



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2023 – 02:33 AM EST

PDB ID : 8G9V
Title : Crystal structures of 17-beta-hydroxysteroid dehydrogenase 13
Deposited on : 2023-02-22
Resolution : 2.65 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

<https://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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

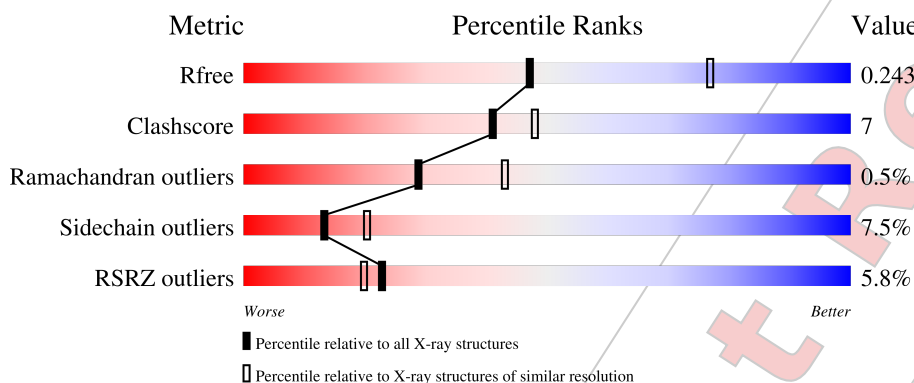
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	315	5% 72% 16% 10%
1	B	315	2% 75% 14% 10%
1	C	315	4% 70% 13% 15%
1	D	315	7% 75% 12% 11%

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Validation Pipeline (wwPDB-VP) : 2.32.1

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Mol	Chain	Length	Quality of chain
1	E	315	
1	F	315	
1	G	315	
1	H	315	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	C	404	-	-	X	-
5	SO4	C	407	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18399 atoms, of which 268 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 17-beta-hydroxysteroid dehydrogenase 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2224	1430	383	401	10			
1	B	283	Total	C	N	O	S	0	0	0
			2215	1424	381	400	10			
1	C	267	Total	C	N	O	S	0	0	0
			2078	1344	354	371	9			
1	D	280	Total	C	N	O	S	0	0	0
			2157	1381	377	389	10			
1	E	293	Total	C	N	O	S	0	0	0
			2308	1488	397	413	10			
1	F	262	Total	C	N	O	S	0	0	0
			2049	1323	347	370	9			
1	G	262	Total	C	N	O	S	0	0	0
			2029	1309	344	367	9			
1	H	289	Total	C	N	O	S	0	0	0
			2271	1463	390	408	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q7Z5P4
A	1	GLY	-	cloning artifact	UNP Q7Z5P4
A	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
A	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
A	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
A	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
A	301	GLY	-	expression tag	UNP Q7Z5P4
A	302	SER	-	expression tag	UNP Q7Z5P4
A	303	GLY	-	expression tag	UNP Q7Z5P4
A	304	HIS	-	expression tag	UNP Q7Z5P4
A	305	HIS	-	expression tag	UNP Q7Z5P4
A	306	HIS	-	expression tag	UNP Q7Z5P4
A	307	HIS	-	expression tag	UNP Q7Z5P4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	308	HIS	-	expression tag	UNP Q7Z5P4
A	309	HIS	-	expression tag	UNP Q7Z5P4
A	310	HIS	-	expression tag	UNP Q7Z5P4
A	311	HIS	-	expression tag	UNP Q7Z5P4
A	312	HIS	-	expression tag	UNP Q7Z5P4
A	313	HIS	-	expression tag	UNP Q7Z5P4
A	314	HIS	-	expression tag	UNP Q7Z5P4
B	0	MET	-	initiating methionine	UNP Q7Z5P4
B	1	GLY	-	cloning artifact	UNP Q7Z5P4
B	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
B	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
B	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
B	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
B	301	GLY	-	expression tag	UNP Q7Z5P4
B	302	SER	-	expression tag	UNP Q7Z5P4
B	303	GLY	-	expression tag	UNP Q7Z5P4
B	304	HIS	-	expression tag	UNP Q7Z5P4
B	305	HIS	-	expression tag	UNP Q7Z5P4
B	306	HIS	-	expression tag	UNP Q7Z5P4
B	307	HIS	-	expression tag	UNP Q7Z5P4
B	308	HIS	-	expression tag	UNP Q7Z5P4
B	309	HIS	-	expression tag	UNP Q7Z5P4
B	310	HIS	-	expression tag	UNP Q7Z5P4
B	311	HIS	-	expression tag	UNP Q7Z5P4
B	312	HIS	-	expression tag	UNP Q7Z5P4
B	313	HIS	-	expression tag	UNP Q7Z5P4
B	314	HIS	-	expression tag	UNP Q7Z5P4
C	0	MET	-	initiating methionine	UNP Q7Z5P4
C	1	GLY	-	cloning artifact	UNP Q7Z5P4
C	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
C	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
C	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
C	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
C	301	GLY	-	expression tag	UNP Q7Z5P4
C	302	SER	-	expression tag	UNP Q7Z5P4
C	303	GLY	-	expression tag	UNP Q7Z5P4
C	304	HIS	-	expression tag	UNP Q7Z5P4
C	305	HIS	-	expression tag	UNP Q7Z5P4
C	306	HIS	-	expression tag	UNP Q7Z5P4
C	307	HIS	-	expression tag	UNP Q7Z5P4
C	308	HIS	-	expression tag	UNP Q7Z5P4
C	309	HIS	-	expression tag	UNP Q7Z5P4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	310	HIS	-	expression tag	UNP Q7Z5P4
C	311	HIS	-	expression tag	UNP Q7Z5P4
C	312	HIS	-	expression tag	UNP Q7Z5P4
C	313	HIS	-	expression tag	UNP Q7Z5P4
C	314	HIS	-	expression tag	UNP Q7Z5P4
D	0	MET	-	initiating methionine	UNP Q7Z5P4
D	1	GLY	-	cloning artifact	UNP Q7Z5P4
D	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
D	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
D	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
D	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
D	301	GLY	-	expression tag	UNP Q7Z5P4
D	302	SER	-	expression tag	UNP Q7Z5P4
D	303	GLY	-	expression tag	UNP Q7Z5P4
D	304	HIS	-	expression tag	UNP Q7Z5P4
D	305	HIS	-	expression tag	UNP Q7Z5P4
D	306	HIS	-	expression tag	UNP Q7Z5P4
D	307	HIS	-	expression tag	UNP Q7Z5P4
D	308	HIS	-	expression tag	UNP Q7Z5P4
D	309	HIS	-	expression tag	UNP Q7Z5P4
D	310	HIS	-	expression tag	UNP Q7Z5P4
D	311	HIS	-	expression tag	UNP Q7Z5P4
D	312	HIS	-	expression tag	UNP Q7Z5P4
D	313	HIS	-	expression tag	UNP Q7Z5P4
D	314	HIS	-	expression tag	UNP Q7Z5P4
E	0	MET	-	initiating methionine	UNP Q7Z5P4
E	1	GLY	-	cloning artifact	UNP Q7Z5P4
E	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
E	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
E	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
E	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
E	301	GLY	-	expression tag	UNP Q7Z5P4
E	302	SER	-	expression tag	UNP Q7Z5P4
E	303	GLY	-	expression tag	UNP Q7Z5P4
E	304	HIS	-	expression tag	UNP Q7Z5P4
E	305	HIS	-	expression tag	UNP Q7Z5P4
E	306	HIS	-	expression tag	UNP Q7Z5P4
E	307	HIS	-	expression tag	UNP Q7Z5P4
E	308	HIS	-	expression tag	UNP Q7Z5P4
E	309	HIS	-	expression tag	UNP Q7Z5P4
E	310	HIS	-	expression tag	UNP Q7Z5P4
E	311	HIS	-	expression tag	UNP Q7Z5P4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	312	HIS	-	expression tag	UNP Q7Z5P4
E	313	HIS	-	expression tag	UNP Q7Z5P4
E	314	HIS	-	expression tag	UNP Q7Z5P4
F	0	MET	-	initiating methionine	UNP Q7Z5P4
F	1	GLY	-	cloning artifact	UNP Q7Z5P4
F	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
F	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
F	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
F	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
F	301	GLY	-	expression tag	UNP Q7Z5P4
F	302	SER	-	expression tag	UNP Q7Z5P4
F	303	GLY	-	expression tag	UNP Q7Z5P4
F	304	HIS	-	expression tag	UNP Q7Z5P4
F	305	HIS	-	expression tag	UNP Q7Z5P4
F	306	HIS	-	expression tag	UNP Q7Z5P4
F	307	HIS	-	expression tag	UNP Q7Z5P4
F	308	HIS	-	expression tag	UNP Q7Z5P4
F	309	HIS	-	expression tag	UNP Q7Z5P4
F	310	HIS	-	expression tag	UNP Q7Z5P4
F	311	HIS	-	expression tag	UNP Q7Z5P4
F	312	HIS	-	expression tag	UNP Q7Z5P4
F	313	HIS	-	expression tag	UNP Q7Z5P4
F	314	HIS	-	expression tag	UNP Q7Z5P4
G	0	MET	-	initiating methionine	UNP Q7Z5P4
G	1	GLY	-	cloning artifact	UNP Q7Z5P4
G	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
G	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
G	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
G	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
G	302	GLY	-	expression tag	UNP Q7Z5P4
G	303	SER	-	expression tag	UNP Q7Z5P4
G	304	GLY	-	expression tag	UNP Q7Z5P4
G	305	HIS	-	expression tag	UNP Q7Z5P4
G	306	HIS	-	expression tag	UNP Q7Z5P4
G	307	HIS	-	expression tag	UNP Q7Z5P4
G	308	HIS	-	expression tag	UNP Q7Z5P4
G	309	HIS	-	expression tag	UNP Q7Z5P4
G	310	HIS	-	expression tag	UNP Q7Z5P4
G	311	HIS	-	expression tag	UNP Q7Z5P4
G	312	HIS	-	expression tag	UNP Q7Z5P4
G	313	HIS	-	expression tag	UNP Q7Z5P4
G	314	HIS	-	expression tag	UNP Q7Z5P4

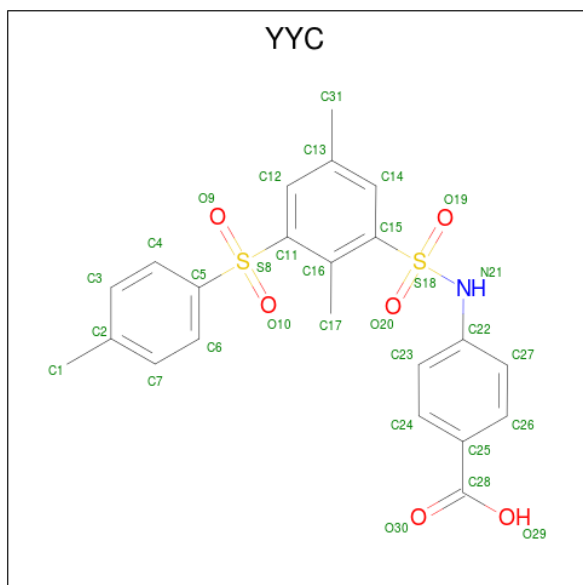
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Chain	Residue	Modelled	Actual	Comment	Reference
G	315	HIS	-	expression tag	UNP Q7Z5P4
H	0	MET	-	initiating methionine	UNP Q7Z5P4
H	1	GLY	-	cloning artifact	UNP Q7Z5P4
H	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
H	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
H	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
H	161	LYS	GLU	engineered mutation	UNP Q7Z5P4
H	301	GLY	-	expression tag	UNP Q7Z5P4
H	302	SER	-	expression tag	UNP Q7Z5P4
H	303	GLY	-	expression tag	UNP Q7Z5P4
H	304	HIS	-	expression tag	UNP Q7Z5P4
H	305	HIS	-	expression tag	UNP Q7Z5P4
H	306	HIS	-	expression tag	UNP Q7Z5P4
H	307	HIS	-	expression tag	UNP Q7Z5P4
H	308	HIS	-	expression tag	UNP Q7Z5P4
H	309	HIS	-	expression tag	UNP Q7Z5P4
H	310	HIS	-	expression tag	UNP Q7Z5P4
H	311	HIS	-	expression tag	UNP Q7Z5P4
H	312	HIS	-	expression tag	UNP Q7Z5P4
H	313	HIS	-	expression tag	UNP Q7Z5P4
H	314	HIS	-	expression tag	UNP Q7Z5P4

- # NAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-{[2,5-dimethyl-3-(4-methylbenzene-1-sulfonyl)benzene-1-sulfonyl]amino}benzoic acid (three-letter code: YYC) (formula: C₂₂H₂₁NO₆S₂) (labeled as "Ligand of Interest" by depositor).



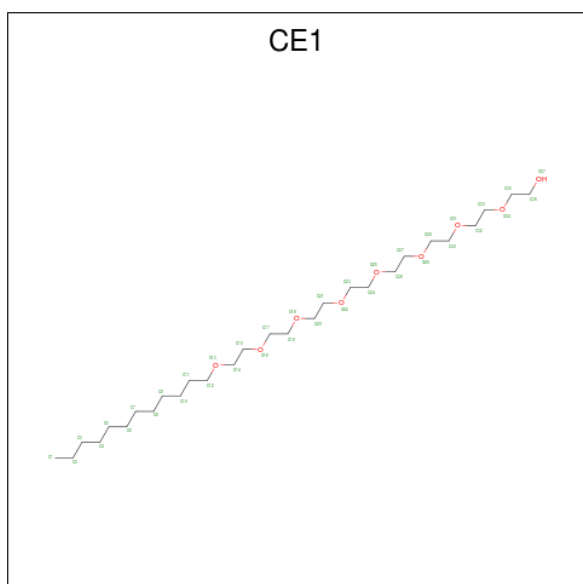
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	20	0
			51	22	20	1	6	2		
3	B	1	Total	C	H	N	O	S	21	0
			52	22	21	1	6	2		
3	C	1	Total	C	H	N	O	S	21	0
			52	22	21	1	6	2		

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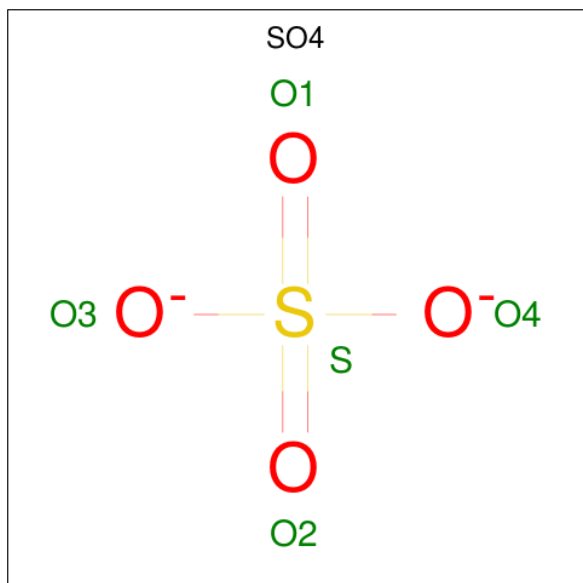
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	20	0
			51	22	20	1	6		
3	E	1	Total	C	H	N	O	21	0
			52	22	21	1	6		
3	F	1	Total	C	H	N	O	20	0
			51	22	20	1	6		
3	G	1	Total	C	H	N	O	21	0
			52	22	21	1	6		
3	H	1	Total	C	H	N	O	21	0
			52	22	21	1	6		

- Molecule 4 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	58	0
			95	28	58	9		
4	C	1	Total	C			0	0
			12	12				
4	D	1	Total	C	H	O	45	0
			76	22	45	9		
4	E	1	Total	C			0	0
			12	12				

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

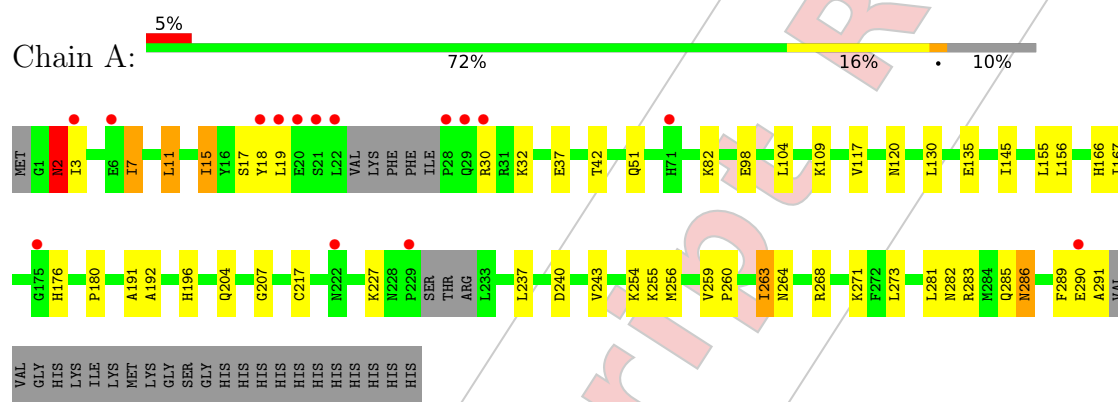
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	5	Total	O	0	0
			5	5		
6	C	3	Total	O	0	0
			3	3		
6	D	4	Total	O	0	0
			4	4		
6	E	2	Total	O	0	0
			2	2		
6	F	4	Total	O	0	0
			4	4		
6	H	1	Total	O	0	0
			1	1		

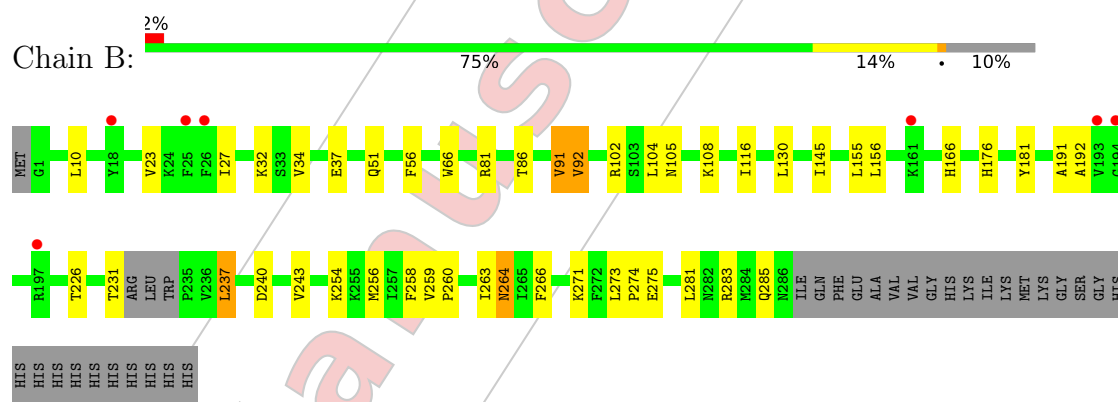
3 Residue-property plots [i](#)

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.

