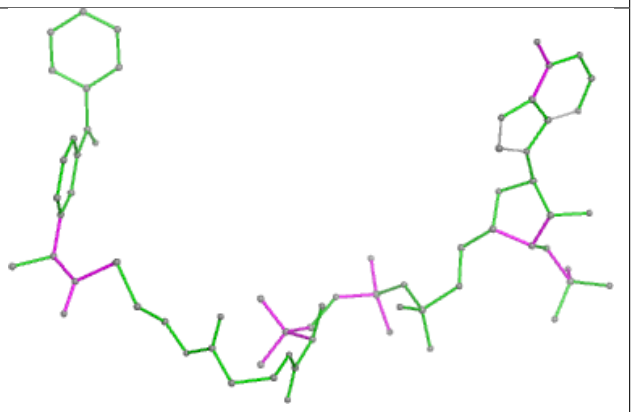


Rings

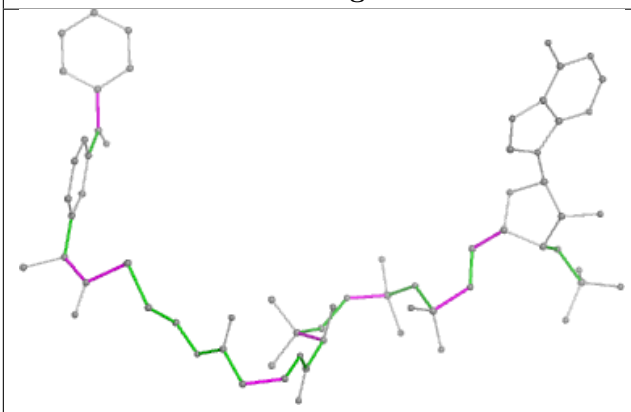
Ligand A1IZD G 401



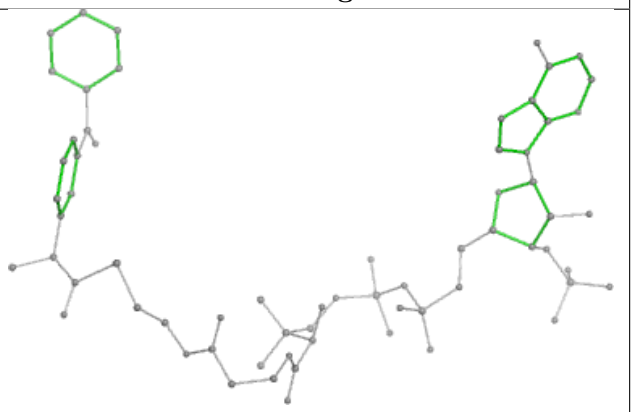
Bond lengths



Bond angles

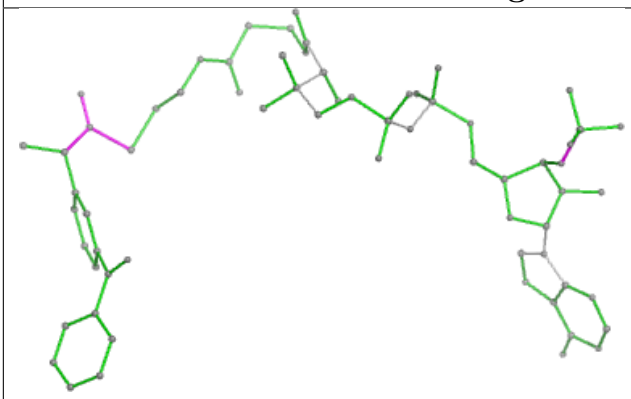


Torsions



Rings

Ligand A1IZD B 401



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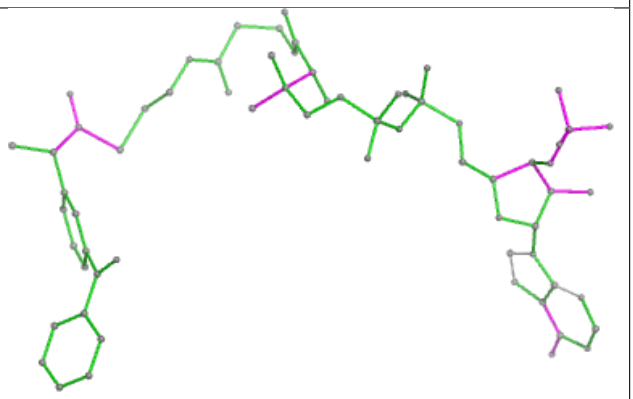

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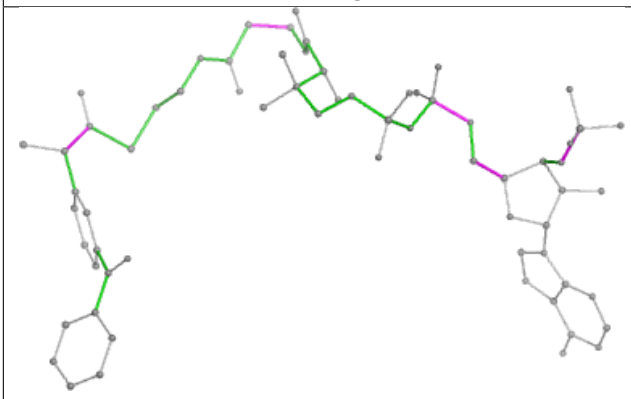

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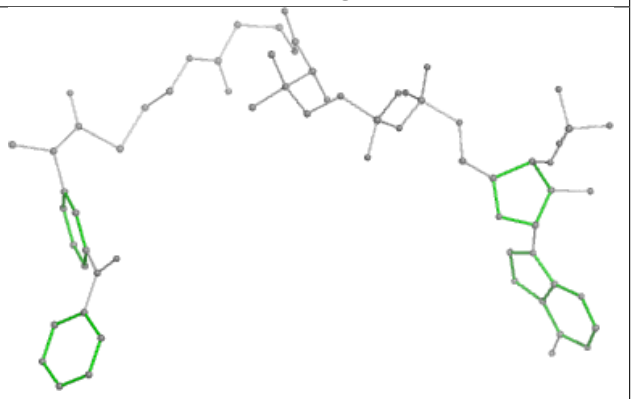
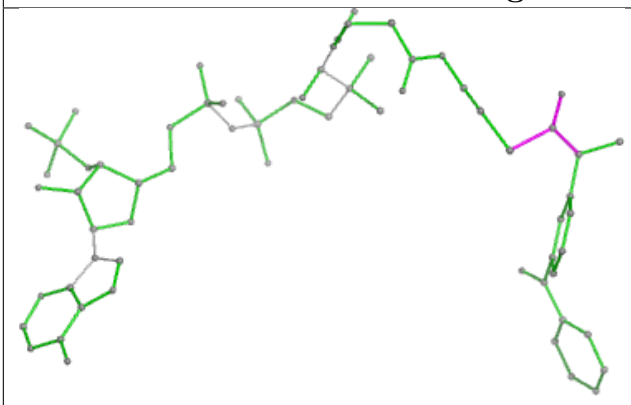


Rings

Ligand A1IZD H 401



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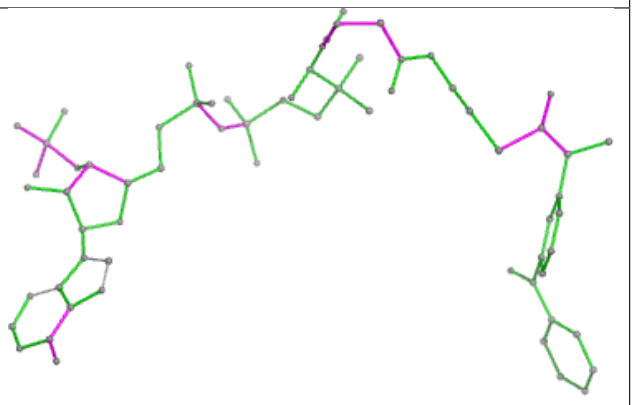

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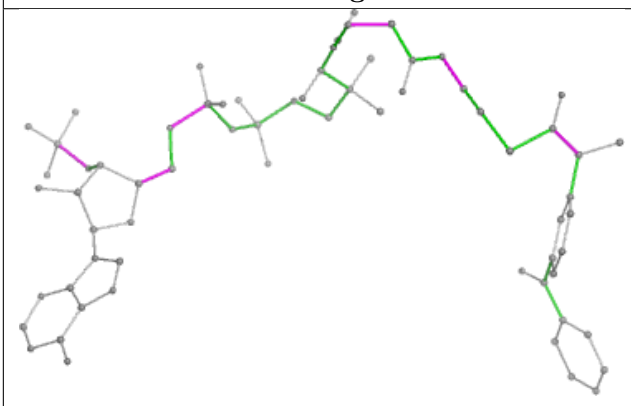
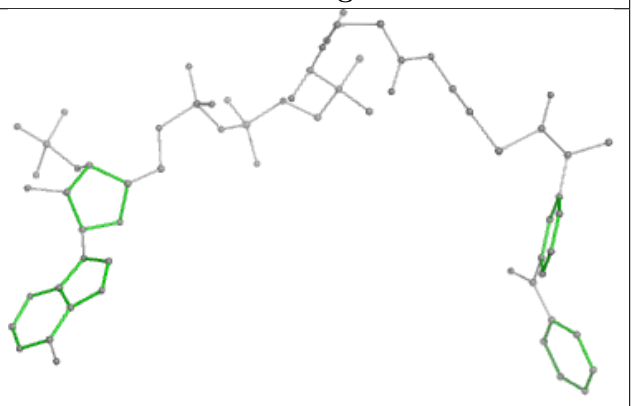
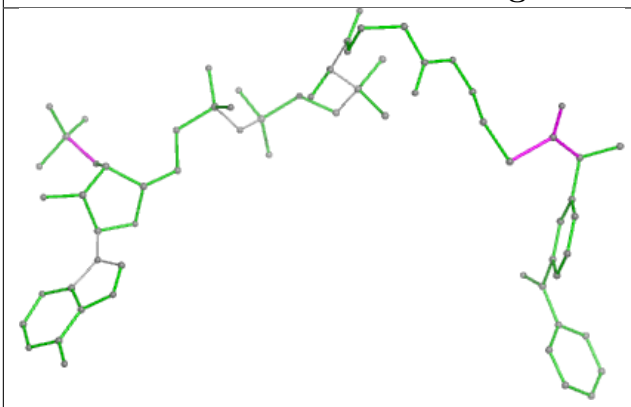


Torsions



Rings

Ligand A1IZD E 401



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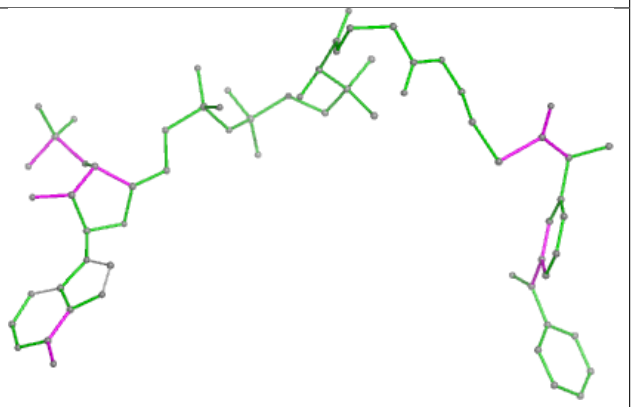
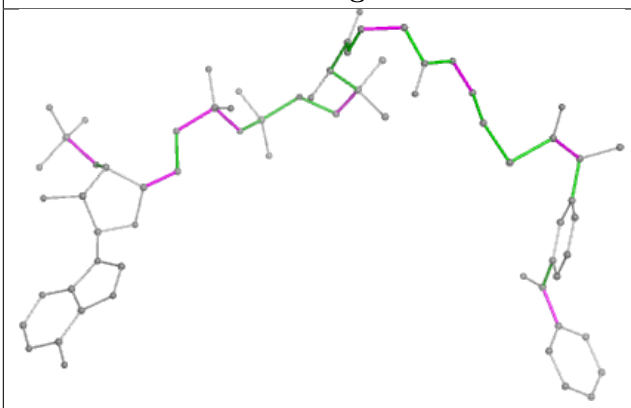


Bond angles



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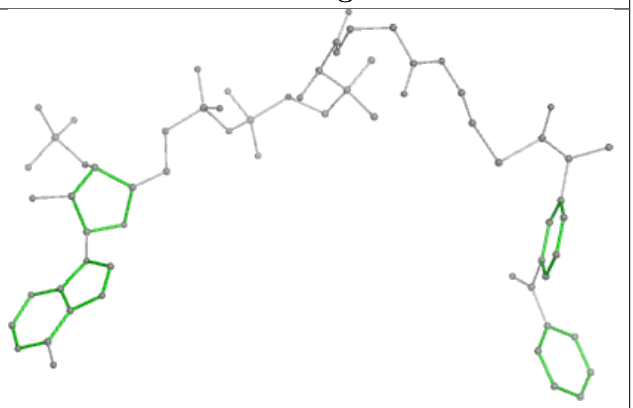
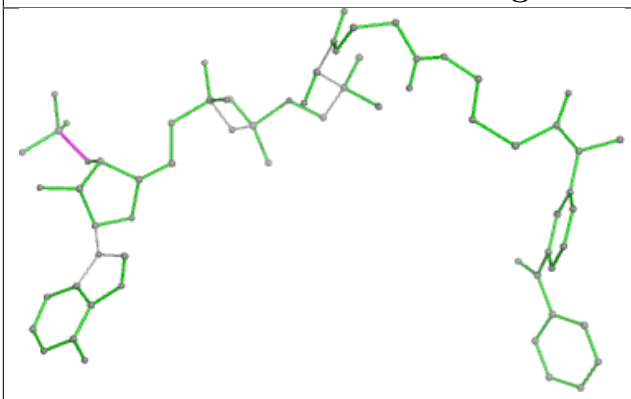
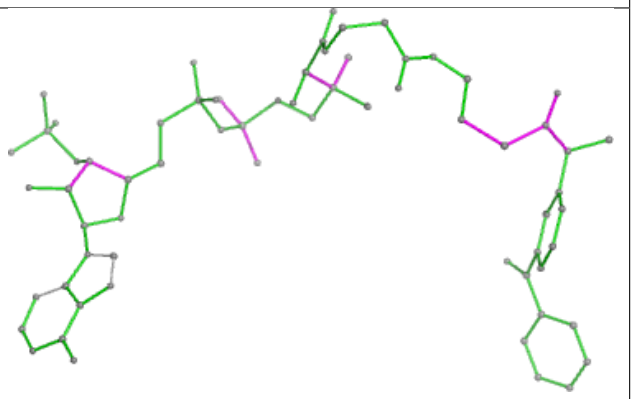


Rings

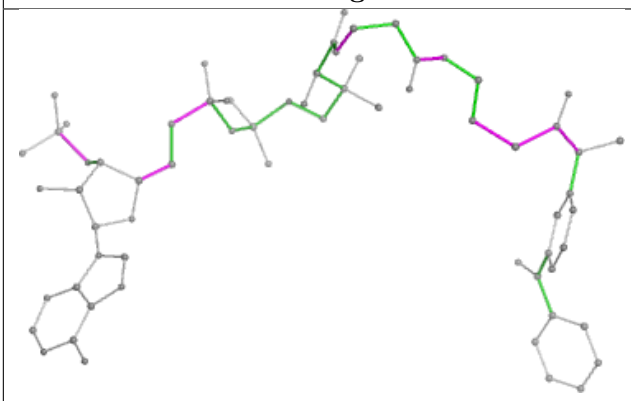
Ligand A1IZD J 401



Bond lengths



Bond angles



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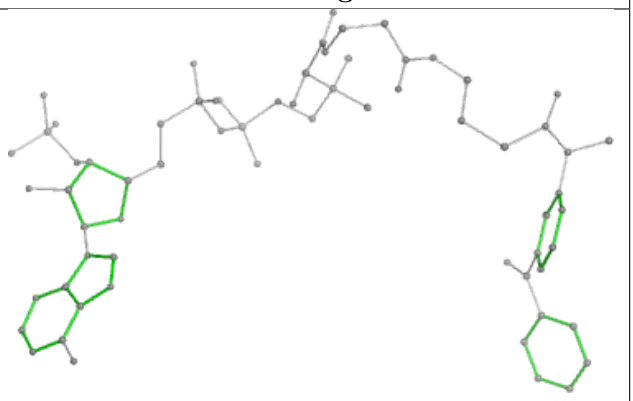
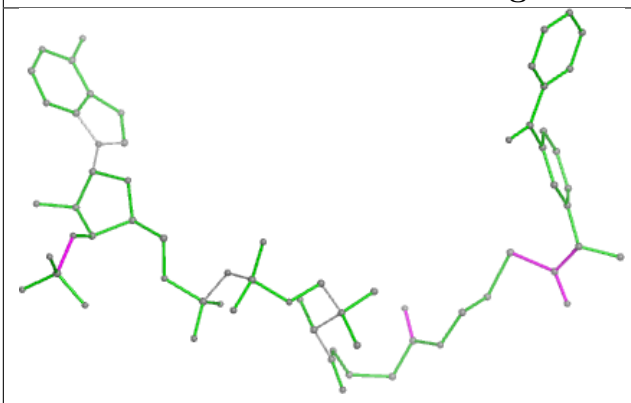