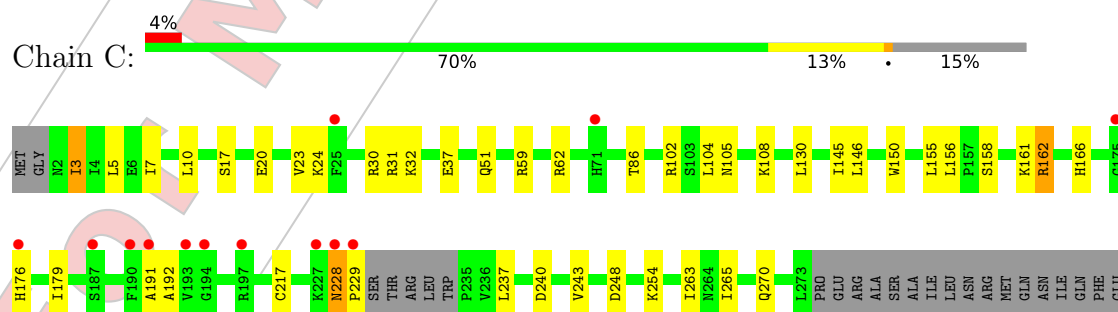
• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



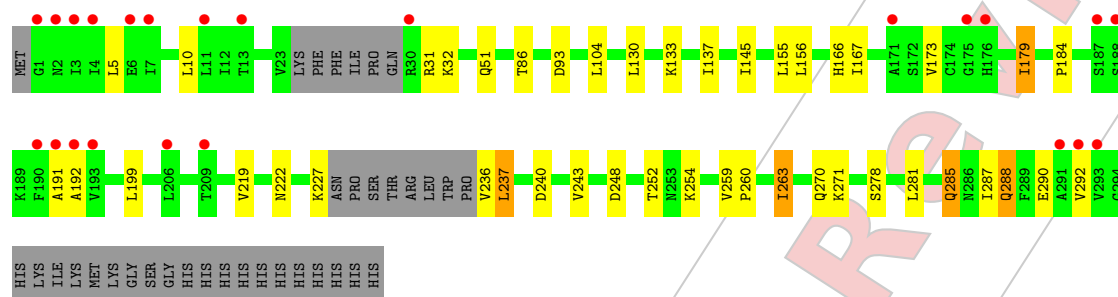
• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



ALA
VAL
VAL
GLY
HIS
LYS
LYS
MET
LYS
GLY
SER
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS

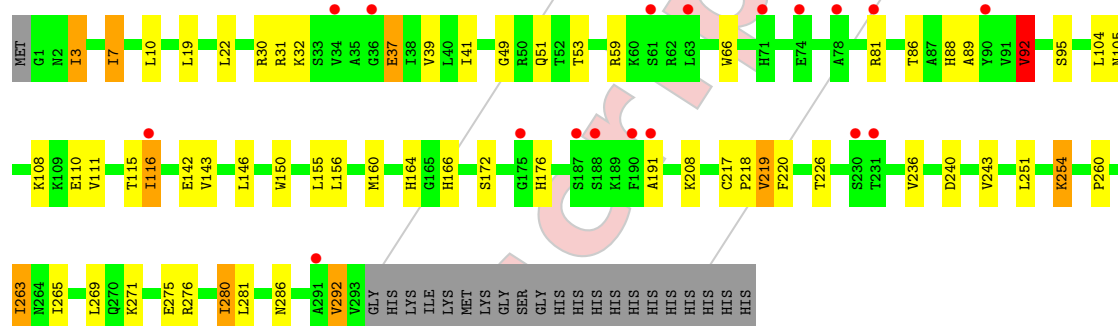
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain D: 7% 75% 12% 11%



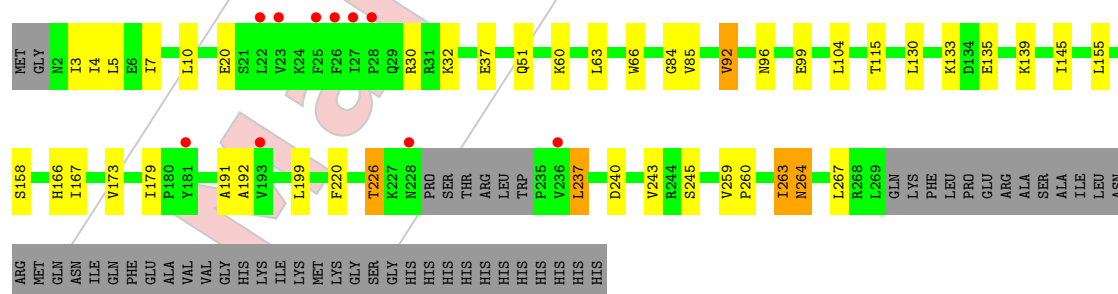
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain E: 6% 73% 17% 7%



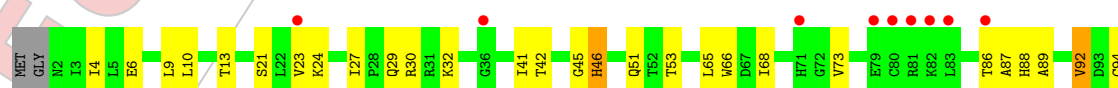
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain F: 3% 69% 13% 17%



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain G: 6% 62% 19% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 161.56Å 100.77Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	37.91 – 2.65 37.91 – 2.65	Depositor EDS
% Data completeness (in resolution range)	76.1 (37.91-2.65) 76.1 (37.91-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.212 , 0.244 0.209 , 0.243	Depositor DCC
R_{free} test set	3399 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18399	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YYC, SO4, CE1, NAD

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	0.43	0/2265	0.61	0/3065
1	B	0.43	0/2256	0.61	0/3054
1	C	0.42	0/2118	0.60	0/2870
1	D	0.43	0/2191	0.58	0/2963
1	E	0.42	0/2353	0.63	0/3188
1	F	0.41	0/2087	0.58	0/2826
1	G	0.43	0/2065	0.61	0/2797
1	H	0.41	0/2316	0.62	0/3141
All	All	0.42	0/17651	0.60	0/23904

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2298	34	0
1	B	2215	0	2291	38	0
1	C	2078	0	2138	28	0
1	D	2157	0	2210	24	0
1	E	2308	0	2393	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2049	0	2120	27	0
1	G	2029	0	2087	45	0
1	H	2271	0	2326	36	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	2	0
3	A	31	20	0	0	0
3	B	31	21	0	0	0
3	C	31	21	0	0	0
3	D	31	20	0	0	0
3	E	31	21	0	0	0
3	F	31	20	0	0	0
3	G	31	21	0	0	0
3	H	31	21	0	0	0
4	A	37	58	58	2	0
4	C	12	0	23	2	0
4	D	31	45	43	4	0
4	E	12	0	23	3	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	20	0	0	4	0
5	E	5	0	0	1	0
5	F	15	0	0	0	0
5	G	10	0	0	1	0
5	H	15	0	0	1	0
6	A	4	0	0	0	0
6	B	5	0	0	0	0
6	C	3	0	0	0	0
6	D	4	0	0	0	0
6	E	2	0	0	0	0
6	F	4	0	0	0	0
6	H	1	0	0	0	0
All	All	18131	268	18218	257	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 7.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:SER:HA	1:G:24:LYS:HE3	1.37	1.06
1:G:142:GLU:HA	1:G:146:LEU:HB2	1.51	0.92
1:E:39:VAL:HG22	1:E:116:ILE:HG23	1.56	0.87
1:E:220:PHE:HB3	1:E:236:VAL:HG23	1.57	0.85
1:A:281:LEU:HD22	4:A:403:CE1:H261	1.61	0.82
1:D:179:ILE:HD11	4:D:403:CE1:H242	1.62	0.81
1:C:32:LYS:HZ1	1:C:166:HIS:HD2	1.29	0.79
1:E:66:TRP:CE3	1:E:92:VAL:HG11	2.18	0.79
1:H:167:ILE:HD13	1:H:199:LEU:HD21	1.66	0.78
1:E:39:VAL:HG22	1:E:116:ILE:CG2	2.16	0.76
1:G:41:ILE:HD13	1:G:53:THR:HG22	1.67	0.76
1:H:223:THR:HG21	2:H:401:NAD:O2N	1.85	0.75
1:E:41:ILE:HD13	1:E:53:THR:HG22	1.67	0.74
1:F:32:LYS:HZ1	1:F:166:HIS:HD2	1.34	0.74
1:G:94:CYS:HA	1:G:100:ILE:HD11	1.69	0.74
1:E:31:ARG:HH12	1:E:59:ARG:HH21	1.32	0.74
1:E:66:TRP:CD2	1:E:92:VAL:HG11	2.22	0.74
1:B:51:GLN:HB2	1:B:243:VAL:HG21	1.70	0.74
1:C:51:GLN:HB2	1:C:243:VAL:HG21	1.69	0.74
1:H:66:TRP:CE3	1:H:92:VAL:HG11	2.23	0.73
1:G:32:LYS:NZ	1:G:166:HIS:HD2	1.86	0.73
1:C:30:ARG:NH2	1:E:286:ASN:HD22	1.85	0.73
1:G:21:SER:HA	1:G:24:LYS:CE	2.16	0.73
1:C:23:VAL:HG21	4:C:403:CE1:H21	1.70	0.72
1:E:104:LEU:HD22	1:E:155:LEU:HD21	1.72	0.72
1:F:167:ILE:HD13	1:F:199:LEU:HD21	1.71	0.72
1:A:32:LYS:HZ1	1:A:166:HIS:HD2	1.38	0.71
1:H:51:GLN:HB2	1:H:243:VAL:HG21	1.73	0.71
1:H:29:GLN:HG2	1:H:252:THR:HB	1.73	0.71
1:D:51:GLN:HB2	1:D:243:VAL:HG21	1.74	0.70
1:A:51:GLN:HB2	1:A:243:VAL:HG21	1.72	0.70
1:E:51:GLN:HB2	1:E:243:VAL:HG21	1.74	0.70
1:C:32:LYS:NZ	1:C:166:HIS:HD2	1.90	0.69
1:B:32:LYS:NZ	1:B:166:HIS:HD2	1.90	0.69
1:F:32:LYS:NZ	1:F:166:HIS:HD2	1.89	0.69
1:C:59:ARG:NH1	5:C:404:SO4:O3	2.25	0.69
1:H:222:ASN:HB2	1:H:236:VAL:HG12	1.75	0.69
1:D:167:ILE:HD13	1:D:199:LEU:HD21	1.73	0.69
1:C:104:LEU:HD22	1:C:155:LEU:HD21	1.74	0.69
1:F:51:GLN:HB2	1:F:243:VAL:HG21	1.74	0.69
1:E:49:GLY:O	1:E:53:THR:HG23	1.93	0.68
1:E:260:PRO:HD2	1:E:263:ILE:CD1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:NZ	1:A:166:HIS:HD2	1.92	0.68
1:G:32:LYS:HZ1	1:G:166:HIS:HD2	1.37	0.68
1:D:137:ILE:HD12	1:D:184:PRO:CG	2.22	0.68
1:H:237:LEU:HD21	1:H:259:VAL:HG12	1.76	0.67
1:D:32:LYS:NZ	1:D:166:HIS:HD2	1.91	0.67
1:A:255:LYS:HD2	1:B:275:GLU:HB3	1.77	0.66
1:E:176:HIS:HE1	1:E:217:CYS:SG	2.20	0.65
1:C:17:SER:HB3	1:C:265:ILE:HD12	1.78	0.65
1:B:260:PRO:O	1:B:263:ILE:HG12	1.97	0.65
1:H:66:TRP:CD2	1:H:92:VAL:HG11	2.33	0.64
1:D:137:ILE:HD12	1:D:184:PRO:HG2	1.79	0.64
1:A:176:HIS:HE1	1:A:217:CYS:SG	2.21	0.64
1:D:32:LYS:HZ1	1:D:166:HIS:HD2	1.43	0.64
1:E:88:HIS:CD2	1:E:111:VAL:HG22	2.32	0.64
1:H:159:MET:HG2	1:H:165:GLY:HA3	1.79	0.63
1:H:114:VAL:HG13	1:H:155:LEU:HD22	1.81	0.63
1:G:66:TRP:CE2	1:G:92:VAL:HG11	2.34	0.63
1:E:105:ASN:HA	1:E:108:LYS:HD2	1.80	0.63
1:G:216:LEU:HD22	1:G:247:LEU:HD22	1.81	0.62
1:A:109:LYS:NZ	1:G:109:LYS:HE2	2.15	0.62
1:A:207:GLY:HA3	1:C:62:ARG:HH12	1.65	0.62
1:E:146:LEU:HB3	1:E:150:TRP:CH2	2.35	0.62
1:E:260:PRO:HD2	1:E:263:ILE:HD13	1.82	0.61
1:D:281:LEU:HD22	4:D:403:CE1:H261	1.82	0.61
1:F:104:LEU:HD22	1:F:155:LEU:HD21	1.81	0.61
1:B:104:LEU:HD22	1:B:155:LEU:HD21	1.82	0.61
1:D:104:LEU:HD22	1:D:155:LEU:HD21	1.81	0.61
1:G:104:LEU:HD22	1:G:155:LEU:HD21	1.81	0.61
1:B:32:LYS:HZ1	1:B:166:HIS:HD2	1.46	0.61
1:G:88:HIS:CD2	1:G:111:VAL:HG22	2.36	0.60
1:G:51:GLN:HB2	1:G:244:VAL:HG21	1.82	0.60
1:F:66:TRP:CE2	1:F:92:VAL:HG11	2.36	0.60
1:B:105:ASN:HA	1:B:108:LYS:HD2	1.82	0.59
1:B:91:VAL:HG22	1:F:60:LYS:HG2	1.83	0.59
1:A:196:HIS:CD2	1:A:256:MET:HE1	2.38	0.59
1:F:96:ASN:HB3	1:F:99:GLU:HB2	1.86	0.58
1:H:146:LEU:HB3	1:H:150:TRP:CH2	2.39	0.58
1:B:66:TRP:CE2	1:B:92:VAL:HG11	2.37	0.58
1:G:243:VAL:HG22	1:G:260:VAL:HG11	1.85	0.57
1:F:66:TRP:CD2	1:F:92:VAL:HG11	2.40	0.57
1:H:39:VAL:HG12	1:H:116:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LEU:HB3	1:H:268:ARG:HE	1.69	0.57
1:A:104:LEU:HD22	1:A:155:LEU:HD21	1.86	0.57
1:C:105:ASN:HA	1:C:108:LYS:HD2	1.86	0.57
1:E:156:LEU:HB3	1:F:130:LEU:HD21	1.87	0.57
1:C:176:HIS:HE1	1:C:217:CYS:SG	2.28	0.56
1:G:130:LEU:HD21	1:H:156:LEU:HB3	1.87	0.56
1:E:191:ALA:HB2	1:F:191:ALA:HB2	1.86	0.56
1:G:66:TRP:CD2	1:G:92:VAL:HG11	2.40	0.56
1:D:237:LEU:HD21	1:D:259:VAL:HG12	1.88	0.56
1:H:3:ILE:O	1:H:7:ILE:HG12	2.06	0.56
1:C:32:LYS:HZ1	1:C:166:HIS:CD2	2.19	0.56
1:H:57:ALA:HB2	1:H:63:LEU:HD21	1.88	0.55
1:G:146:LEU:HB3	1:G:150:TRP:CH2	2.42	0.55
1:E:32:LYS:NZ	1:E:166:HIS:HD2	2.05	0.54
1:A:282:ASN:O	1:A:286:ASN:OD1	2.25	0.54
1:G:96:ASN:HB3	1:G:99:GLU:HB3	1.90	0.54
1:G:145:ILE:HD13	1:G:149:PHE:CE2	2.43	0.54
1:C:32:LYS:NZ	1:C:166:HIS:CD2	2.75	0.54
1:H:222:ASN:HB2	1:H:236:VAL:CG1	2.37	0.54
1:E:37:GLU:HG2	1:E:116:ILE:HG22	1.89	0.53
1:C:146:LEU:HB3	1:C:150:TRP:CH2	2.43	0.53
1:H:173:VAL:CG1	1:H:263:ILE:HD13	2.39	0.53
1:G:42:THR:O	1:G:120:ASN:HB3	2.09	0.52
1:B:237:LEU:HD21	1:B:259:VAL:HG12	1.90	0.52
1:E:142:GLU:HA	1:E:146:LEU:HB2	1.90	0.52
1:G:261:PRO:HD2	1:G:264:ILE:HD13	1.90	0.52
1:C:30:ARG:HH22	1:E:286:ASN:HD22	1.55	0.52
1:B:23:VAL:HG23	1:B:27:ILE:HD13	1.92	0.52
1:H:114:VAL:HG21	1:H:155:LEU:HD13	1.91	0.52
1:C:130:LEU:HD21	1:D:156:LEU:HB3	1.92	0.52
1:H:104:LEU:HD22	1:H:155:LEU:HD21	1.92	0.52
1:A:196:HIS:HD2	1:A:256:MET:HE1	1.74	0.51
1:A:130:LEU:HD21	1:B:156:LEU:HB3	1.93	0.51
1:F:220:PHE:CE1	1:F:226:THR:HG23	2.45	0.51
1:H:41:ILE:HG12	1:H:118:VAL:HG13	1.91	0.51
1:B:34:VAL:HG21	1:B:56:PHE:HE1	1.75	0.51
1:H:197:ARG:NH2	5:H:405:SO4:O4	2.43	0.51
1:E:31:ARG:HG3	1:E:251:LEU:HD13	1.92	0.51
1:G:249:ASP:O	1:G:253:THR:HB	2.10	0.51
1:A:11:LEU:O	1:A:15:ILE:HG12	2.10	0.51
1:F:237:LEU:HD21	1:F:259:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LYS:NZ	1:D:166:HIS:CD2	2.77	0.51
1:G:95:SER:HB2	1:G:142:GLU:HG3	1.93	0.51
1:E:3:ILE:O	1:E:7:ILE:HG23	2.11	0.50
1:G:127:ALA:HB3	1:G:132:THR:HG22	1.93	0.50
1:D:137:ILE:CD1	1:D:184:PRO:HG2	2.40	0.50
1:E:32:LYS:HZ1	1:E:166:HIS:HD2	1.59	0.50
1:H:114:VAL:CG2	1:H:155:LEU:HD13	2.41	0.50
1:C:20:GLU:HG3	4:C:403:CE1:H12	1.94	0.50
1:B:37:GLU:HG2	1:B:116:ILE:HD11	1.94	0.50
1:B:263:ILE:HA	1:B:266:PHE:HD2	1.77	0.50
1:F:32:LYS:NZ	1:F:166:HIS:CD2	2.76	0.50
1:B:145:ILE:HD13	1:B:192:ALA:HA	1.92	0.50
1:D:270:GLN:HG3	4:D:403:CE1:H182	1.93	0.50
1:B:66:TRP:CD2	1:B:92:VAL:HG11	2.47	0.49
1:F:63:LEU:HD12	1:F:85:VAL:HG11	1.92	0.49
1:B:32:LYS:NZ	1:B:166:HIS:CD2	2.76	0.49
1:C:59:ARG:NH1	5:C:404:SO4:S	2.80	0.49
1:H:265:ILE:HG13	1:H:269:LEU:HD12	1.94	0.49
1:E:172:SER:HA	1:E:218:PRO:HD2	1.94	0.49
1:G:45:GLY:O	1:G:46:HIS:HB2	2.11	0.49
1:G:96:ASN:O	1:G:100:ILE:HG12	2.11	0.49
1:A:196:HIS:CD2	1:A:256:MET:CE	2.95	0.48
1:B:34:VAL:HG23	1:B:116:ILE:CD1	2.43	0.48
1:E:292:VAL:O	1:E:292:VAL:HG13	2.13	0.48
1:B:181:TYR:HB2	1:C:161:LYS:HG2	1.96	0.48
1:H:262:TYR:O	1:H:265:ILE:HG22	2.14	0.48
1:D:222:ASN:HB2	1:D:236:VAL:CG2	2.44	0.47
1:B:23:VAL:HG23	1:B:27:ILE:CD1	2.44	0.47
1:G:32:LYS:NZ	1:G:166:HIS:CD2	2.76	0.47
1:A:204:GLN:HE21	1:B:283:ARG:HH21	1.62	0.47
1:C:145:ILE:HD13	1:C:192:ALA:HA	1.95	0.47
1:F:66:TRP:CG	1:F:92:VAL:HG13	2.50	0.47
1:H:145:ILE:HD13	1:H:192:ALA:HA	1.97	0.47
1:A:7:ILE:O	1:A:11:LEU:HB2	2.14	0.47
1:A:32:LYS:NZ	1:A:166:HIS:CD2	2.77	0.47
1:A:273:LEU:HD13	4:A:403:CE1:H142	1.96	0.47
1:E:276:ARG:O	1:E:280:ILE:HG23	2.15	0.47
1:A:145:ILE:HD13	1:A:192:ALA:HA	1.97	0.47
1:B:66:TRP:CG	1:B:92:VAL:HG13	2.50	0.47
1:C:31:ARG:HH22	1:C:248:ASP:CG	2.18	0.47
1:H:159:MET:CG	1:H:165:GLY:HA3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:GLN:OE1	4:D:403:CE1:H292	2.15	0.47
1:F:264:ASN:HD22	1:F:264:ASN:H	1.61	0.47
1:G:66:TRP:CG	1:G:92:VAL:HG13	2.50	0.47
1:H:2:ASN:O	1:H:6:GLU:HG2	2.15	0.47
1:C:20:GLU:HG2	1:C:24:LYS:HE2	1.97	0.47
1:G:65:LEU:O	1:G:66:TRP:HD1	1.98	0.46
1:G:66:TRP:CD2	1:G:92:VAL:CG1	2.99	0.46
1:E:265:ILE:HG12	1:E:269:LEU:HD12	1.97	0.46
1:E:280:ILE:HD11	4:E:601:CE1:H111	1.97	0.46
1:F:66:TRP:CD2	1:F:92:VAL:CG1	2.98	0.46
1:E:37:GLU:OE2	1:E:164:HIS:HE1	1.98	0.46
1:F:220:PHE:HE1	1:F:226:THR:HG23	1.80	0.46
1:B:37:GLU:HG2	1:B:116:ILE:CD1	2.46	0.46
1:C:20:GLU:O	1:C:24:LYS:HG2	2.16	0.46
1:G:145:ILE:HD13	1:G:149:PHE:HE2	1.81	0.46
1:A:237:LEU:HD21	1:A:259:VAL:HG12	1.98	0.45
1:C:162:ARG:NH1	5:C:407:SO4:O3	2.50	0.45
1:D:145:ILE:HD13	1:D:192:ALA:HA	1.98	0.45
1:G:65:LEU:HD11	1:G:87:ALA:HB1	1.98	0.45
1:H:263:ILE:HG22	1:H:267:LEU:HD22	1.98	0.45
1:A:191:ALA:HB2	1:B:191:ALA:HB2	1.99	0.45
1:A:15:ILE:HG21	1:B:274:PRO:HG2	1.99	0.45
1:A:109:LYS:NZ	1:G:109:LYS:CE	2.80	0.45
1:E:280:ILE:HD11	4:E:601:CE1:H91	1.99	0.45
1:F:264:ASN:HA	1:F:267:LEU:HD12	1.99	0.45
1:E:39:VAL:HG13	1:E:116:ILE:HG12	1.99	0.44
1:F:66:TRP:CG	1:F:92:VAL:CG1	3.00	0.44
1:B:176:HIS:CE1	1:B:256:MET:CE	3.01	0.44
1:E:37:GLU:OE2	1:E:164:HIS:CE1	2.70	0.44
1:A:2:ASN:HD22	1:A:3:ILE:H	1.66	0.44
1:E:254:LYS:NZ	5:E:604:SO4:O2	2.37	0.44
1:H:34:VAL:HG11	1:H:56:PHE:CE1	2.53	0.44
1:B:23:VAL:HA	1:B:27:ILE:HD12	1.99	0.44
1:A:156:LEU:HB3	1:B:130:LEU:HD21	2.00	0.43
1:A:180:PRO:HG2	1:A:285:GLN:NE2	2.33	0.43
1:C:228:ASN:H	1:C:229:PRO:CD	2.31	0.43
1:A:260:PRO:HD2	1:A:263:ILE:CG2	2.48	0.43
1:H:96:ASN:HB3	1:H:99:GLU:HB3	1.99	0.43
1:B:176:HIS:CE1	1:B:256:MET:HE1	2.54	0.43
1:C:156:LEU:HB3	1:D:130:LEU:HD11	2.00	0.43
1:G:152:THR:O	1:G:156:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:THR:HG21	1:G:65:LEU:HD23	1.99	0.43
1:B:176:HIS:HE1	1:B:256:MET:CE	2.32	0.43
1:H:145:ILE:HG23	1:H:146:LEU:HD13	1.99	0.43
1:A:117:VAL:CG1	1:A:167:ILE:HD13	2.49	0.43
1:E:176:HIS:CE1	1:E:217:CYS:SG	3.06	0.43
1:H:34:VAL:O	1:H:34:VAL:HG12	2.18	0.43
1:E:260:PRO:HD2	1:E:263:ILE:HD11	2.00	0.43
1:G:133:LYS:HD2	1:G:133:LYS:HA	1.71	0.43
1:C:191:ALA:HB2	1:D:191:ALA:HB2	1.99	0.42
1:E:41:ILE:CD1	1:E:53:THR:HG22	2.44	0.42
1:A:32:LYS:HZ1	1:A:166:HIS:CD2	2.27	0.42
1:B:102:ARG:NH1	1:F:84:GLY:O	2.52	0.42
1:G:23:VAL:HA	1:G:27:ILE:HD12	2.02	0.42
1:G:13:THR:HG21	5:G:404:SO4:O2	2.18	0.42
1:A:260:PRO:HD2	1:A:263:ILE:HG23	2.02	0.42
1:H:5:LEU:HD12	1:H:5:LEU:HA	1.95	0.42
1:H:223:THR:HG21	2:H:401:NAD:PN	2.60	0.42
1:B:260:PRO:HD2	1:B:263:ILE:CG2	2.49	0.42
1:C:3:ILE:O	1:C:7:ILE:HG12	2.19	0.42
1:G:114:VAL:HB	1:G:155:LEU:HD22	2.02	0.42
1:G:66:TRP:CG	1:G:92:VAL:CG1	3.02	0.42
1:A:117:VAL:HG12	1:A:167:ILE:HD13	2.02	0.42
1:B:66:TRP:CD2	1:B:92:VAL:CG1	3.03	0.42
1:D:285:GLN:HE21	1:D:285:GLN:HB3	1.65	0.41
1:E:160:MET:HG3	1:E:208:LYS:HE3	2.02	0.41
5:C:406:SO4:O3	1:E:276:ARG:NH1	2.53	0.41
1:B:32:LYS:HZ3	1:B:166:HIS:CD2	2.37	0.41
1:F:37:GLU:HG3	1:F:115:THR:HB	2.02	0.41
1:E:219:VAL:CG1	1:E:220:PHE:N	2.83	0.41
1:B:260:PRO:HD2	1:B:263:ILE:HG23	2.03	0.41
1:D:219:VAL:HG13	1:D:263:ILE:HD12	2.03	0.41
1:F:260:PRO:HD2	1:F:263:ILE:CD1	2.51	0.41
1:B:258:PHE:CD2	1:B:264:ASN:HB3	2.55	0.41
1:F:32:LYS:HZ1	1:F:166:HIS:CD2	2.24	0.41
1:H:22:LEU:HD22	1:H:26:PHE:HE2	1.86	0.41
1:D:93:ASP:OD1	2:D:401:NAD:N6A	2.53	0.41
1:E:31:ARG:HH12	1:E:59:ARG:NH2	2.08	0.41
1:A:289:PHE:C	1:A:291:ALA:H	2.25	0.40
1:G:65:LEU:HD11	1:G:87:ALA:CB	2.51	0.40
1:G:219:VAL:HG22	1:G:238:LEU:HD22	2.03	0.40
1:G:226:THR:HG22	1:G:227:LYS:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:O	1:A:120:ASN:HB3	2.21	0.40
1:B:34:VAL:HG21	1:B:56:PHE:CE1	2.54	0.40
1:F:145:ILE:HD13	1:F:192:ALA:HA	2.04	0.40
1:G:216:LEU:HB2	1:G:247:LEU:HD13	2.03	0.40
1:E:280:ILE:CG1	4:E:601:CE1:H111	2.51	0.40
1:D:31:ARG:NH2	1:D:248:ASP:OD1	2.54	0.40
1:D:260:PRO:HD2	1:D:263:ILE:HG23	2.04	0.40
1:E:3:ILE:H	1:E:3:ILE:HD12	1.86	0.40
1:F:3:ILE:O	1:F:7:ILE:HG13	2.22	0.40
1:E:95:SER:HB3	1:E:143:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/315 (88%)	265 (96%)	9 (3%)	3 (1%)	14	20
1	B	279/315 (89%)	268 (96%)	11 (4%)	0	100	100
1	C	263/315 (84%)	252 (96%)	9 (3%)	2 (1%)	19	28
1	D	274/315 (87%)	268 (98%)	6 (2%)	0	100	100
1	E	291/315 (92%)	274 (94%)	14 (5%)	3 (1%)	15	22
1	F	258/315 (82%)	251 (97%)	7 (3%)	0	100	100
1	G	258/315 (82%)	242 (94%)	13 (5%)	3 (1%)	13	18
1	H	287/315 (91%)	275 (96%)	12 (4%)	0	100	100
All	All	2187/2520 (87%)	2095 (96%)	81 (4%)	11 (0%)	29	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	C	3	ILE
1	C	228	ASN
1	E	92	VAL
1	G	89	ALA
1	A	18	TYR
1	A	290	GLU
1	G	46	HIS
1	E	89	ALA
1	E	110	GLU
1	G	172	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/275 (90%)	226 (92%)	20 (8%)	11	17
1	B	246/275 (90%)	231 (94%)	15 (6%)	18	29
1	C	228/275 (83%)	215 (94%)	13 (6%)	20	31
1	D	232/275 (84%)	213 (92%)	19 (8%)	11	16
1	E	256/275 (93%)	234 (91%)	22 (9%)	10	15
1	F	228/275 (83%)	210 (92%)	18 (8%)	12	18
1	G	223/275 (81%)	206 (92%)	17 (8%)	13	20
1	H	250/275 (91%)	230 (92%)	20 (8%)	12	18
All	All	1909/2200 (87%)	1765 (92%)	144 (8%)	13	20

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	7	ILE
1	A	11	LEU
1	A	15	ILE
1	A	17	SER

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	30	ARG
1	A	37	GLU
1	A	82	LYS
1	A	98	GLU
1	A	135	GLU
1	A	227	LYS
1	A	240	ASP
1	A	254	LYS
1	A	263	ILE
1	A	264	ASN
1	A	268	ARG
1	A	271	LYS
1	A	283	ARG
1	A	286	ASN
1	B	10	LEU
1	B	81	ARG
1	B	86	THR
1	B	91	VAL
1	B	92	VAL
1	B	226	THR
1	B	231	THR
1	B	237	LEU
1	B	240	ASP
1	B	254	LYS
1	B	264	ASN
1	B	271	LYS
1	B	273	LEU
1	B	281	LEU
1	B	285	GLN
1	C	5	LEU
1	C	10	LEU
1	C	37	GLU
1	C	86	THR
1	C	102	ARG
1	C	158	SER
1	C	162	ARG
1	C	179	ILE
1	C	237	LEU
1	C	240	ASP
1	C	254	LYS
1	C	263	ILE

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Mol	Chain	Res	Type
1	C	270	GLN
1	D	5	LEU
1	D	10	LEU
1	D	86	THR
1	D	133	LYS
1	D	173	VAL
1	D	179	ILE
1	D	227	LYS
1	D	237	LEU
1	D	240	ASP
1	D	252	THR
1	D	254	LYS
1	D	263	ILE
1	D	271	LYS
1	D	278	SER
1	D	285	GLN
1	D	287	ILE
1	D	288	GLN
1	D	290	GLU
1	D	292	VAL
1	E	3	ILE
1	E	7	ILE
1	E	10	LEU
1	E	19	LEU
1	E	22	LEU
1	E	30	ARG
1	E	37	GLU
1	E	81	ARG
1	E	86	THR
1	E	92	VAL
1	E	115	THR
1	E	116	ILE
1	E	219	VAL
1	E	226	THR
1	E	240	ASP
1	E	254	LYS
1	E	263	ILE
1	E	271	LYS
1	E	275	GLU
1	E	280	ILE
1	E	281	LEU
1	E	292	VAL

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Mol	Chain	Res	Type
1	F	4	ILE
1	F	5	LEU
1	F	10	LEU
1	F	20	GLU
1	F	30	ARG
1	F	92	VAL
1	F	133	LYS
1	F	135	GLU
1	F	139	LYS
1	F	158	SER
1	F	173	VAL
1	F	179	ILE
1	F	226	THR
1	F	237	LEU
1	F	240	ASP
1	F	245	SER
1	F	263	ILE
1	F	264	ASN
1	G	4	ILE
1	G	6	GLU
1	G	10	LEU
1	G	29	GLN
1	G	30	ARG
1	G	68	ILE
1	G	73	VAL
1	G	86	THR
1	G	92	VAL
1	G	99	GLU
1	G	133	LYS
1	G	145	ILE
1	G	179	ILE
1	G	241	ASP
1	G	253	THR
1	G	264	ILE
1	G	268	LEU
1	H	10	LEU
1	H	30	ARG
1	H	31	ARG
1	H	61	SER
1	H	86	THR
1	H	102	ARG
1	H	103	SER

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Mol	Chain	Res	Type
1	H	146	LEU
1	H	159	MET
1	H	173	VAL
1	H	206	LEU
1	H	223	THR
1	H	237	LEU
1	H	254	LYS
1	H	267	LEU
1	H	268	ARG
1	H	270	GLN
1	H	280	ILE
1	H	281	LEU
1	H	290	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	105	ASN
1	A	164	HIS
1	A	166	HIS
1	A	176	HIS
1	A	196	HIS
1	A	204	GLN
1	A	264	ASN
1	A	285	GLN
1	A	286	ASN
1	B	166	HIS
1	B	264	ASN
1	B	282	ASN
1	C	166	HIS
1	C	176	HIS
1	D	148	HIS
1	D	166	HIS
1	D	285	GLN
1	E	88	HIS
1	E	166	HIS
1	E	176	HIS
1	E	264	ASN
1	F	120	ASN
1	F	164	HIS
1	F	166	HIS