Rings

Ligand A1IZD F 401



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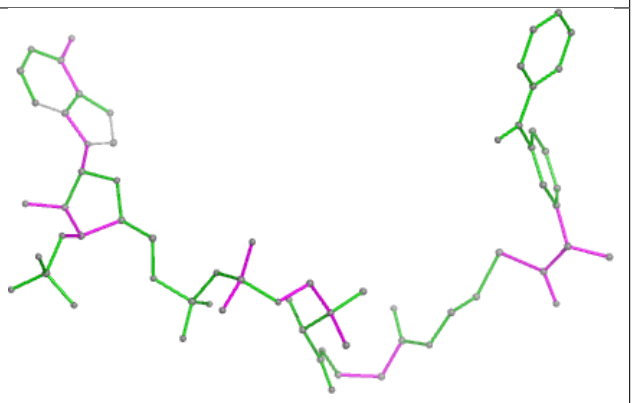
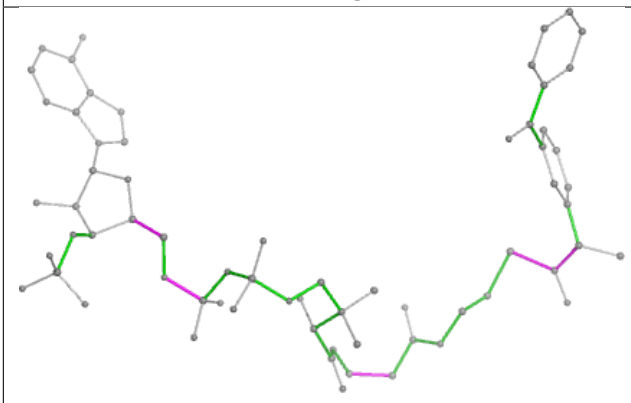


Bond angles



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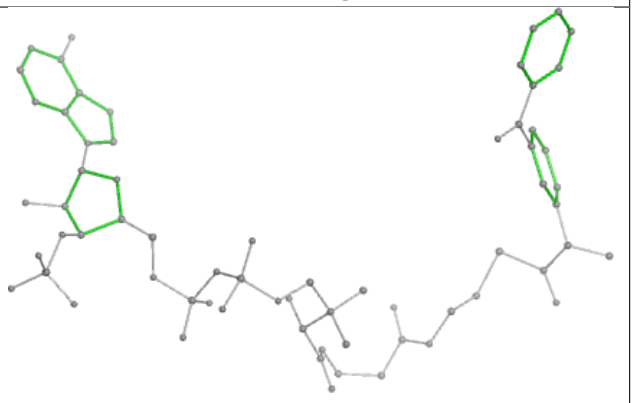
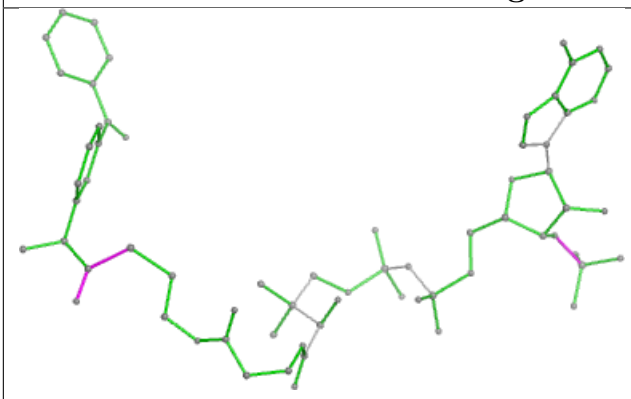


Rings

Ligand A1IZD C 401



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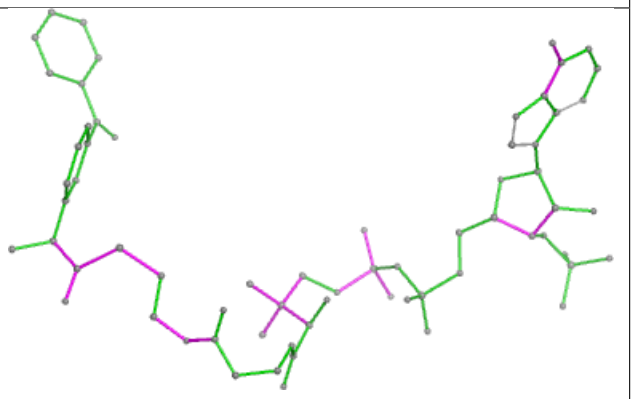

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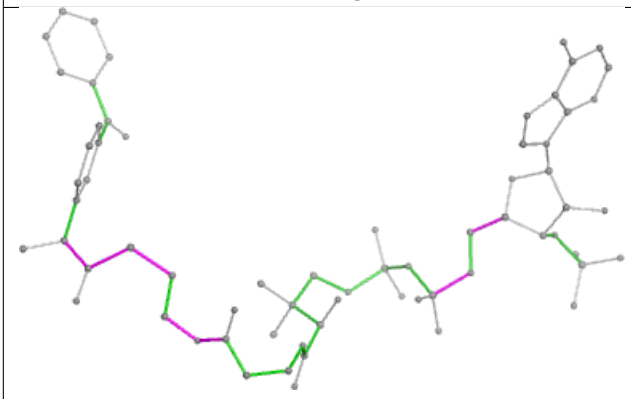