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Mol	Chain	Res	Type
1	F	264	ASN
1	G	119	ASN
1	G	166	HIS
1	H	106	GLN
1	H	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 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	NAD	A	401	-	42,48,48	0.56	0	50,73,73	0.63	1 (2%)
2	NAD	C	401	-	42,48,48	0.54	0	50,73,73	0.61	1 (2%)
3	YYC	C	402	-	33,33,33	0.68	2 (6%)	48,50,50	0.56	1 (2%)
5	SO4	C	404	-	4,4,4	0.34	0	6,6,6	0.26	0
5	SO4	H	403	-	4,4,4	0.20	0	6,6,6	0.20	0
5	SO4	B	404	-	4,4,4	0.11	0	6,6,6	0.28	0
5	SO4	F	403	-	4,4,4	0.13	0	6,6,6	0.39	0
3	YYC	B	402	-	33,33,33	0.70	2 (6%)	48,50,50	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	401	-	42,48,48	0.56	0	50,73,73	0.66	1 (2%)
4	CE1	E	601	-	11,11,36	0.25	0	10,10,35	0.17	0
5	SO4	C	405	-	4,4,4	0.22	0	6,6,6	0.16	0
3	YYC	H	402	-	33,33,33	0.73	2 (6%)	48,50,50	0.61	2 (4%)
2	NAD	F	401	-	42,48,48	0.55	0	50,73,73	0.62	1 (2%)
5	SO4	H	405	-	4,4,4	0.12	0	6,6,6	0.16	0
3	YYC	G	402	-	33,33,33	0.68	2 (6%)	48,50,50	0.60	2 (4%)
5	SO4	F	405	-	4,4,4	0.14	0	6,6,6	0.32	0
4	CE1	C	403	-	11,11,36	0.42	0	10,10,35	0.27	0
5	SO4	A	405	-	4,4,4	0.17	0	6,6,6	0.29	0
4	CE1	D	403	-	30,30,36	0.33	0	29,29,35	0.22	0
5	SO4	G	404	-	4,4,4	0.15	0	6,6,6	0.17	0
3	YYC	A	402	-	33,33,33	0.63	2 (6%)	48,50,50	0.61	2 (4%)
5	SO4	E	604	-	4,4,4	0.16	0	6,6,6	0.23	0
5	SO4	F	404	-	4,4,4	0.10	0	6,6,6	0.15	0
3	YYC	E	603	-	33,33,33	0.74	2 (6%)	48,50,50	0.56	2 (4%)
5	SO4	A	404	-	4,4,4	0.26	0	6,6,6	0.13	0
5	SO4	C	407	-	4,4,4	0.09	0	6,6,6	0.14	0
2	NAD	G	401	-	42,48,48	0.59	0	50,73,73	0.66	1 (2%)
3	YYC	F	402	-	33,33,33	0.65	2 (6%)	48,50,50	0.60	2 (4%)
2	NAD	D	401	-	42,48,48	0.59	0	50,73,73	0.69	1 (2%)
5	SO4	H	404	-	4,4,4	0.17	0	6,6,6	0.25	0
5	SO4	C	406	-	4,4,4	0.18	0	6,6,6	0.36	0
2	NAD	E	602	-	42,48,48	0.56	0	50,73,73	0.62	1 (2%)
5	SO4	G	403	-	4,4,4	0.15	0	6,6,6	0.29	0
5	SO4	B	403	-	4,4,4	0.11	0	6,6,6	0.20	0
4	CE1	A	403	-	36,36,36	0.39	0	35,35,35	0.22	0
2	NAD	H	401	-	42,48,48	0.56	0	50,73,73	0.61	1 (2%)
3	YYC	D	402	-	33,33,33	0.69	2 (6%)	48,50,50	0.63	2 (4%)

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	NAD	A	401	-	-	6/26/62/62	0/5/5/5
2	NAD	C	401	-	-	6/26/62/62	0/5/5/5
3	YYC	C	402	-	-	11/27/27/27	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YYC	B	402	-	-	8/27/27/27	0/3/3/3
2	NAD	B	401	-	-	7/26/62/62	0/5/5/5
4	CE1	E	601	-	-	2/9/9/34	-
3	YYC	H	402	-	-	6/27/27/27	0/3/3/3
2	NAD	F	401	-	-	8/26/62/62	0/5/5/5
3	YYC	G	402	-	-	11/27/27/27	0/3/3/3
4	CE1	C	403	-	-	3/9/9/34	-
4	CE1	D	403	-	-	12/28/28/34	-
3	YYC	A	402	-	-	12/27/27/27	0/3/3/3
3	YYC	E	603	-	-	6/27/27/27	0/3/3/3
2	NAD	G	401	-	-	5/26/62/62	0/5/5/5
3	YYC	F	402	-	-	11/27/27/27	0/3/3/3
2	NAD	D	401	-	-	5/26/62/62	0/5/5/5
2	NAD	E	602	-	-	6/26/62/62	0/5/5/5
4	CE1	A	403	-	-	13/34/34/34	-
2	NAD	H	401	-	-	6/26/62/62	0/5/5/5
3	YYC	D	402	-	-	10/27/27/27	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	YYC	O30-C28	3.18	1.32	1.22
3	H	402	YYC	O30-C28	3.11	1.31	1.22
3	E	603	YYC	O30-C28	3.09	1.31	1.22
3	G	402	YYC	O30-C28	2.85	1.31	1.22
3	E	603	YYC	O29-C28	-2.82	1.21	1.30
3	A	402	YYC	O30-C28	2.78	1.31	1.22
3	D	402	YYC	O30-C28	2.77	1.30	1.22
3	H	402	YYC	O29-C28	-2.68	1.22	1.30
3	C	402	YYC	O30-C28	2.66	1.30	1.22
3	F	402	YYC	O30-C28	2.65	1.30	1.22
3	C	402	YYC	O29-C28	-2.54	1.22	1.30
3	F	402	YYC	O29-C28	-2.43	1.23	1.30
3	D	402	YYC	O29-C28	-2.43	1.23	1.30
3	G	402	YYC	O29-C28	-2.42	1.23	1.30
3	B	402	YYC	O29-C28	-2.09	1.24	1.30
3	A	402	YYC	O29-C28	-2.07	1.24	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	YYC	O29-C28-C25	2.56	121.48	114.85
3	F	402	YYC	O29-C28-C25	2.55	121.46	114.85
3	G	402	YYC	O29-C28-C25	2.51	121.36	114.85
3	A	402	YYC	O30-C28-C25	-2.48	114.85	121.45
3	F	402	YYC	O30-C28-C25	-2.44	114.95	121.45
3	D	402	YYC	O30-C28-C25	-2.39	115.09	121.45
3	D	402	YYC	O29-C28-C25	2.34	120.93	114.85
3	E	603	YYC	O29-C28-C25	2.33	120.88	114.85
2	G	401	NAD	C5A-C6A-N6A	2.29	123.84	120.35
2	C	401	NAD	C5A-C6A-N6A	2.28	123.81	120.35
2	H	401	NAD	C5A-C6A-N6A	2.28	123.81	120.35
2	F	401	NAD	C5A-C6A-N6A	2.27	123.81	120.35
2	D	401	NAD	C5A-C6A-N6A	2.24	123.76	120.35
3	G	402	YYC	O30-C28-C25	-2.24	115.47	121.45
2	B	401	NAD	C5A-C6A-N6A	2.22	123.73	120.35
2	E	602	NAD	C5A-C6A-N6A	2.21	123.70	120.35
2	A	401	NAD	C5A-C6A-N6A	2.19	123.69	120.35
3	E	603	YYC	O30-C28-C25	-2.15	115.73	121.45
3	H	402	YYC	O29-C28-C25	2.13	120.39	114.85
3	C	402	YYC	O29-C28-C25	2.11	120.32	114.85
3	H	402	YYC	O30-C28-C25	-2.10	115.87	121.45

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	E	602	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	E	602	NAD	C5D-O5D-PN-O2N
2	E	602	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	C5D-O5D-PN-O2N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C5D-O5D-PN-O1N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	C5D-O5D-PN-O1N
2	H	401	NAD	C5D-O5D-PN-O2N
2	H	401	NAD	O4D-C1D-N1N-C2N
3	C	402	YYC	C14-C15-S18-N21
3	D	402	YYC	C14-C15-S18-N21
3	F	402	YYC	C14-C15-S18-N21
3	G	402	YYC	C14-C15-S18-N21
3	H	402	YYC	C14-C15-S18-N21
4	A	403	CE1	C6-C7-C8-C9
3	A	402	YYC	C14-C15-S18-N21
3	B	402	YYC	C14-C15-S18-N21
3	E	603	YYC	C14-C15-S18-N21
4	D	403	CE1	O19-C20-C21-O22
4	A	403	CE1	O19-C20-C21-O22
4	A	403	CE1	O16-C17-C18-O19
4	D	403	CE1	O16-C17-C18-O19
4	A	403	CE1	O34-C35-C36-O37
4	E	601	CE1	C6-C7-C8-C9
4	A	403	CE1	C3-C4-C5-C6
4	D	403	CE1	O34-C35-C36-O37
3	E	603	YYC	C22-N21-S18-O19
3	G	402	YYC	C22-N21-S18-O20
3	C	402	YYC	C22-N21-S18-O20
3	D	402	YYC	C22-N21-S18-O19
3	D	402	YYC	C22-N21-S18-O20
3	F	402	YYC	C22-N21-S18-O20
3	G	402	YYC	C22-N21-S18-O19
3	C	402	YYC	C22-N21-S18-O19
3	F	402	YYC	C22-N21-S18-O19
3	E	603	YYC	C22-N21-S18-O20
3	A	402	YYC	C22-N21-S18-O20
3	A	402	YYC	C4-C5-S8-O9
3	G	402	YYC	C6-C5-S8-O9
4	A	403	CE1	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	402	YYC	C6-C5-S8-O9
3	F	402	YYC	C6-C5-S8-O9
3	A	402	YYC	C22-N21-S18-O19
3	A	402	YYC	C6-C5-S8-O9
3	C	402	YYC	C6-C5-S8-O9
3	F	402	YYC	C4-C5-S8-O9
3	G	402	YYC	C4-C5-S8-O9
3	A	402	YYC	C16-C15-S18-N21
3	B	402	YYC	C16-C15-S18-N21
3	C	402	YYC	C16-C15-S18-N21
3	D	402	YYC	C16-C15-S18-N21
3	E	603	YYC	C16-C15-S18-N21
3	F	402	YYC	C16-C15-S18-N21
3	G	402	YYC	C16-C15-S18-N21
3	H	402	YYC	C16-C15-S18-N21
3	C	402	YYC	C4-C5-S8-O9
3	D	402	YYC	C4-C5-S8-O9
4	A	403	CE1	C2-C3-C4-C5
2	D	401	NAD	PN-O3-PA-O5B
3	C	402	YYC	C22-N21-S18-C15
3	D	402	YYC	C22-N21-S18-C15
3	F	402	YYC	C22-N21-S18-C15
3	G	402	YYC	C22-N21-S18-C15
4	A	403	CE1	C20-C21-O22-C23
4	D	403	CE1	C20-C21-O22-C23
2	G	401	NAD	C5D-O5D-PN-O3
4	A	403	CE1	C23-C24-O25-C26
4	D	403	CE1	C21-C20-O19-C18
3	H	402	YYC	C22-N21-S18-O20
4	D	403	CE1	C23-C24-O25-C26
3	B	402	YYC	C4-C5-S8-O9
2	G	401	NAD	C5D-O5D-PN-O2N
4	A	403	CE1	C21-C20-O19-C18
3	B	402	YYC	C6-C5-S8-O9
3	A	402	YYC	C22-N21-S18-C15
4	A	403	CE1	C18-C17-O16-C15
4	D	403	CE1	C18-C17-O16-C15
3	E	603	YYC	C22-N21-S18-C15
3	D	402	YYC	C6-C5-S8-C11
3	F	402	YYC	C6-C5-S8-C11
3	G	402	YYC	C6-C5-S8-C11
3	A	402	YYC	C4-C5-S8-C11

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Mol	Chain	Res	Type	Atoms
4	C	403	CE1	C3-C4-C5-C6
3	A	402	YYC	C6-C5-S8-C11
3	C	402	YYC	C6-C5-S8-C11
3	F	402	YYC	C4-C5-S8-C11
3	B	402	YYC	C16-C15-S18-O20
3	D	402	YYC	C16-C15-S18-O19
3	G	402	YYC	C4-C5-S8-C11
3	C	402	YYC	C4-C5-S8-C11
3	D	402	YYC	C4-C5-S8-C11
3	H	402	YYC	C16-C15-S18-O19
4	E	601	CE1	C5-C6-C7-C8
2	C	401	NAD	O4B-C4B-C5B-O5B
3	H	402	YYC	C22-N21-S18-O19
2	G	401	NAD	O4B-C4B-C5B-O5B
3	A	402	YYC	C16-C15-S18-O20
3	C	402	YYC	C16-C15-S18-O19
3	E	603	YYC	C16-C15-S18-O19
2	B	401	NAD	PA-O3-PN-O1N
2	F	401	NAD	PA-O3-PN-O1N
2	H	401	NAD	PA-O3-PN-O1N
2	H	401	NAD	O4B-C4B-C5B-O5B
4	D	403	CE1	C24-C23-O22-C21
4	C	403	CE1	C11-C10-C9-C8
3	H	402	YYC	C22-N21-S18-C15
3	F	402	YYC	C16-C15-S18-O19
3	G	402	YYC	C16-C15-S18-O19
2	A	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
4	A	403	CE1	C24-C23-O22-C21
4	D	403	CE1	C11-C12-O13-C14
2	A	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C5D-O5D-PN-O3
2	E	602	NAD	C5D-O5D-PN-O3
2	F	401	NAD	C5D-O5D-PN-O3
2	F	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	C5D-O5D-PN-O3
3	F	402	YYC	C16-C15-S18-O20
2	B	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	E	602	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PA-O3-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	E	602	NAD	PA-O3-PN-O1N
3	B	402	YYC	C4-C5-S8-C11
4	C	403	CE1	C1-C2-C3-C4
3	B	402	YYC	C14-C15-S18-O20
3	A	402	YYC	C16-C15-S18-O19
3	C	402	YYC	C16-C15-S18-O20
3	G	402	YYC	C16-C15-S18-O20
3	B	402	YYC	C6-C5-S8-C11
4	D	403	CE1	O13-C14-C15-O16
3	A	402	YYC	C26-C25-C28-O29
4	D	403	CE1	O28-C29-C30-O31
4	A	403	CE1	O13-C14-C15-O16
4	D	403	CE1	O22-C23-C24-O25

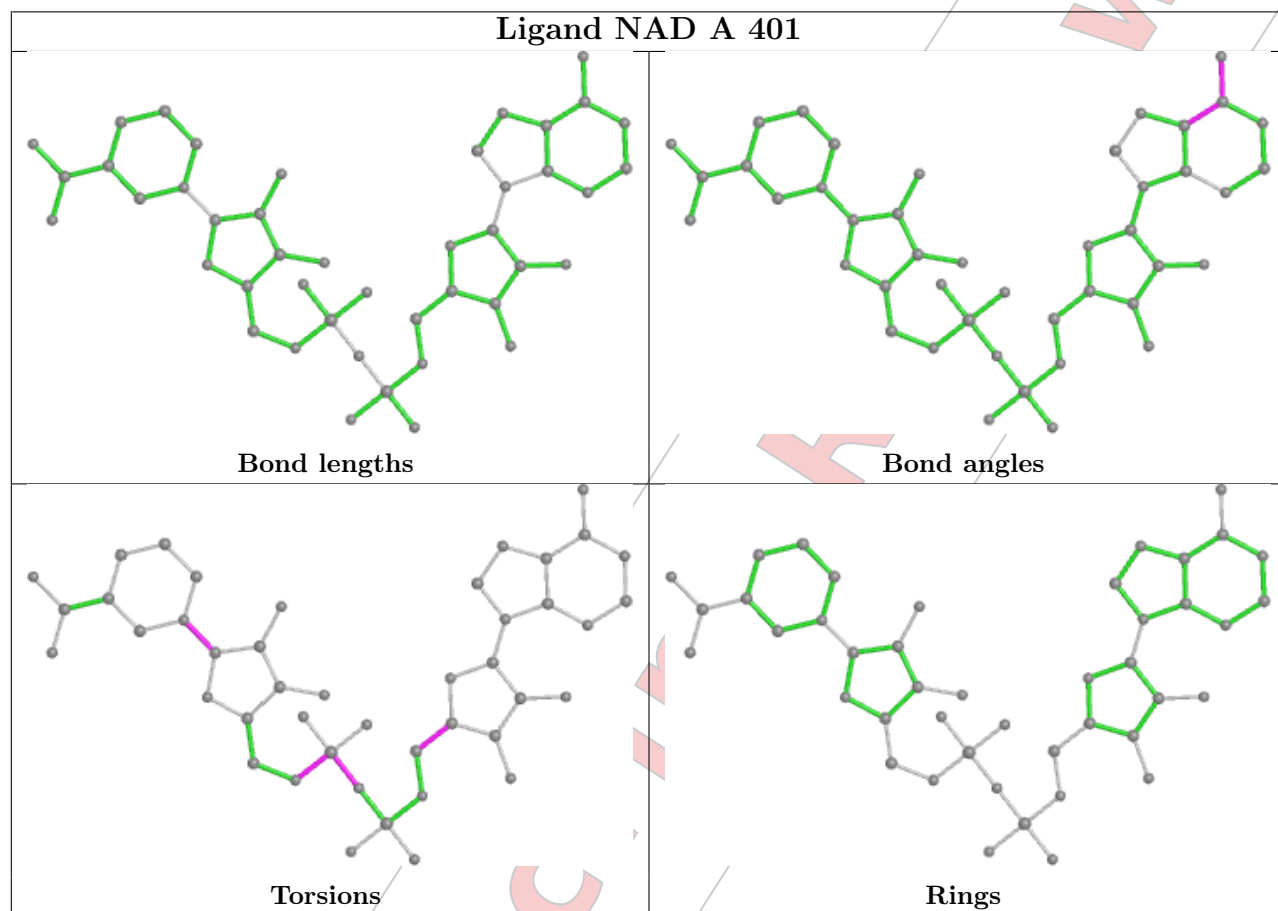
There are no ring outliers.

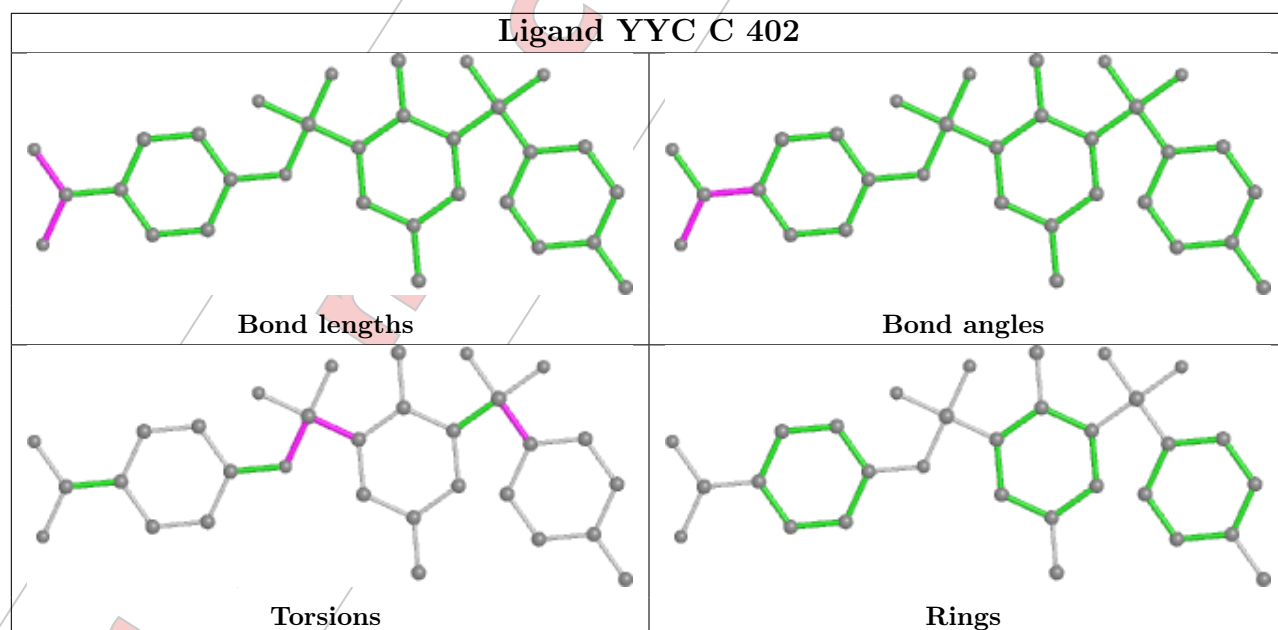
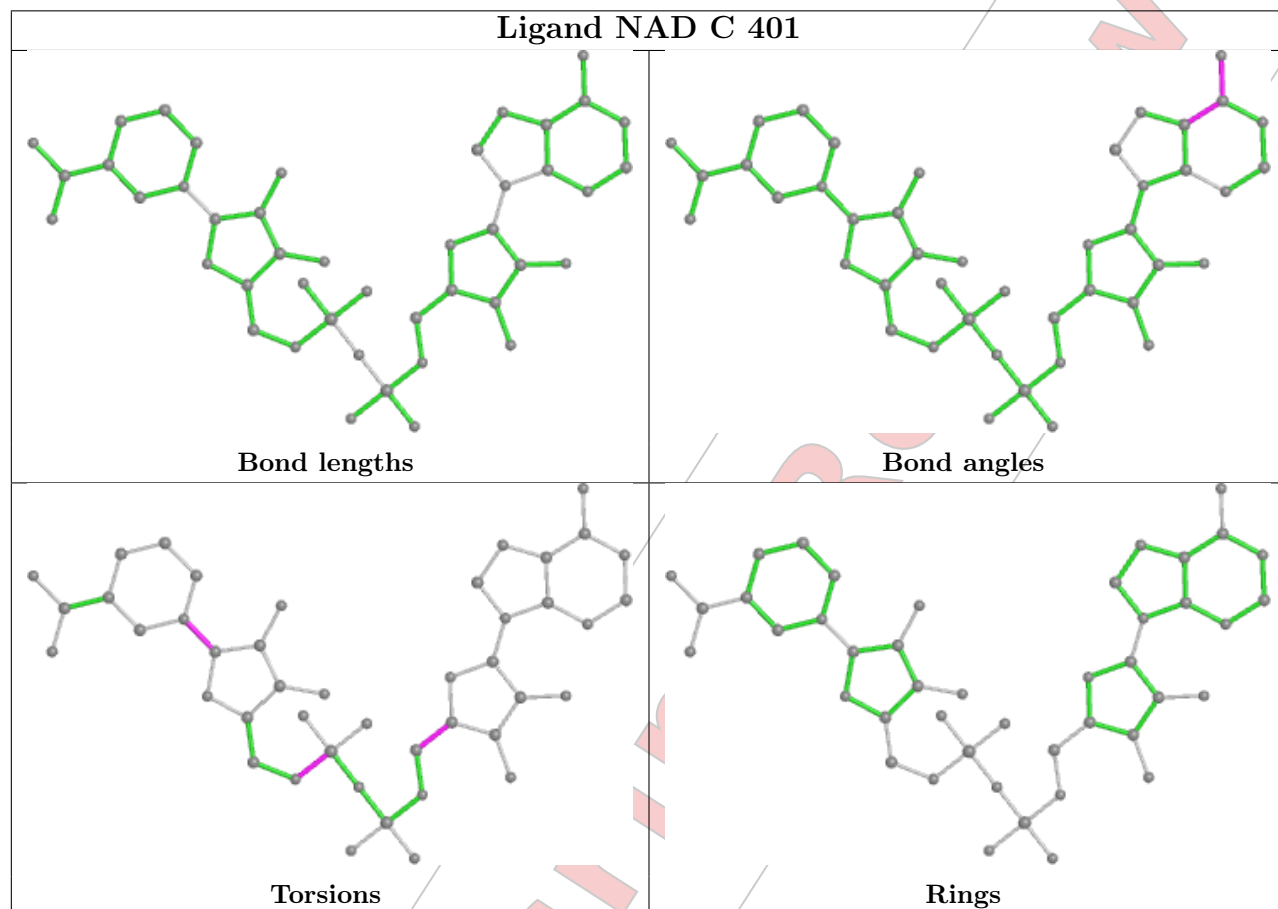
12 monomers are involved in 21 short contacts:

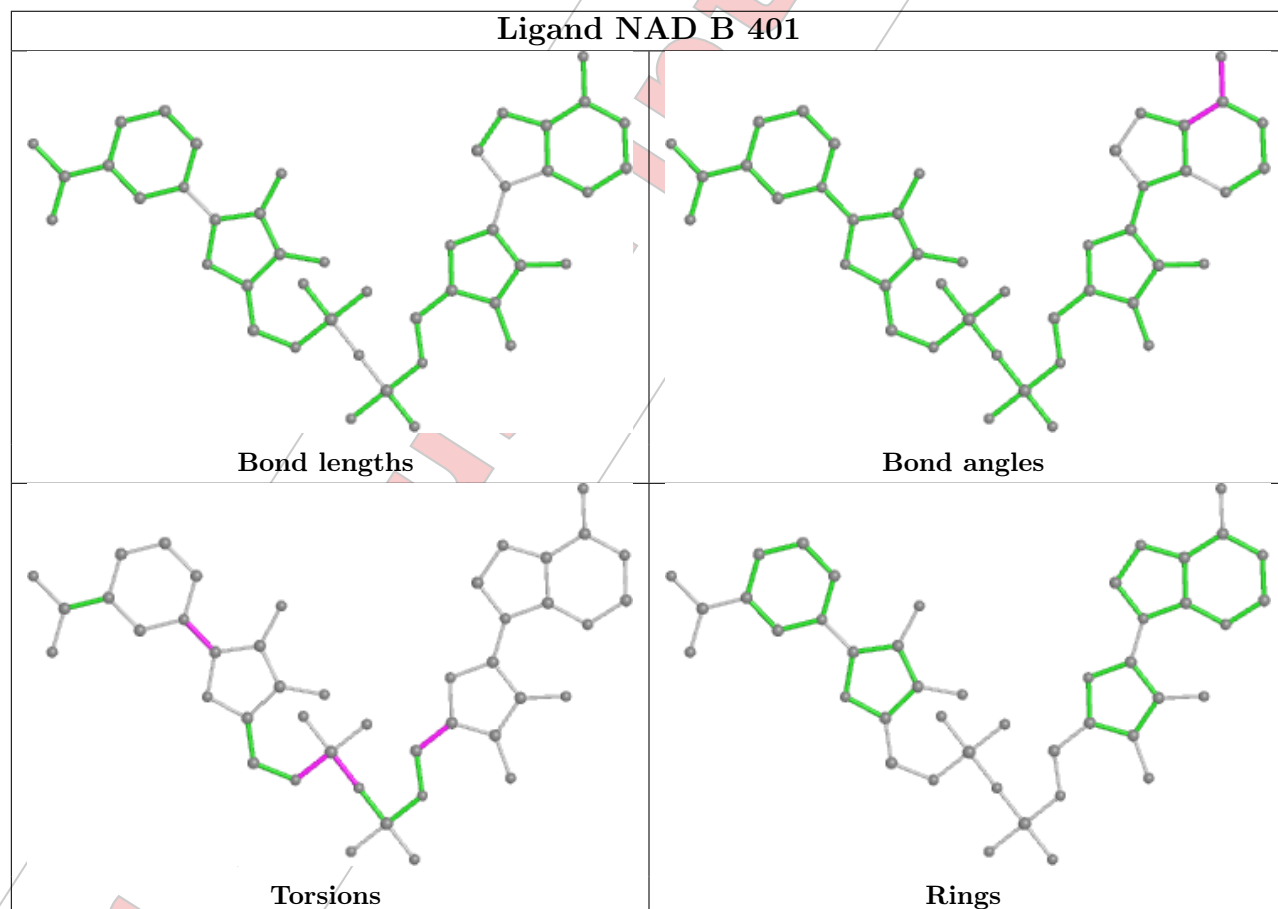
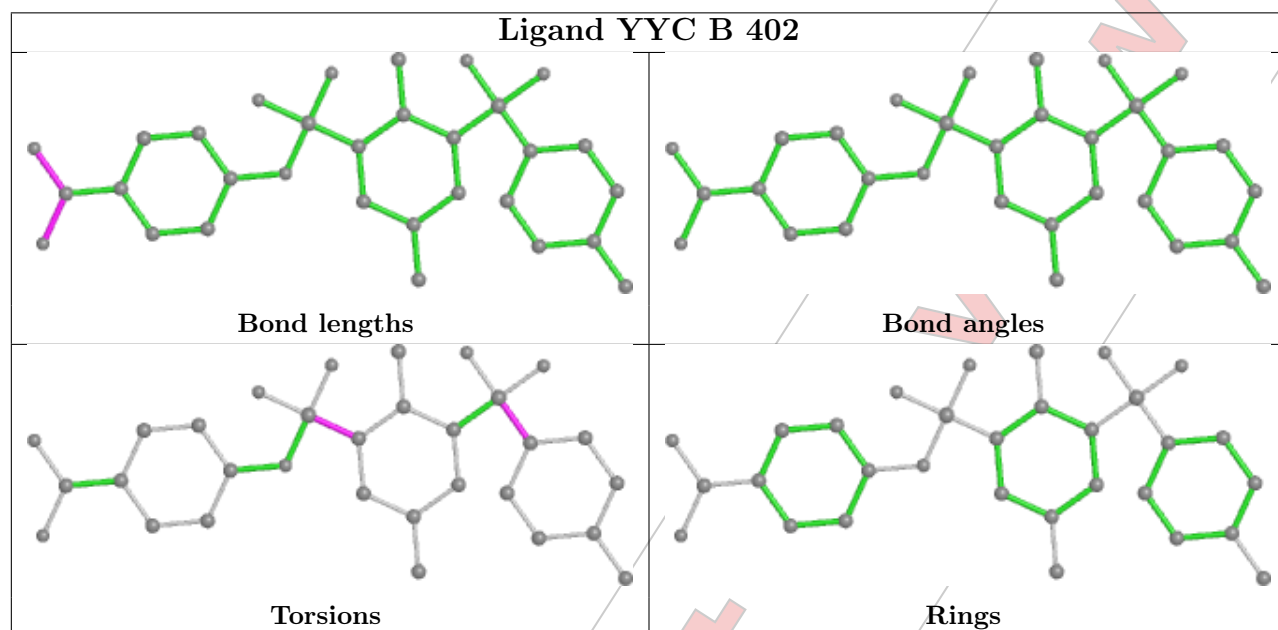
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	SO4	2	0
4	E	601	CE1	3	0
5	H	405	SO4	1	0
4	C	403	CE1	2	0
4	D	403	CE1	4	0
5	G	404	SO4	1	0
5	E	604	SO4	1	0
5	C	407	SO4	1	0
2	D	401	NAD	1	0
5	C	406	SO4	1	0
4	A	403	CE1	2	0
2	H	401	NAD	2	0

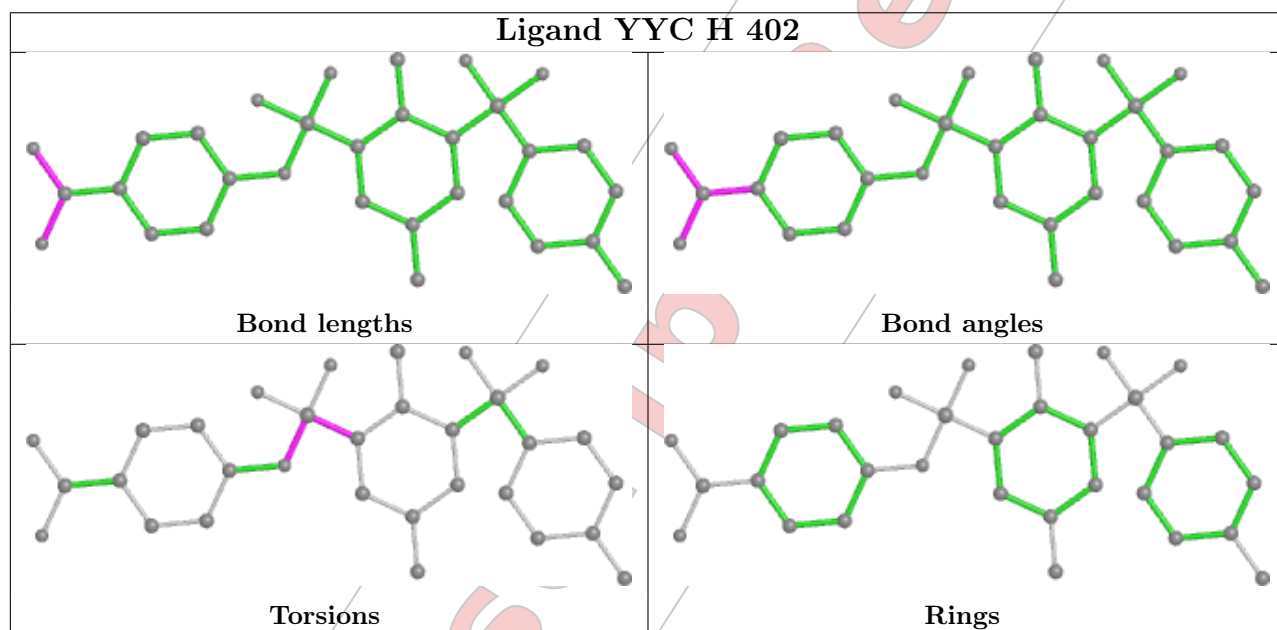
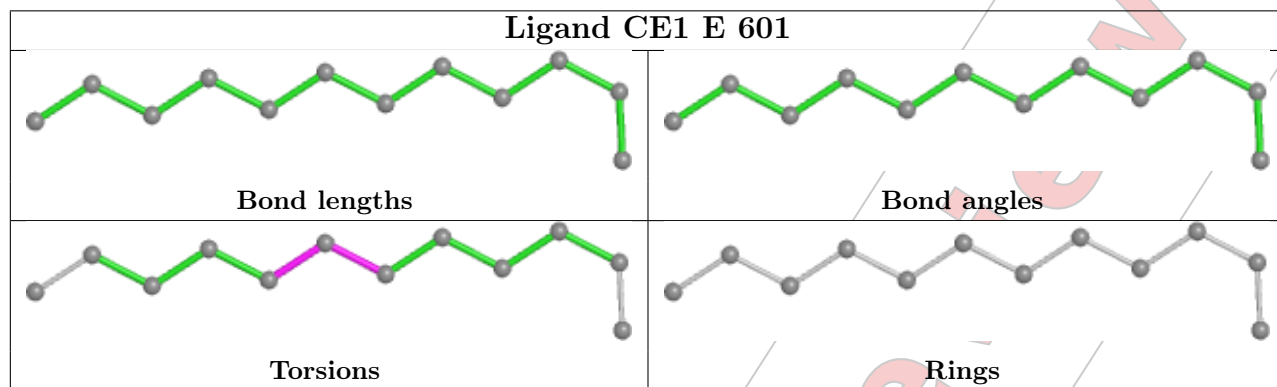
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