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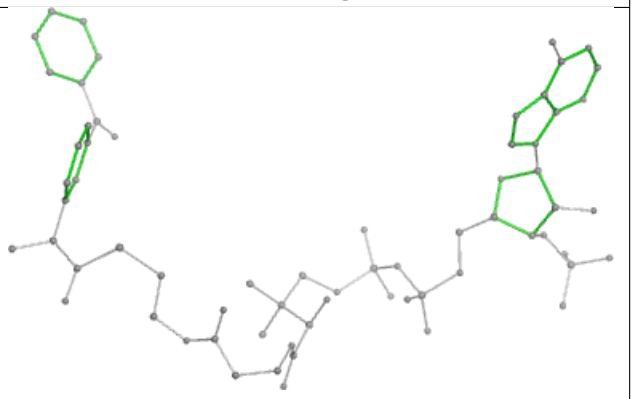
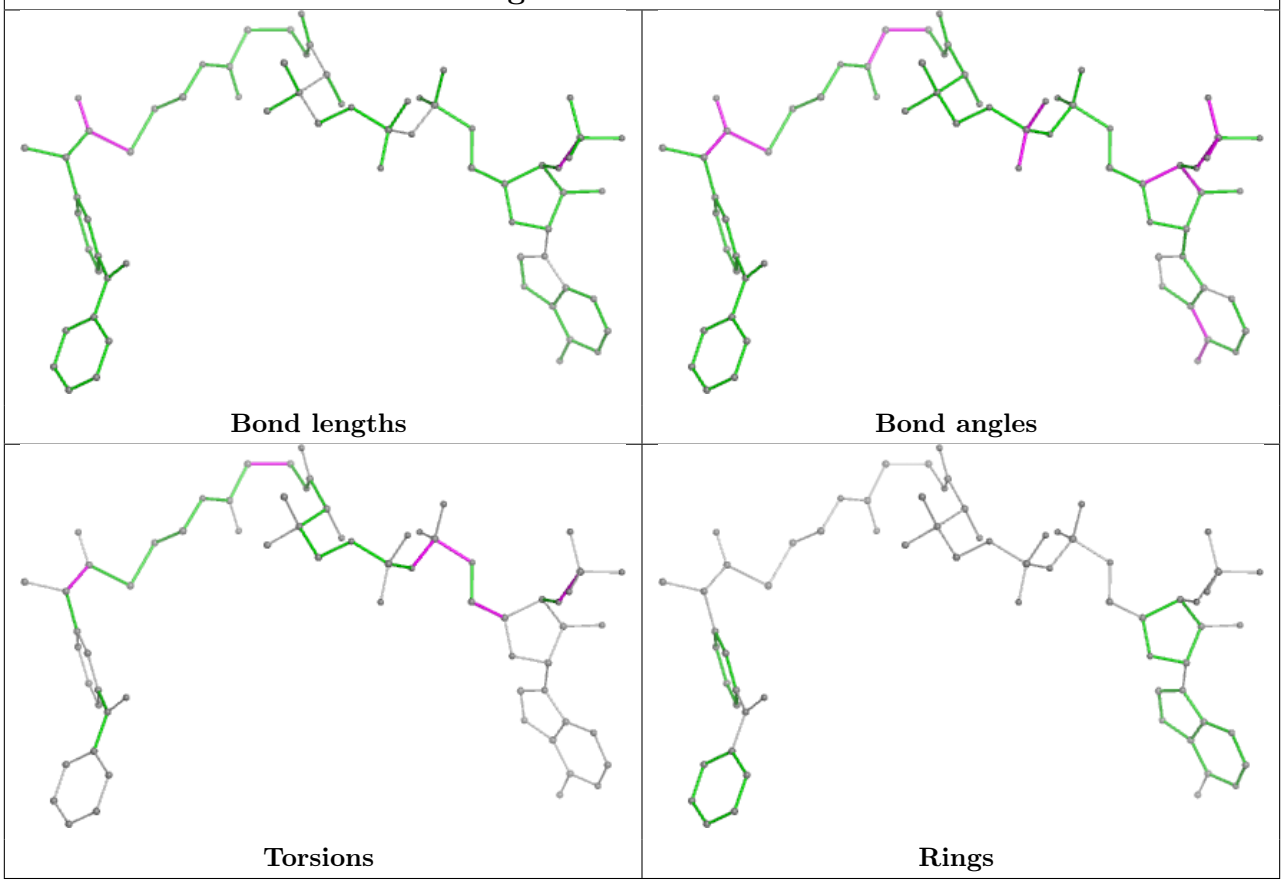


Rings

Ligand A1IZD K 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^{th} 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	354/364 (97%)	0.52	49 (13%) 8 8	23, 41, 83, 105	2 (0%)
1	B	354/364 (97%)	0.42	30 (8%) 18 19	20, 40, 80, 109	1 (0%)
1	C	357/364 (98%)	0.51	52 (14%) 7 7	20, 41, 87, 115	2 (0%)
1	D	357/364 (98%)	0.50	45 (12%) 9 10	21, 41, 82, 118	1 (0%)
1	E	355/364 (97%)	0.51	39 (10%) 12 13	23, 42, 84, 107	2 (0%)
1	F	356/364 (97%)	0.58	51 (14%) 7 8	22, 43, 84, 135	1 (0%)
1	G	355/364 (97%)	0.92	90 (25%) 2 2	21, 44, 93, 122	2 (0%)
1	H	356/364 (97%)	0.81	77 (21%) 3 3	21, 44, 94, 123	1 (0%)
1	I	359/364 (98%)	0.26	23 (6%) 27 28	21, 38, 76, 120	2 (0%)
1	J	357/364 (98%)	0.20	19 (5%) 33 35	21, 38, 75, 115	1 (0%)
1	K	354/364 (97%)	0.35	31 (8%) 17 18	19, 40, 79, 113	2 (0%)
1	L	358/364 (98%)	0.43	41 (11%) 11 12	21, 41, 78, 113	1 (0%)
All	All	4272/4368 (97%)	0.50	547 (12%) 9 9	19, 41, 84, 135	18 (0%)

The worst 5 of 547 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	ALA	8.0
1	C	346	ALA	7.4
1	F	346	ALA	6.8
1	D	42	VAL	6.5
1	B	346	ALA	6.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

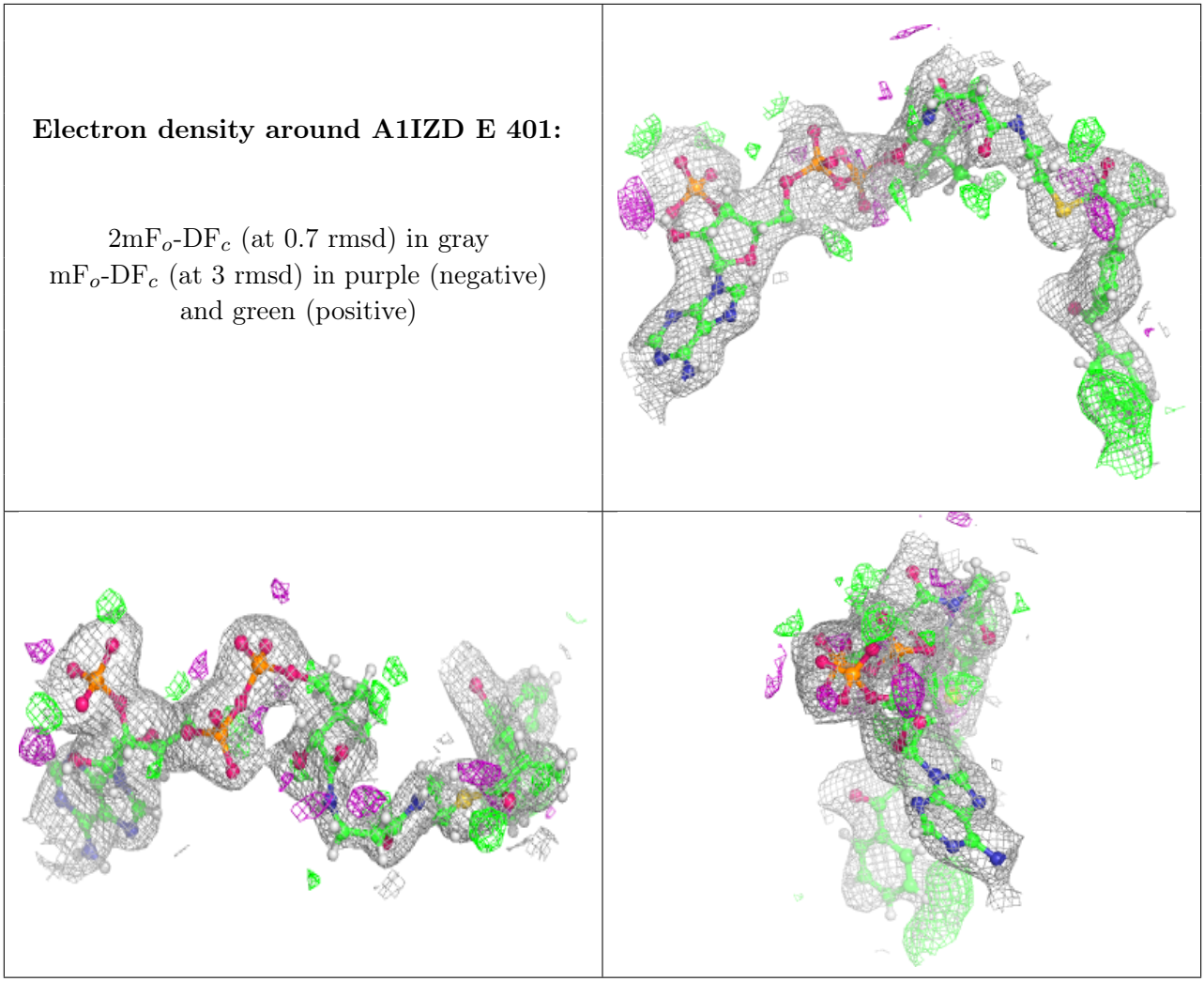
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A1IZD	E	401	66/66	0.89	0.16	51,72,91,98	2
2	A1IZD	H	401	66/66	0.90	0.15	57,72,95,100	2
2	A1IZD	G	401	66/66	0.92	0.15	35,59,108,119	2
2	A1IZD	A	401	66/66	0.92	0.13	40,60,86,90	2
2	A1IZD	C	401	66/66	0.93	0.13	39,57,94,100	2
2	A1IZD	F	401	66/66	0.93	0.12	31,53,81,97	2
2	A1IZD	L	401	66/66	0.93	0.12	35,53,79,88	2
2	A1IZD	I	401	66/66	0.94	0.11	33,52,86,89	2
2	A1IZD	B	401	66/66	0.95	0.11	35,53,92,101	2
2	A1IZD	J	401	66/66	0.95	0.10	36,47,78,82	2
2	A1IZD	D	401	66/66	0.95	0.10	31,52,80,87	2
2	A1IZD	K	401	66/66	0.96	0.09	34,52,82,87	2

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.