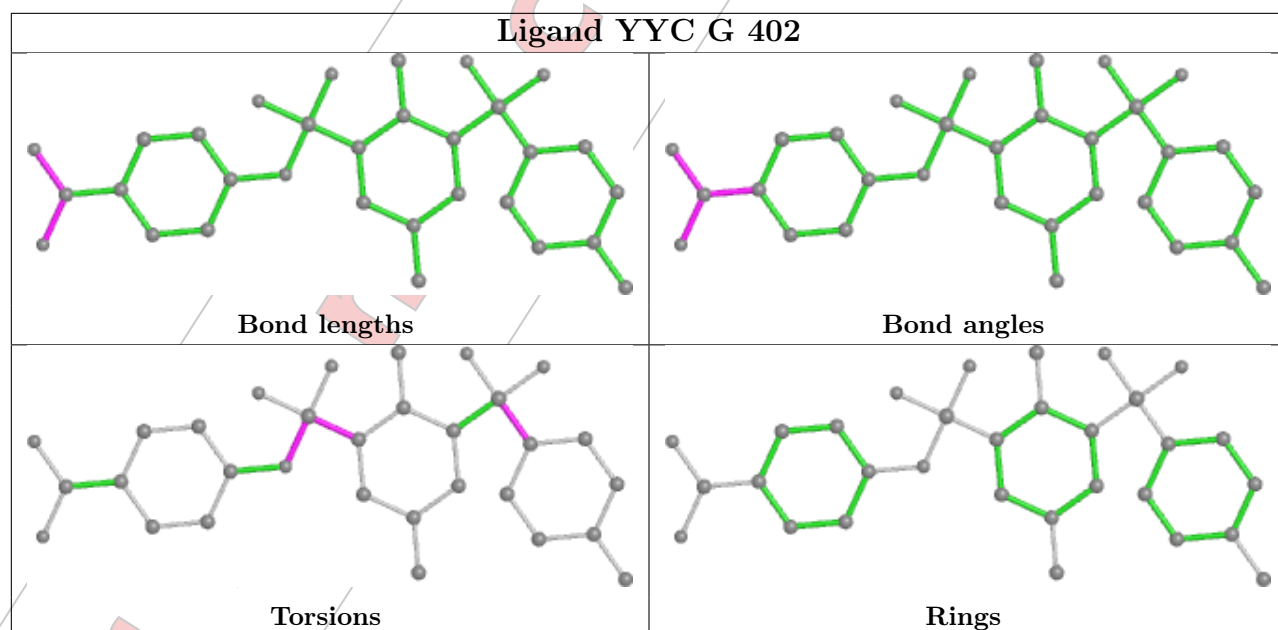
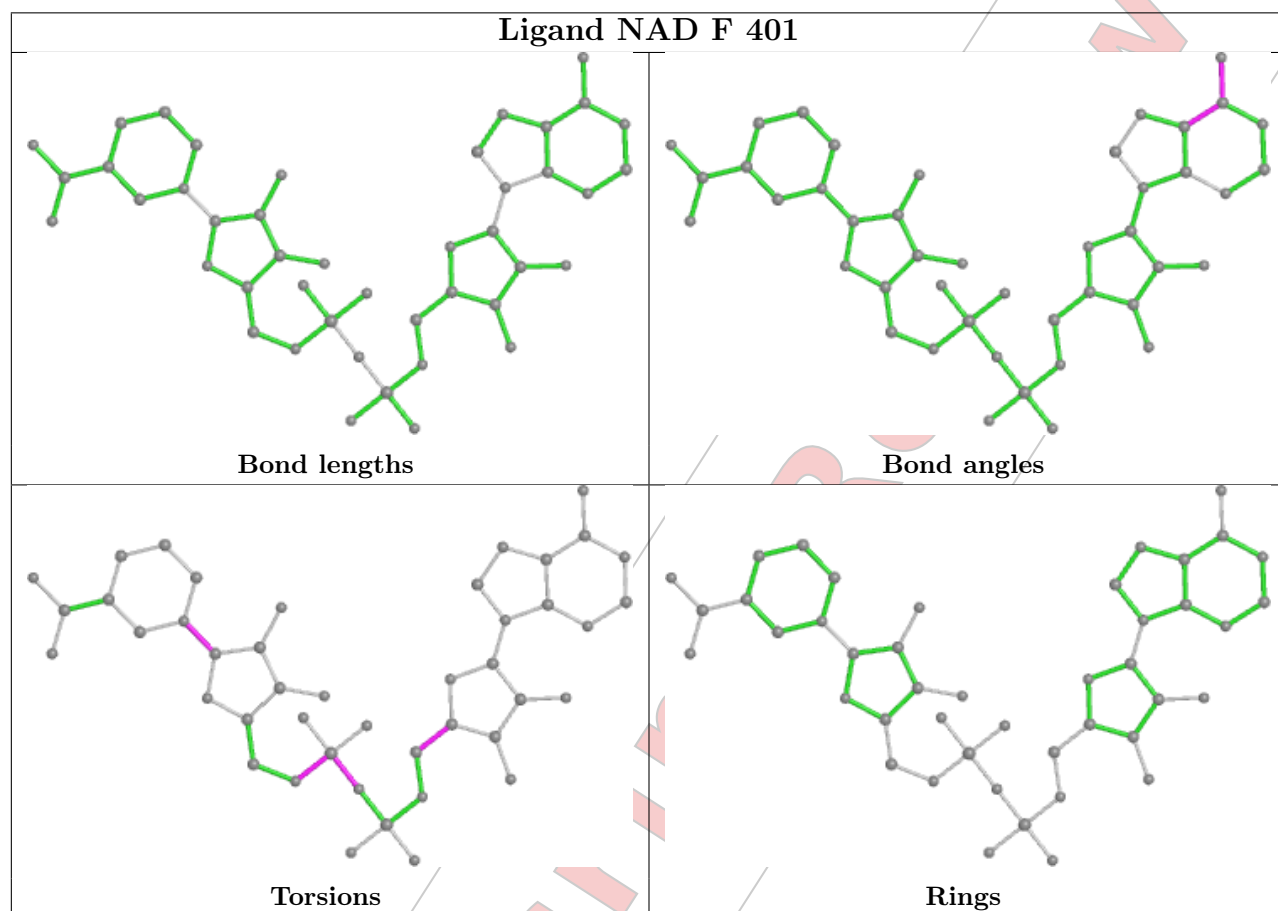
equivalents in the CSD to analyse the geometry.

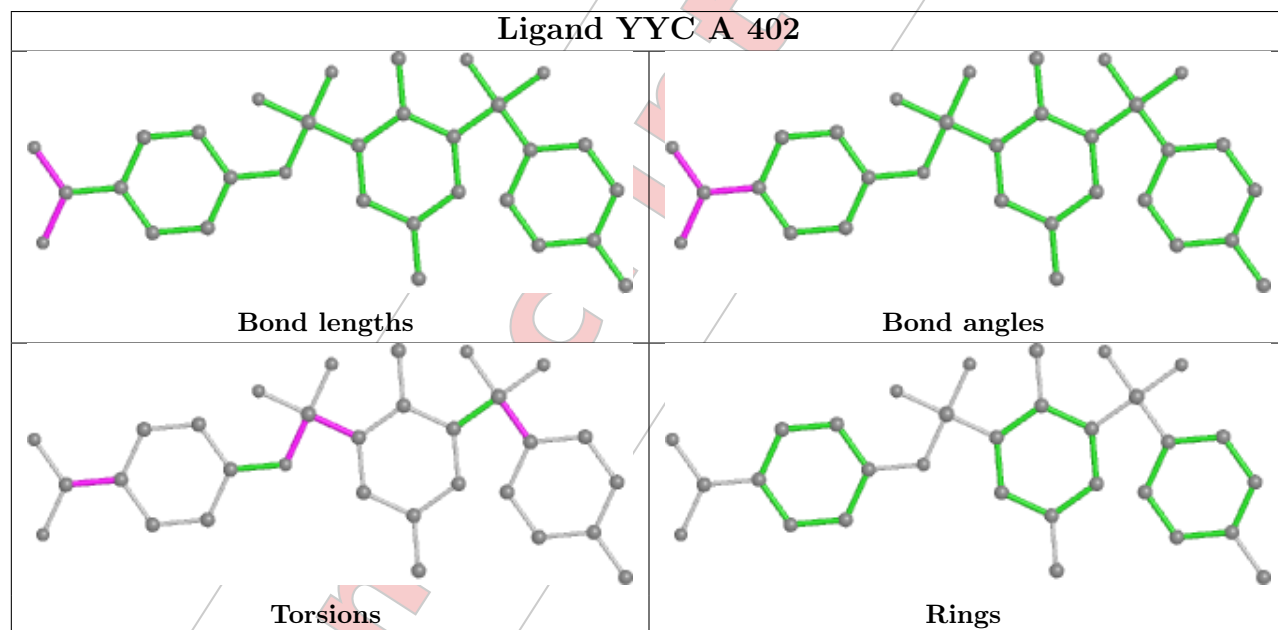
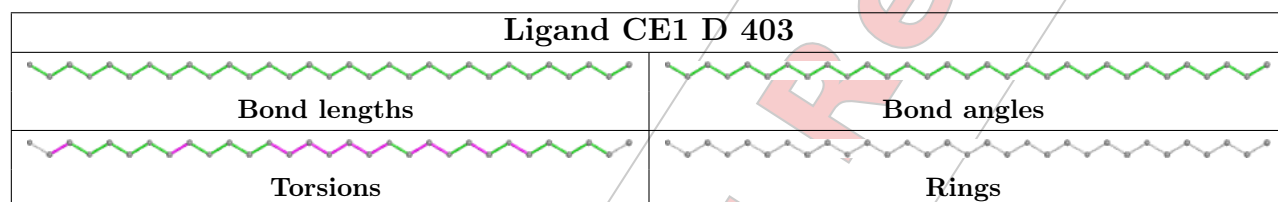
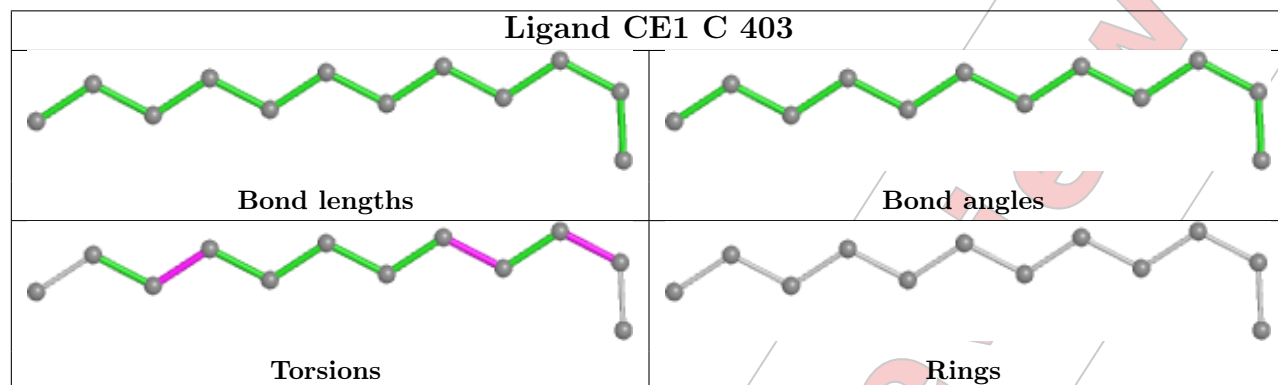


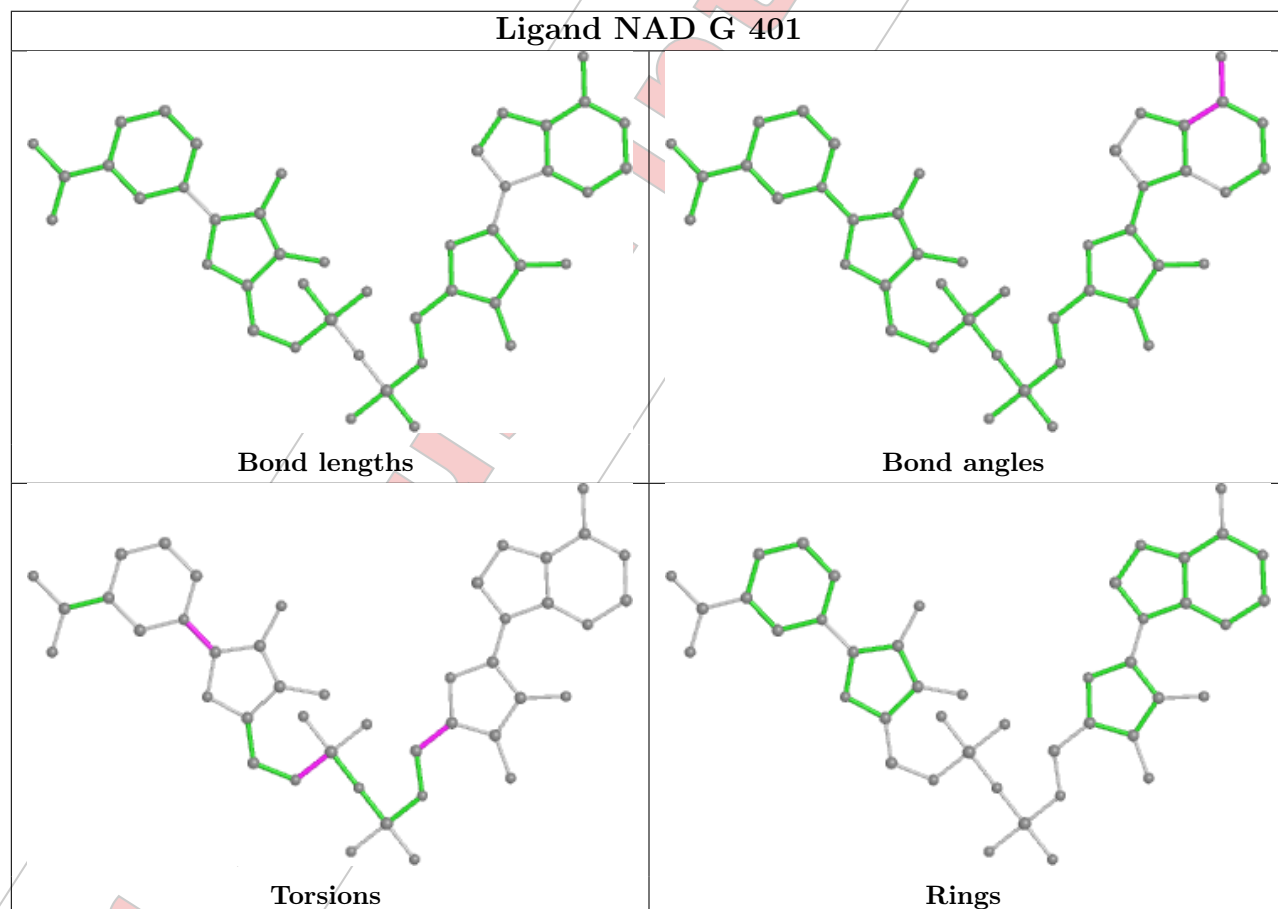
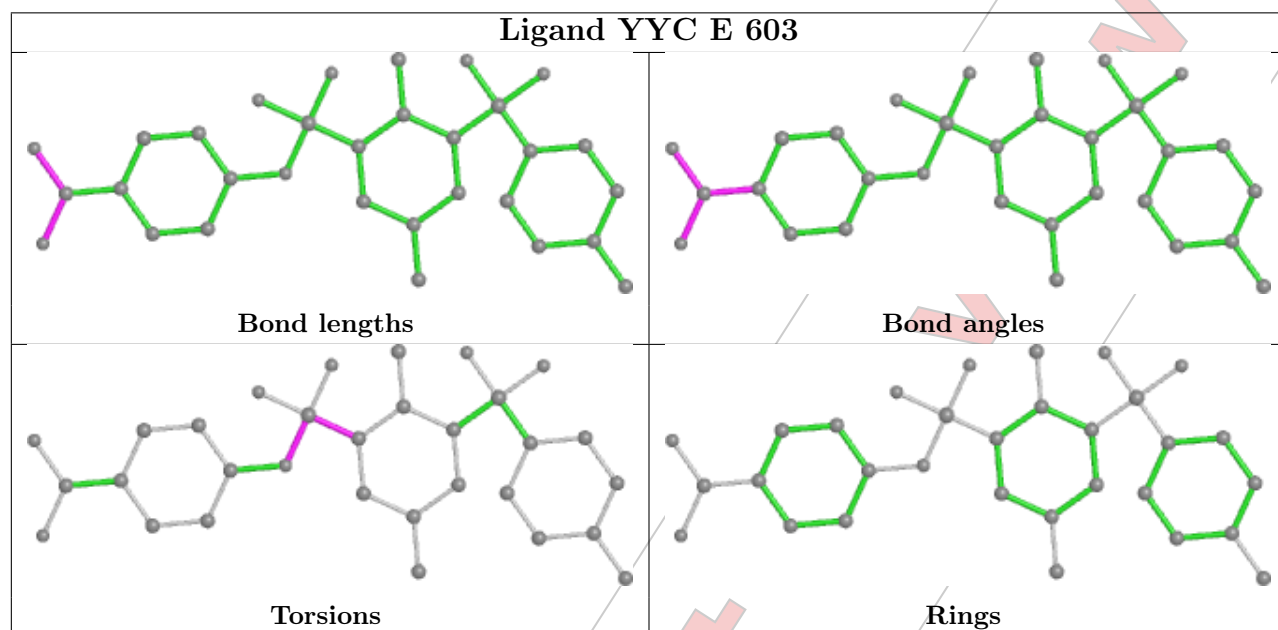


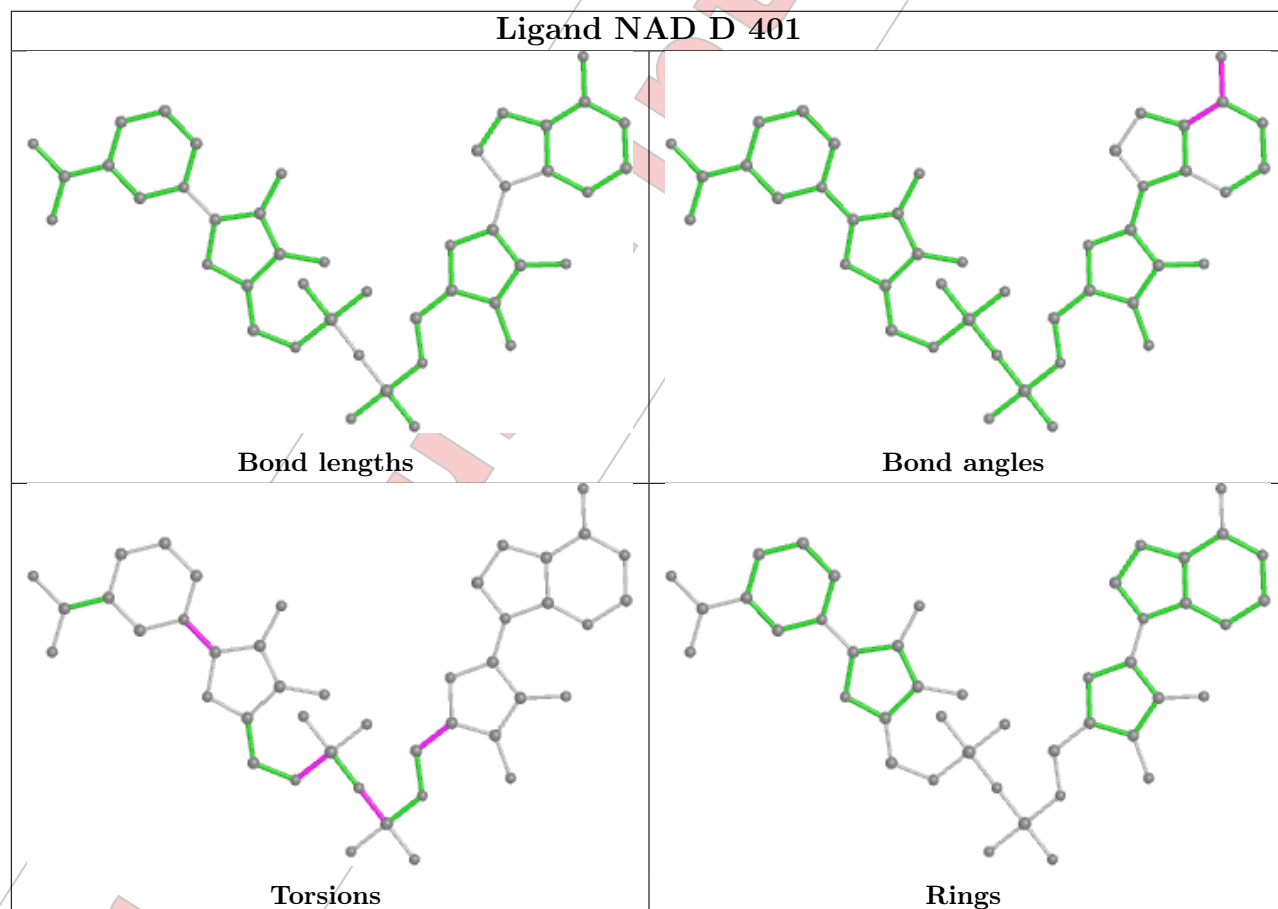
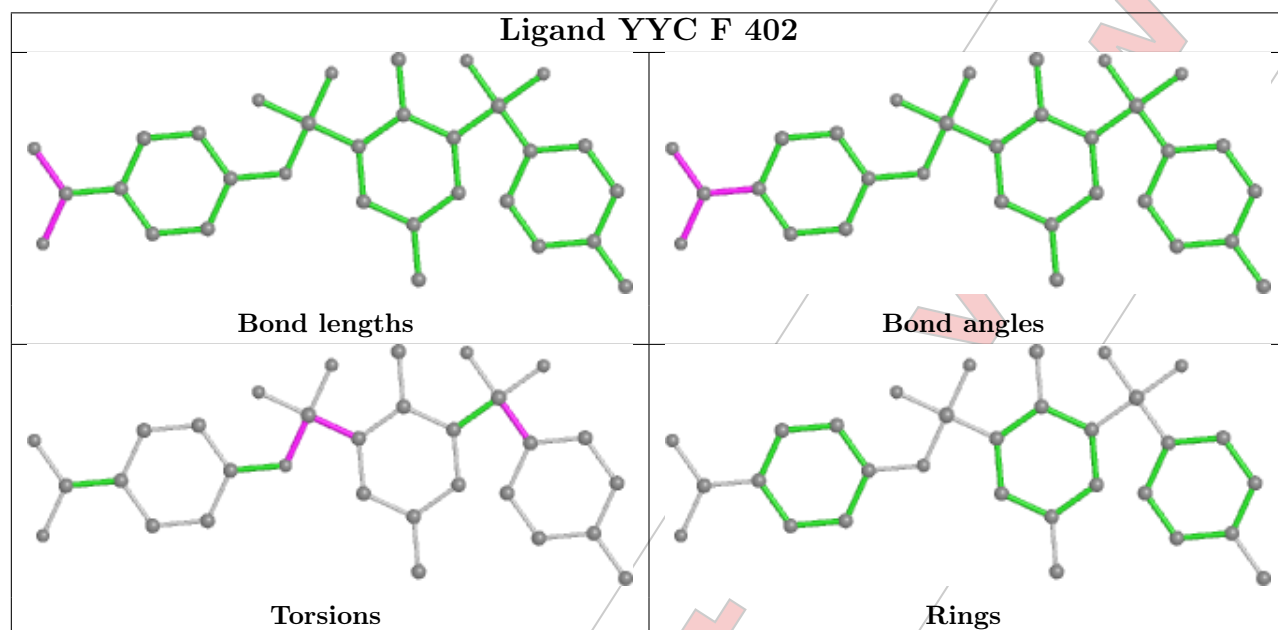


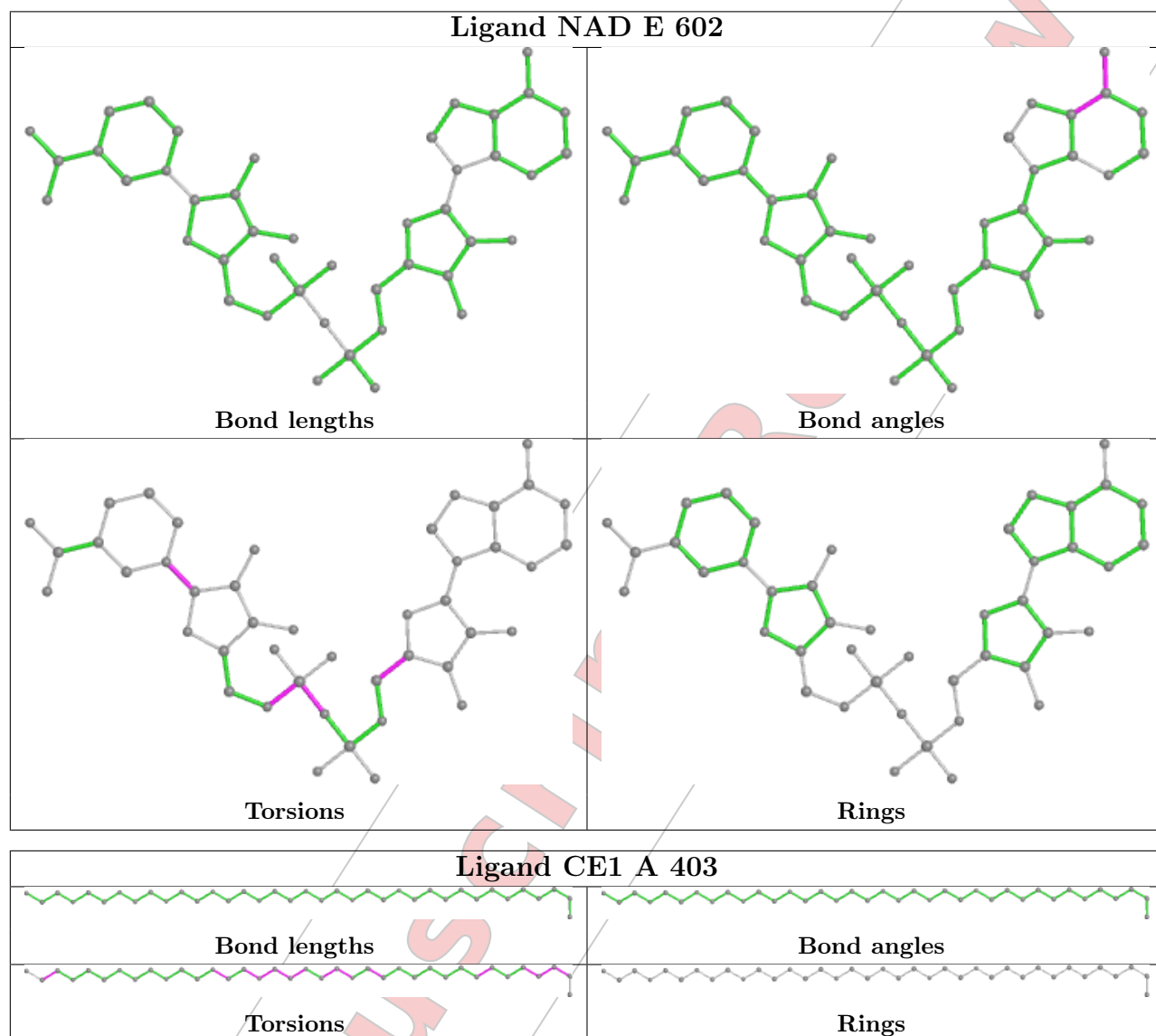


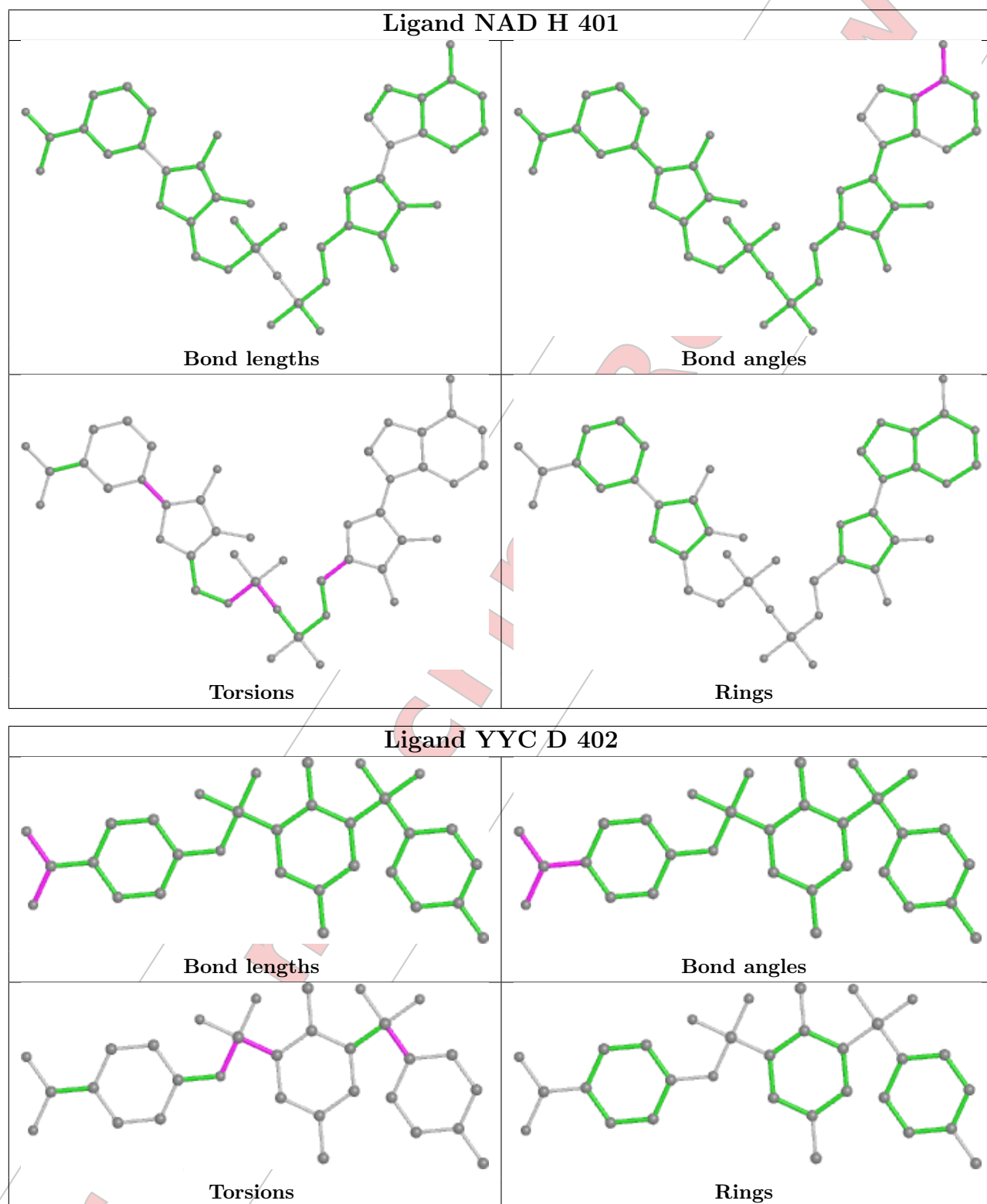












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

For Manuscript Review

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	283/315 (89%)	0.26	15 (5%) 26 23	37, 53, 83, 110	0
1	B	283/315 (89%)	0.04	7 (2%) 57 53	37, 51, 69, 84	0
1	C	267/315 (84%)	0.11	13 (4%) 29 25	38, 54, 75, 89	0
1	D	280/315 (88%)	0.37	23 (8%) 11 9	39, 54, 105, 117	0
1	E	293/315 (93%)	0.30	18 (6%) 21 18	44, 66, 89, 101	0
1	F	262/315 (83%)	0.08	10 (3%) 40 36	42, 55, 78, 88	0
1	G	262/315 (83%)	0.44	20 (7%) 13 10	50, 69, 93, 104	0
1	H	289/315 (91%)	0.40	23 (7%) 12 9	43, 70, 99, 109	0
All	All	2219/2520 (88%)	0.25	129 (5%) 23 20	37, 58, 90, 117	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	ILE	6.0
1	G	83	LEU	5.6
1	H	83	LEU	5.1
1	C	229	PRO	5.0
1	D	4	ILE	4.7
1	A	30	ARG	4.6
1	D	11	LEU	4.5
1	A	29	GLN	4.3
1	G	240	THR	4.2
1	E	90	TYR	4.1
1	F	26	PHE	4.1
1	H	206	LEU	3.9
1	B	26	PHE	3.9
1	A	21	SER	3.8
1	D	7	ILE	3.8
1	A	20	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	231	THR	3.6
1	H	34	VAL	3.6
1	G	241	ASP	3.6
1	H	161	LYS	3.6
1	G	135	GLU	3.6
1	D	30	ARG	3.6
1	C	228	ASN	3.5
1	D	2	ASN	3.4
1	H	107	VAL	3.4
1	E	230	SER	3.3
1	A	28	PRO	3.3
1	C	197	ARG	3.3
1	H	109	LYS	3.3
1	C	194	GLY	3.3
1	D	193	VAL	3.2
1	H	78	ALA	3.2
1	H	230	SER	3.2
1	G	23	VAL	3.1
1	F	22	LEU	3.1
1	D	293	VAL	3.1
1	A	3	ILE	3.1
1	C	193	VAL	3.1
1	G	71	HIS	3.1
1	F	228	ASN	3.1
1	E	191	ALA	3.0
1	C	175	GLY	3.0
1	D	190	PHE	3.0
1	A	222	ASN	3.0
1	G	227	LYS	3.0
1	G	86	THR	3.0
1	D	171	ALA	2.9
1	D	292	VAL	2.9
1	G	181	TYR	2.9
1	G	137	ILE	2.9
1	A	6	GLU	2.9
1	D	291	ALA	2.9
1	E	36	GLY	2.8
1	H	81	ARG	2.8
1	H	236	VAL	2.8
1	A	18	TYR	2.8
1	G	80	CYS	2.8
1	D	206	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	79	GLU	2.8
1	C	190	PHE	2.8
1	H	162	ARG	2.8
1	E	190	PHE	2.7
1	H	187	SER	2.7
1	B	197	ARG	2.7
1	D	13	THR	2.7
1	D	176	HIS	2.7
1	E	74	GLU	2.7
1	F	28	PRO	2.7
1	D	175	GLY	2.7
1	D	188	SER	2.7
1	E	187	SER	2.7
1	E	175	GLY	2.7
1	E	71	HIS	2.6
1	A	175	GLY	2.6
1	C	187	SER	2.6
1	E	81	ARG	2.6
1	H	76	THR	2.6
1	F	236	VAL	2.6
1	F	181	TYR	2.5
1	G	222	ASN	2.5
1	H	30	ARG	2.5
1	H	154	ALA	2.5
1	D	6	GLU	2.5
1	F	25	PHE	2.5
1	D	1	GLY	2.4
1	D	192	ALA	2.4
1	G	161	LYS	2.4
1	C	227	LYS	2.4
1	A	229	PRO	2.4
1	F	23	VAL	2.4
1	A	71	HIS	2.4
1	C	176	HIS	2.4
1	B	161	LYS	2.4
1	D	209	THR	2.4
1	B	193	VAL	2.4
1	B	25	PHE	2.4
1	F	27	ILE	2.4
1	C	191	ALA	2.4
1	E	61	SER	2.4
1	H	89	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	25	PHE	2.4
1	D	187	SER	2.3
1	A	290	GLU	2.3
1	F	193	VAL	2.3
1	G	36	GLY	2.3
1	H	157	PRO	2.3
1	A	19	LEU	2.3
1	B	18	TYR	2.3
1	E	231	THR	2.2
1	E	34	VAL	2.2
1	G	160	MET	2.2
1	E	116	ILE	2.2
1	G	179	ILE	2.2
1	H	38	ILE	2.2
1	E	291	ALA	2.2
1	E	188	SER	2.2
1	E	78	ALA	2.2
1	H	57	ALA	2.2
1	B	194	GLY	2.2
1	H	102	ARG	2.2
1	G	244	VAL	2.1
1	E	63	LEU	2.1
1	G	82	LYS	2.0
1	G	81	ARG	2.0
1	D	191	ALA	2.0
1	H	36	GLY	2.0
1	A	22	LEU	2.0
1	C	71	HIS	2.0
1	H	82	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