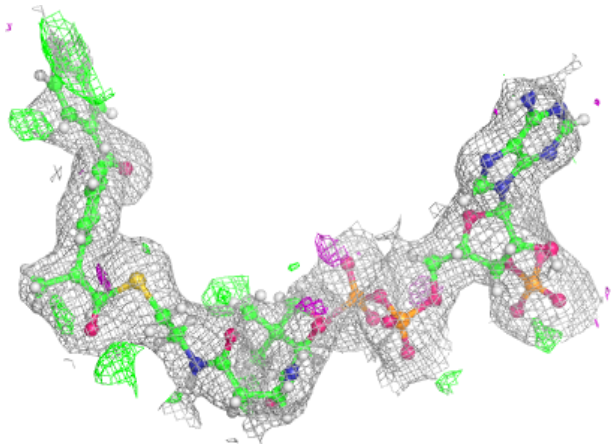
Electron density around A1IZD E 401:

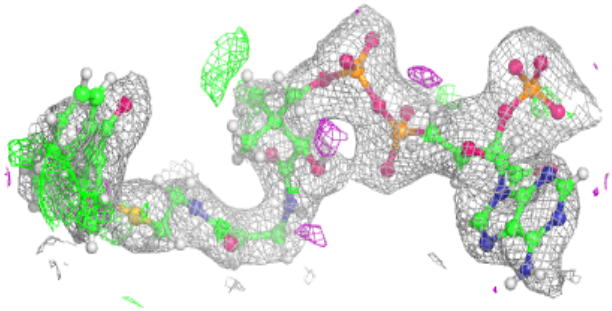
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

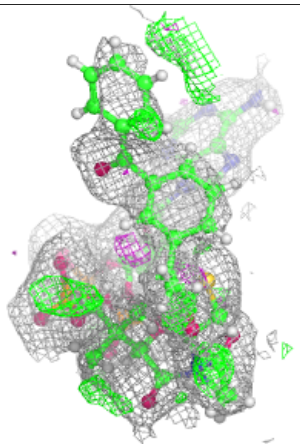


Electron density around A1IZD H 401:

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

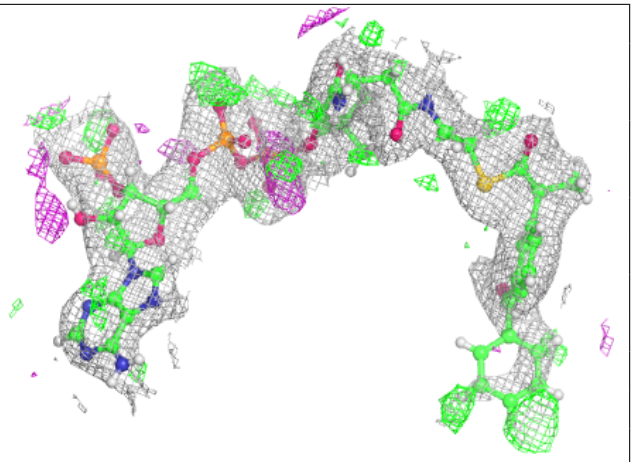


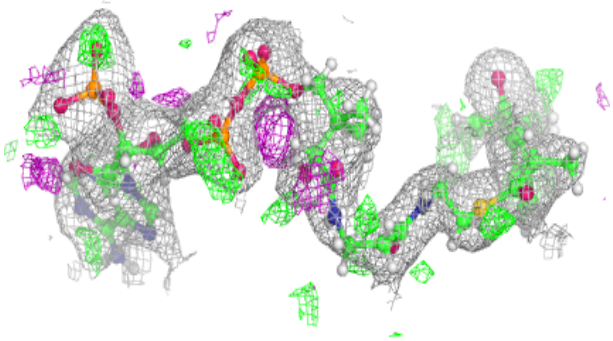


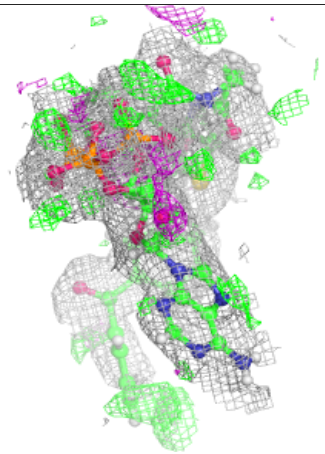


Electron density around A1IZD G 401:

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

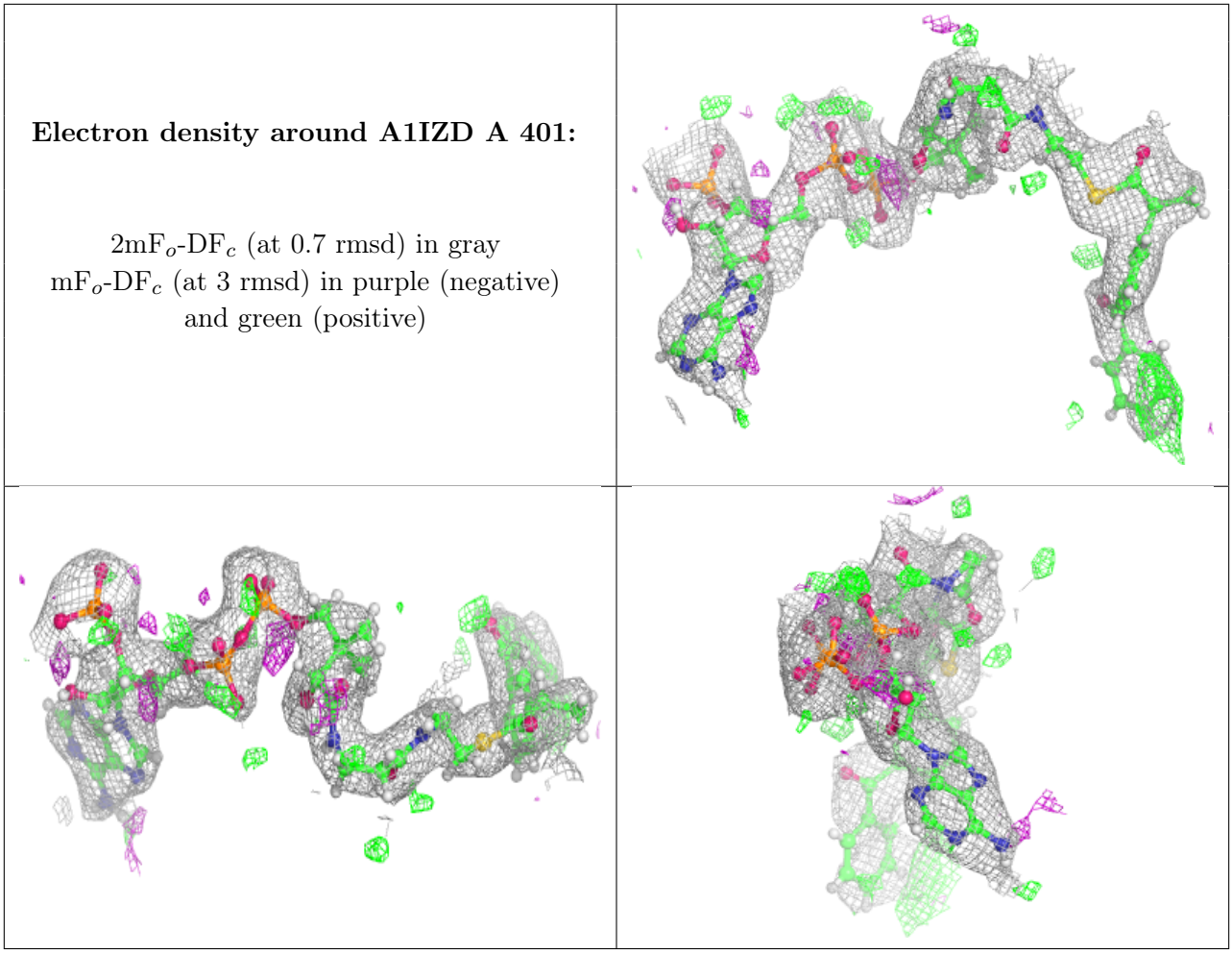






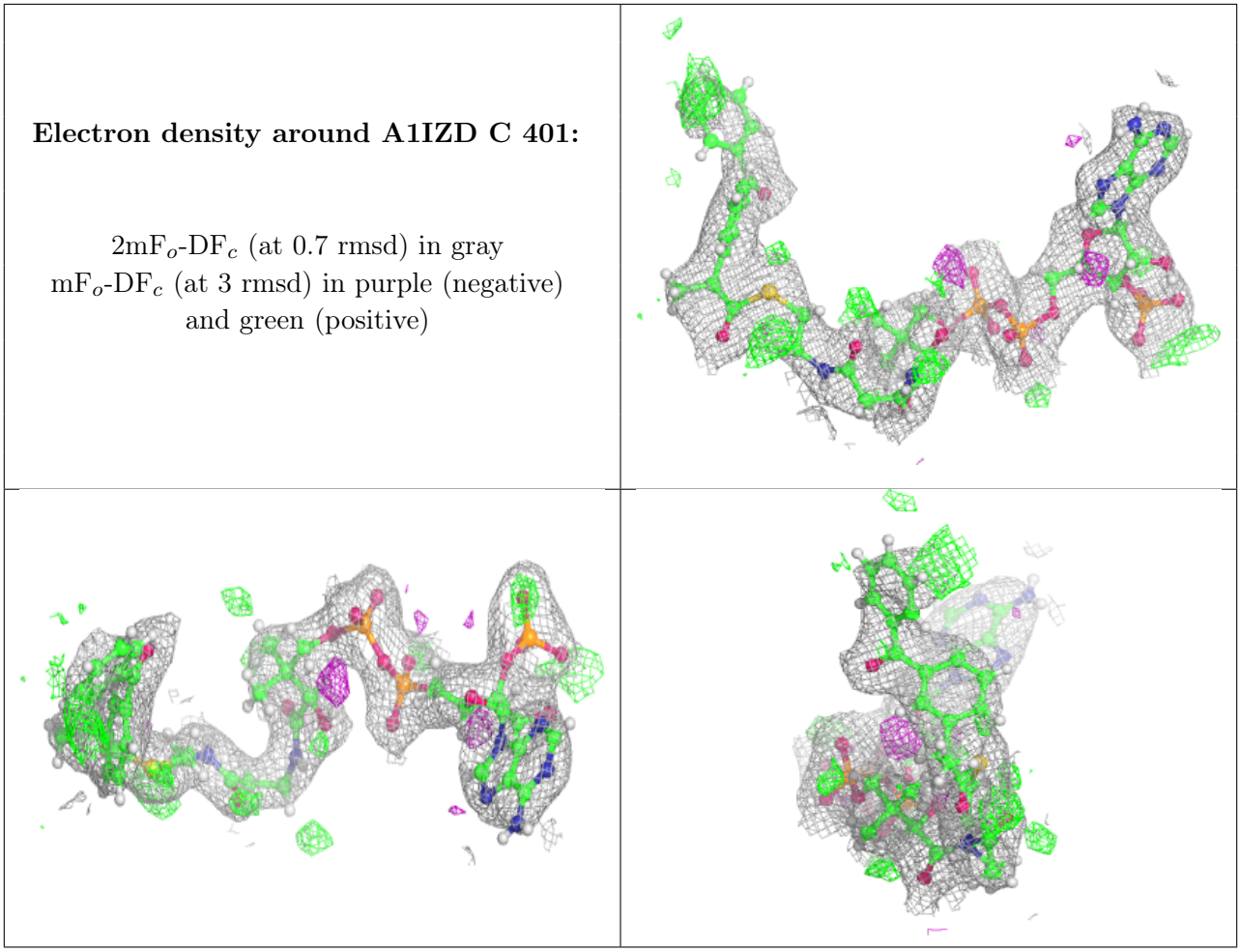
Electron density around A1IZD A 401:

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



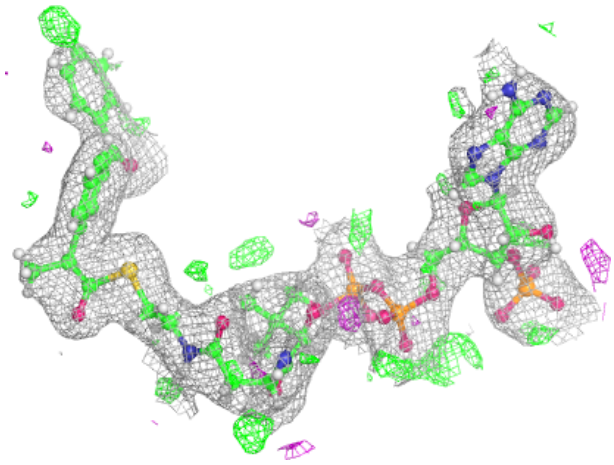
Electron density around A1IZD C 401:

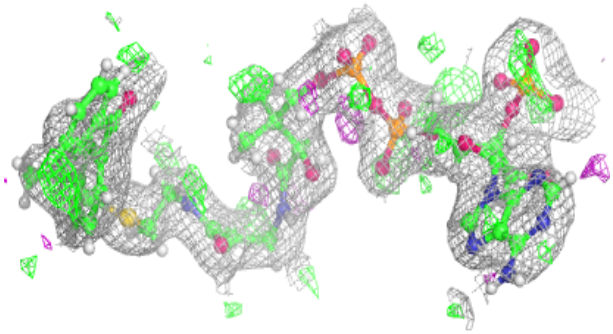
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

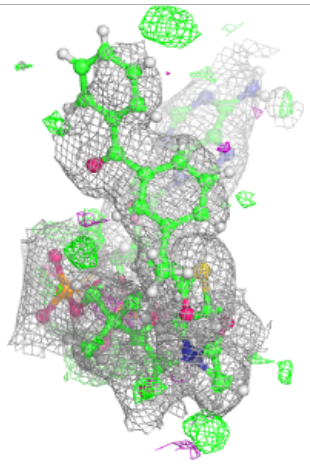


Electron density around A1IZD F 401:

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

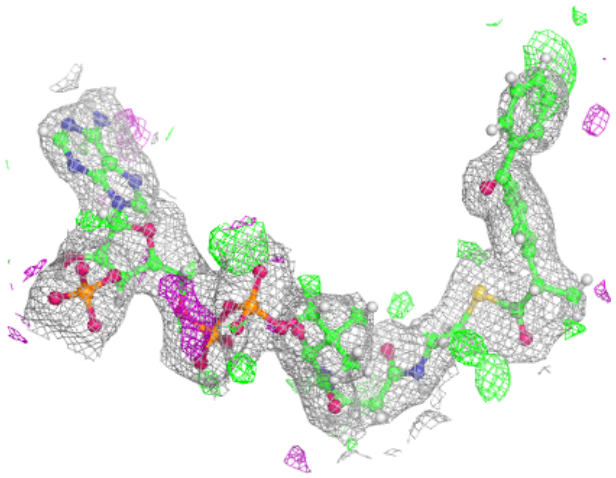


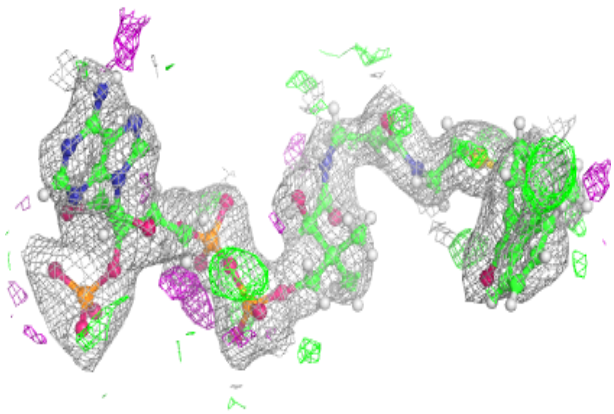


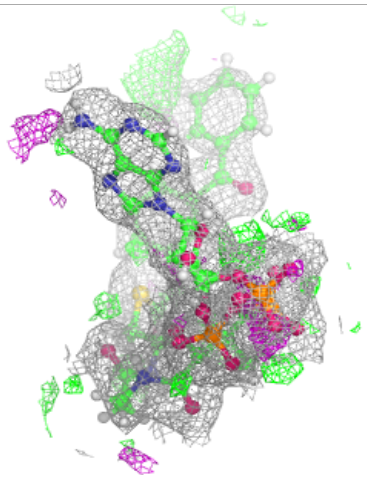


Electron density around A1IZD L 401:

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

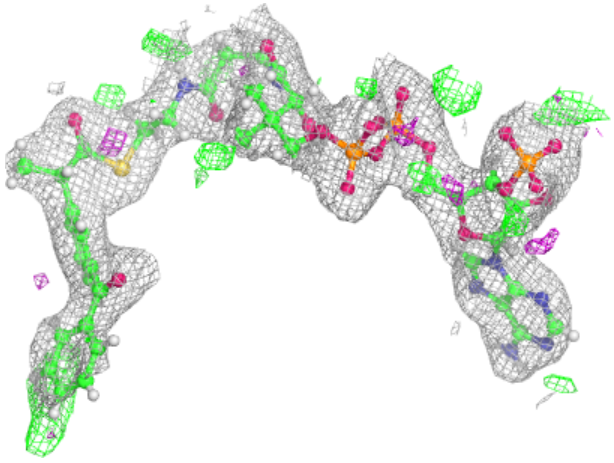


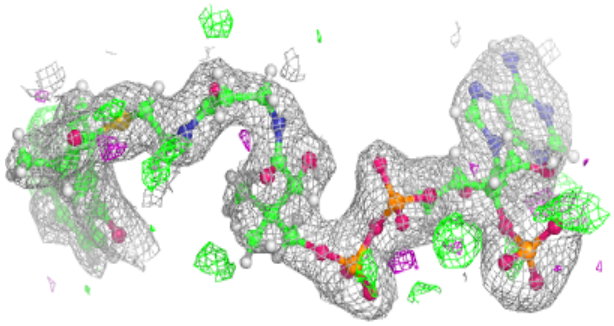


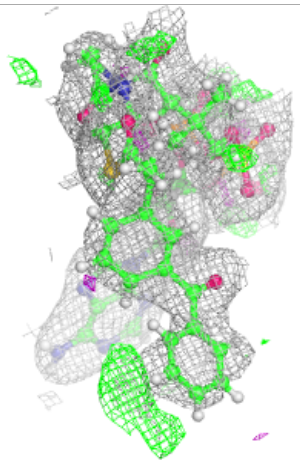


Electron density around A1IZD I 401:

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

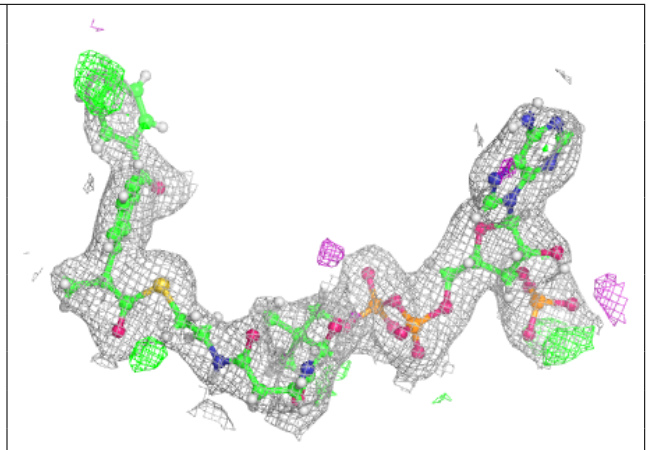


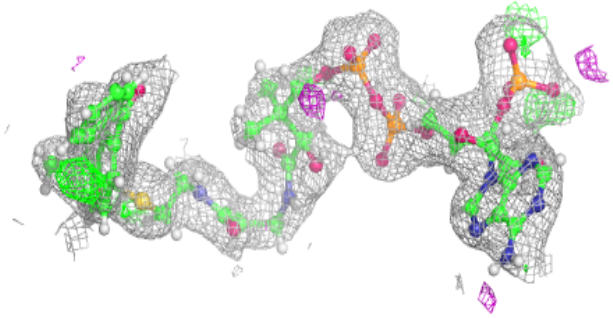


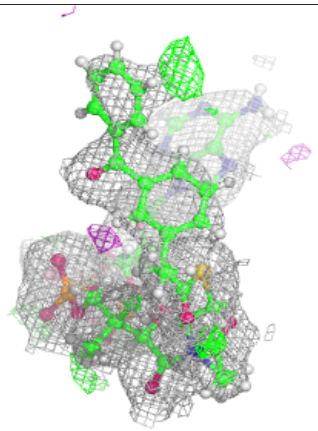


Electron density around A1IZD B 401:

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

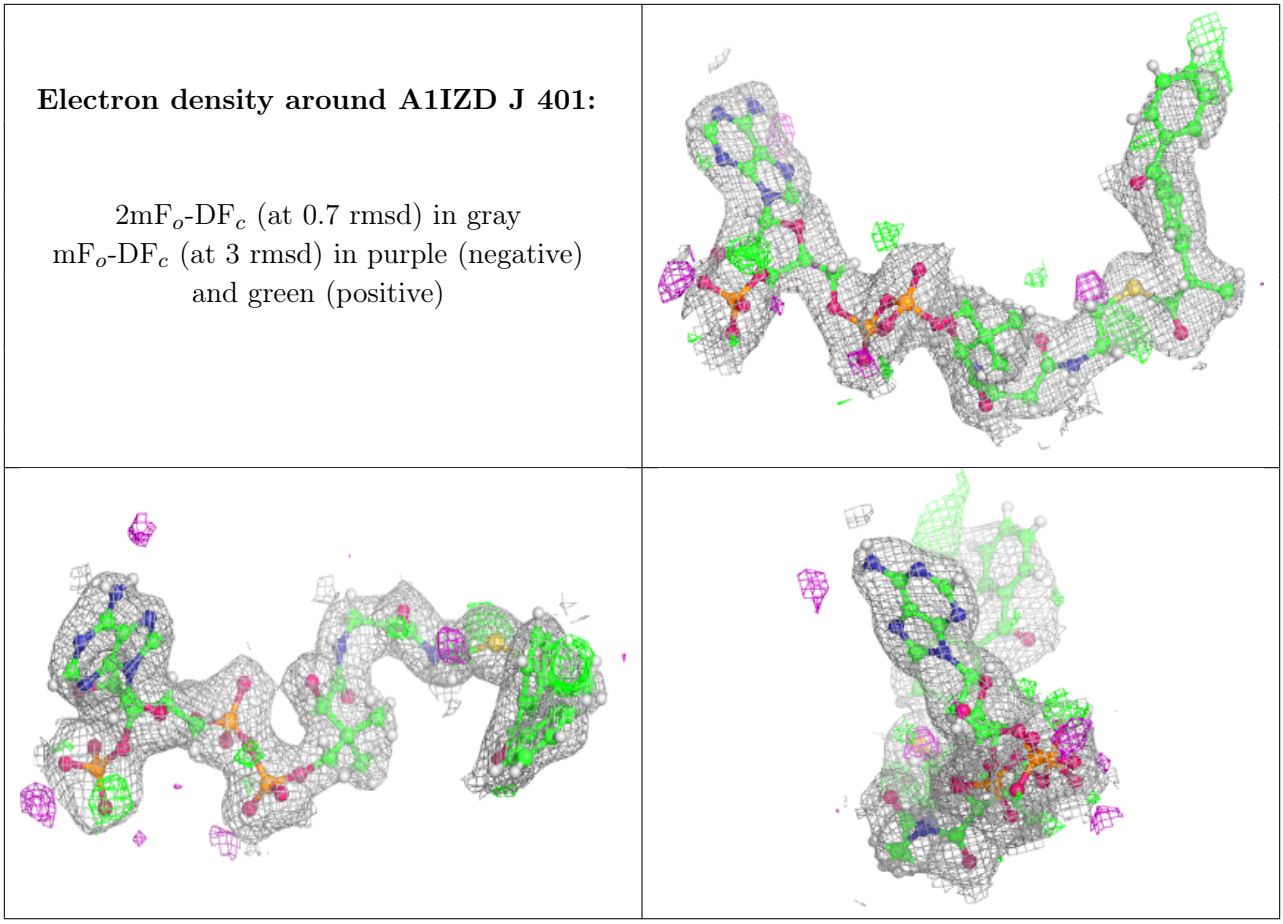






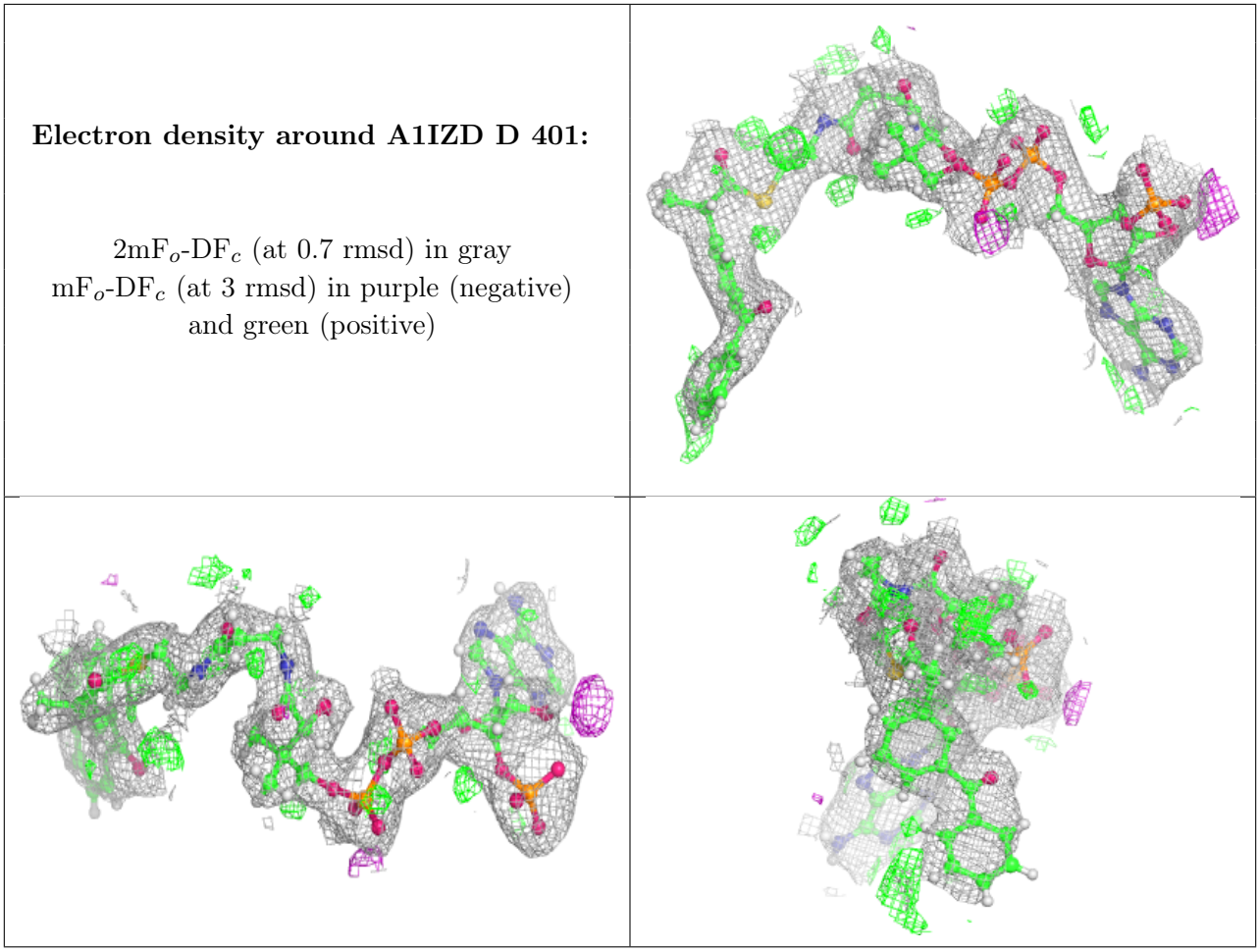
Electron density around A1IZD J 401:

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



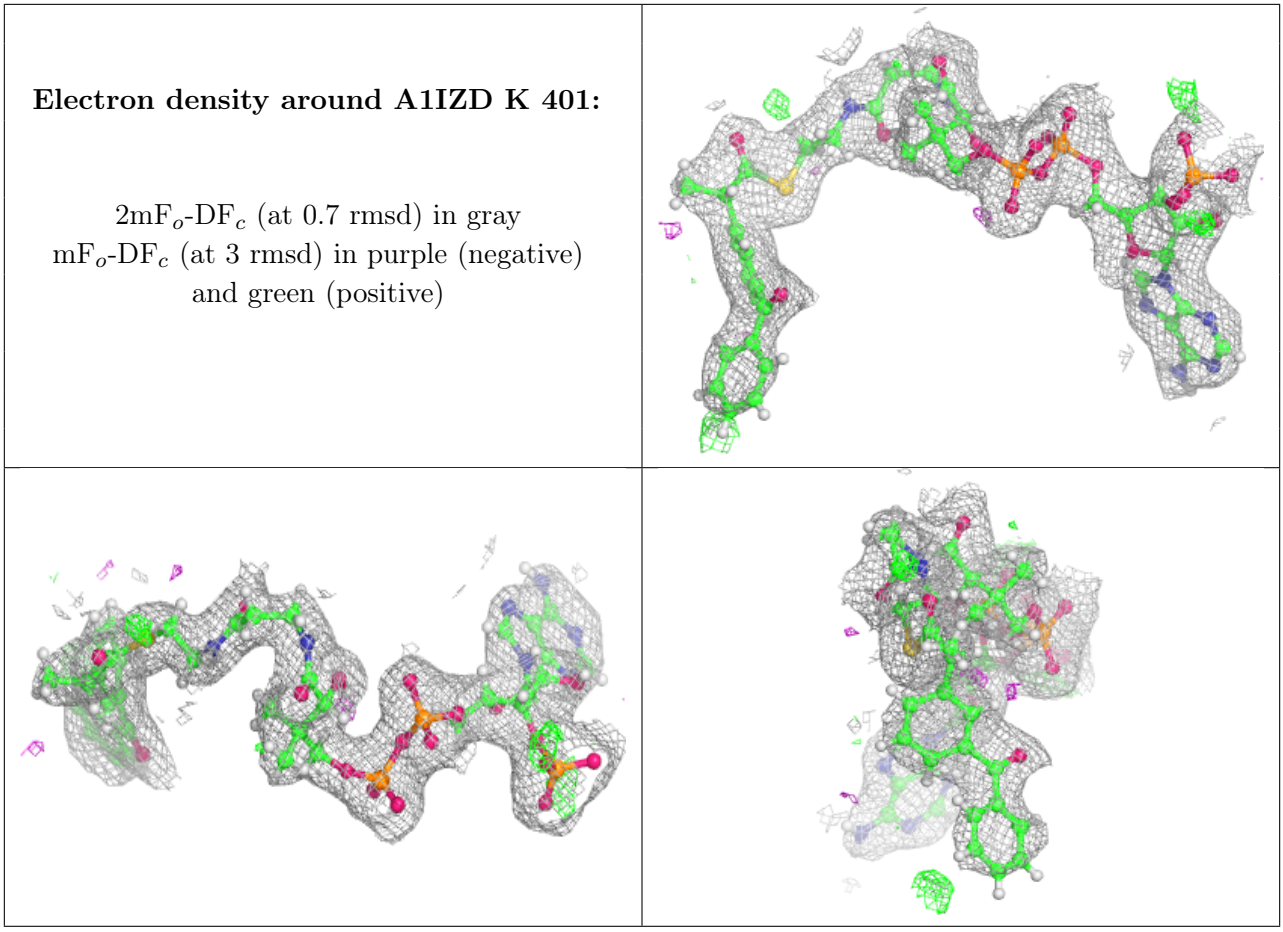
Electron density around A1IZD D 401:

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



Electron density around A1IZD 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.