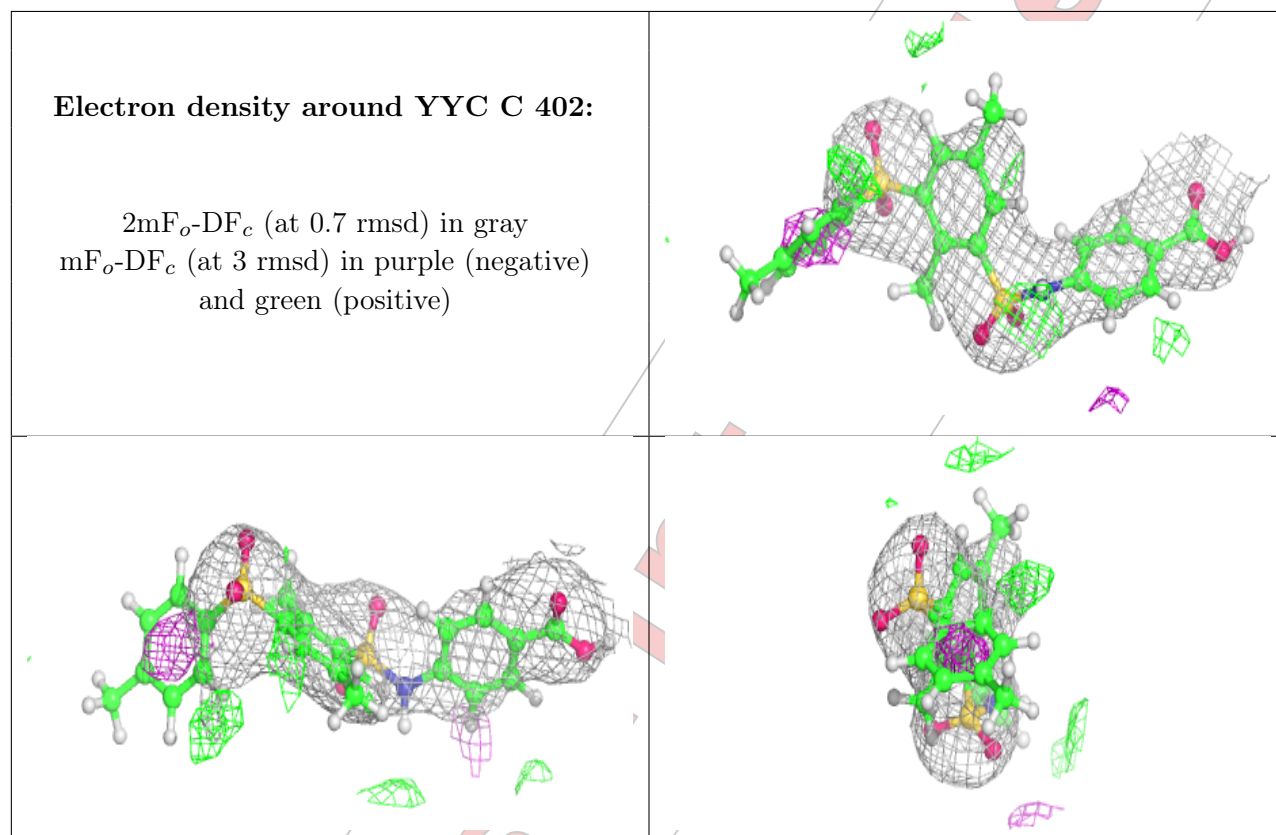
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

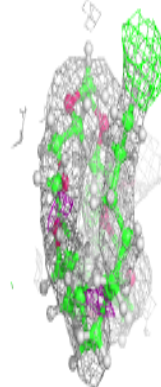
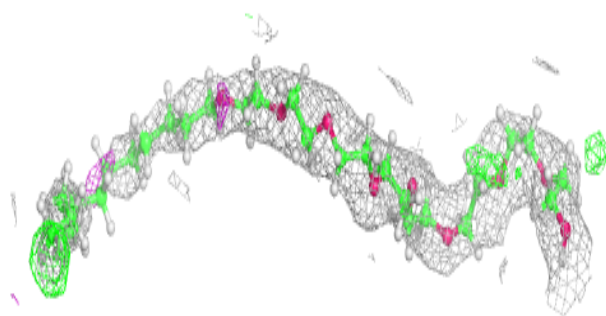
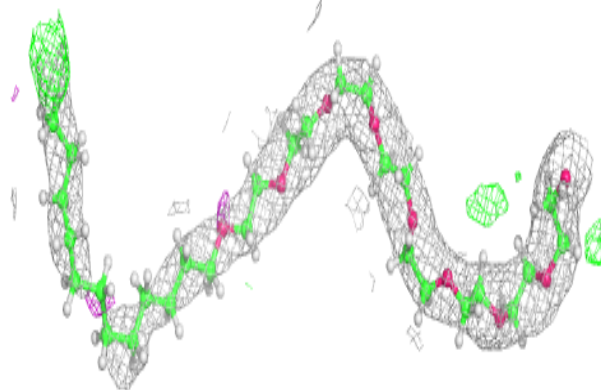
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	407	5/5	0.65	0.47	157,157,157,157	0
5	SO4	H	405	5/5	0.83	0.19	130,130,130,130	0
5	SO4	G	404	5/5	0.84	0.28	132,132,132,132	0
3	YYC	C	402	31/31	0.87	0.26	77,86,97,98	21
4	CE1	A	403	37/37	0.88	0.21	51,60,62,63	58
4	CE1	D	403	31/37	0.89	0.19	51,55,59,60	45
4	CE1	E	601	12/37	0.90	0.39	46,47,49,49	0
3	YYC	F	402	31/31	0.91	0.26	74,76,84,85	20
5	SO4	E	604	5/5	0.91	0.16	100,100,101,101	0
4	CE1	C	403	12/37	0.92	0.17	47,47,48,48	0
3	YYC	G	402	31/31	0.93	0.20	89,91,100,102	21
5	SO4	H	403	5/5	0.93	0.14	107,107,107,107	0
5	SO4	B	404	5/5	0.93	0.15	103,103,103,104	0
5	SO4	B	403	5/5	0.95	0.13	93,93,93,93	0
2	NAD	H	401	44/44	0.95	0.17	60,70,75,76	0
5	SO4	C	405	5/5	0.95	0.37	96,97,97,97	0
2	NAD	G	401	44/44	0.95	0.15	73,76,81,81	0
2	NAD	E	602	44/44	0.96	0.16	61,69,72,72	0
5	SO4	A	405	5/5	0.96	0.17	93,93,94,94	0
2	NAD	C	401	44/44	0.97	0.14	52,59,62,63	0
2	NAD	A	401	44/44	0.97	0.13	45,48,51,51	0
5	SO4	C	404	5/5	0.97	0.15	75,75,75,75	0
3	YYC	H	402	31/31	0.97	0.14	55,60,64,64	21
5	SO4	C	406	5/5	0.97	0.21	78,78,78,79	0
3	YYC	A	402	31/31	0.97	0.16	49,52,54,55	20
3	YYC	B	402	31/31	0.97	0.17	46,49,51,53	21
5	SO4	F	403	5/5	0.97	0.13	64,64,64,64	0
5	SO4	F	405	5/5	0.97	0.14	82,83,83,83	0
2	NAD	F	401	44/44	0.97	0.14	52,53,56,56	0
3	YYC	D	402	31/31	0.97	0.16	48,49,53,54	20
5	SO4	H	404	5/5	0.97	0.20	80,80,80,80	0
3	YYC	E	603	31/31	0.97	0.16	48,54,57,57	21
2	NAD	D	401	44/44	0.98	0.15	43,45,46,47	0
5	SO4	A	404	5/5	0.98	0.18	83,83,83,83	0
2	NAD	B	401	44/44	0.98	0.14	37,41,44,44	0
5	SO4	G	403	5/5	0.98	0.13	64,65,65,65	0
5	SO4	F	404	5/5	0.99	0.11	55,55,56,56	0

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



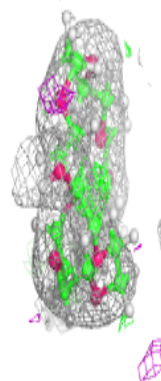
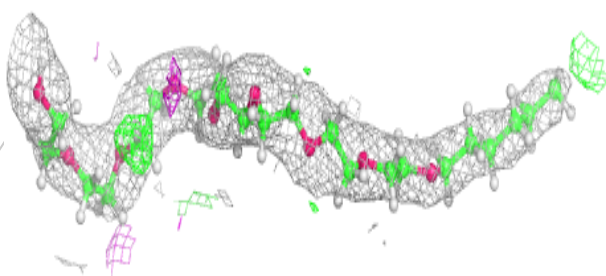
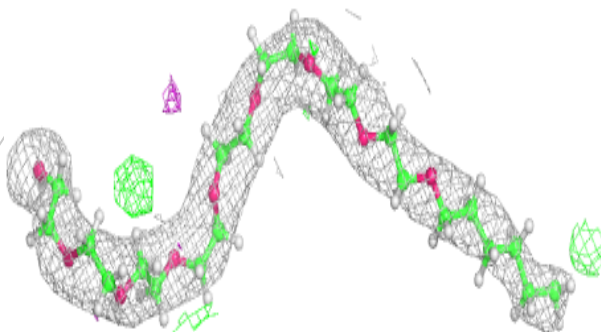
Electron density around CE1 A 403:

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



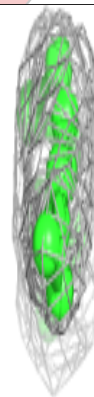
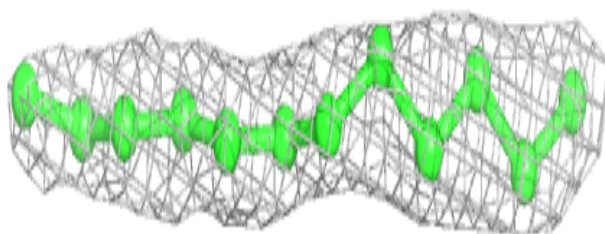
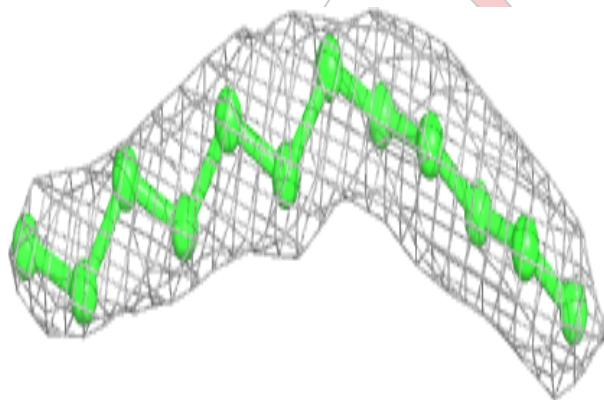
Electron density around CE1 D 403:

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



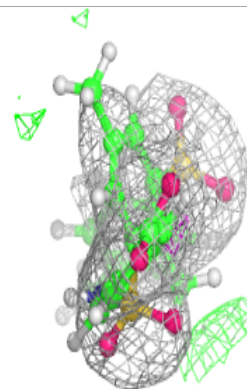
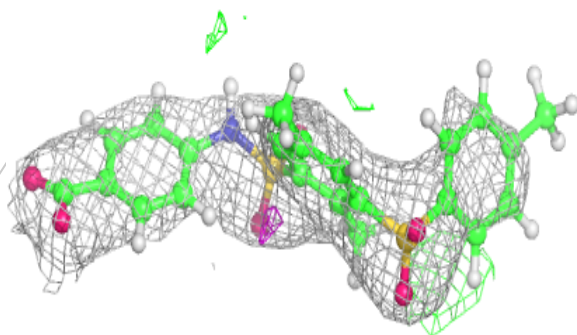
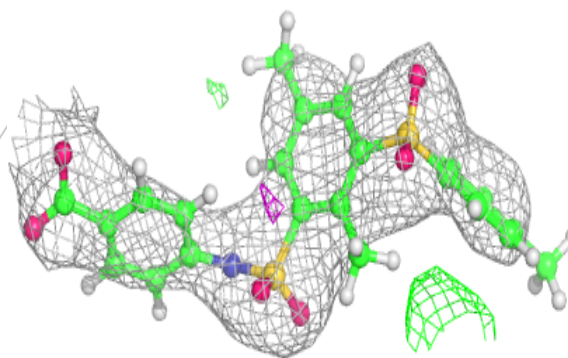
Electron density around CE1 E 601:

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



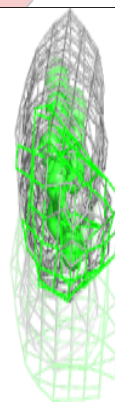
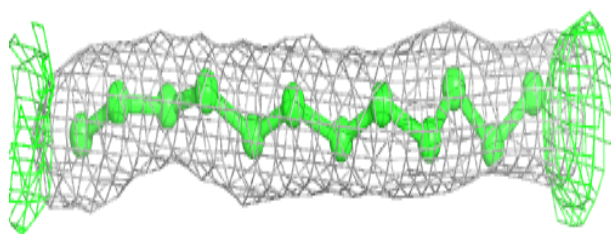
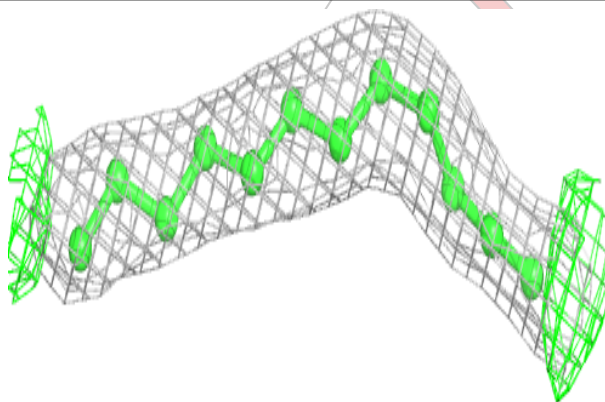
Electron density around YYC F 402:

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



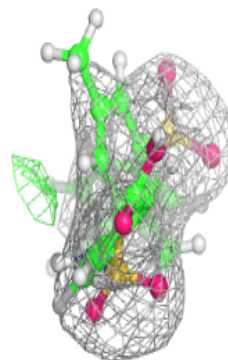
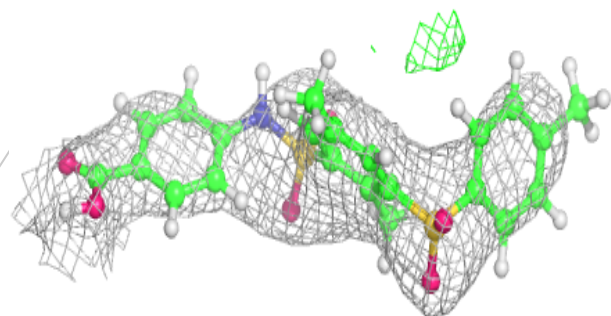
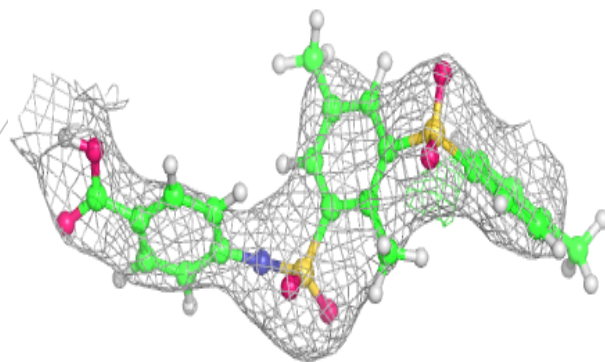
Electron density around CE1 C 403:

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



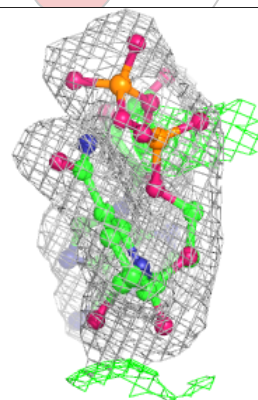
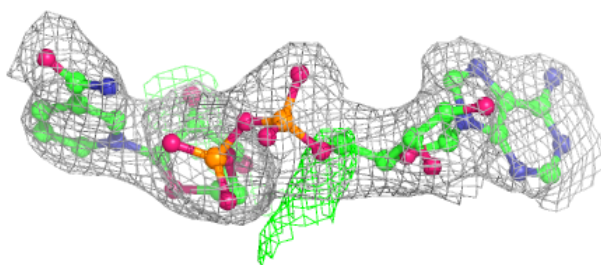
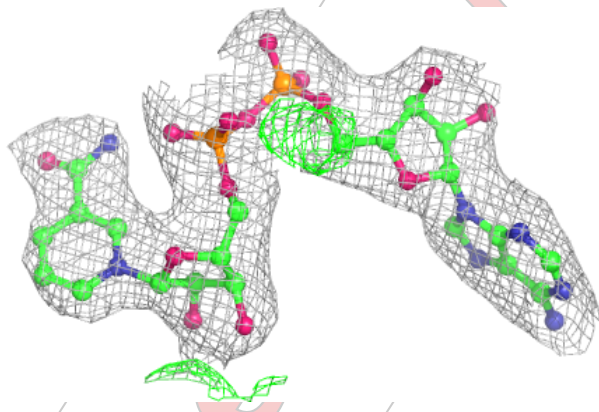
Electron density around YYC G 402:

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 and green (positive)



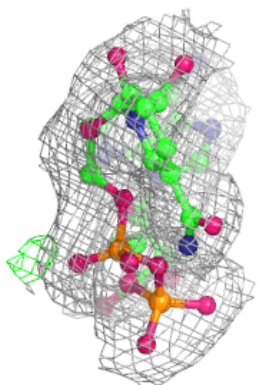
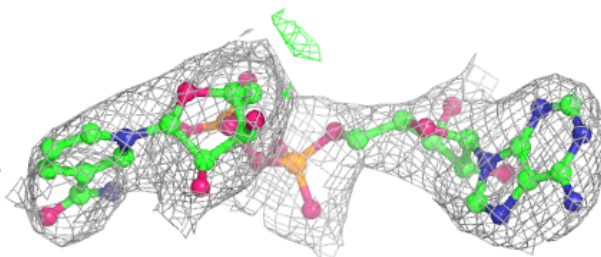
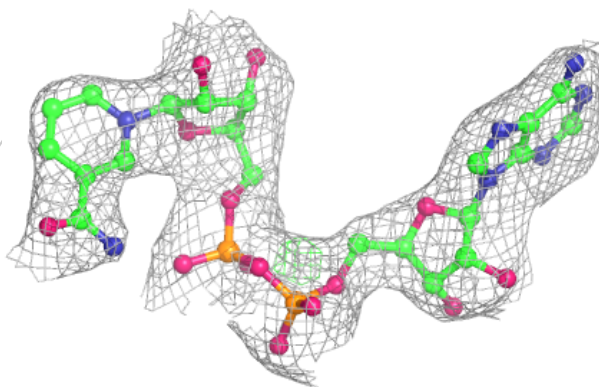
Electron density around NAD H 401:

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



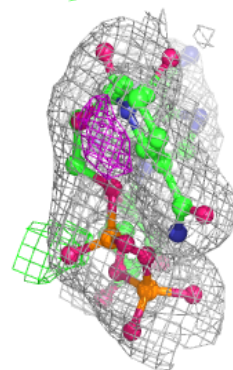
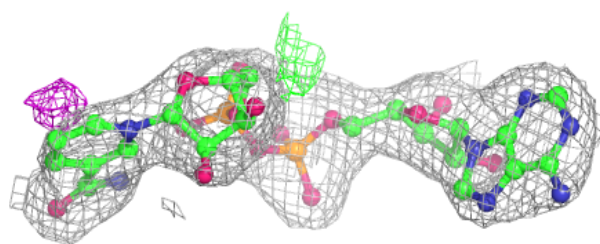
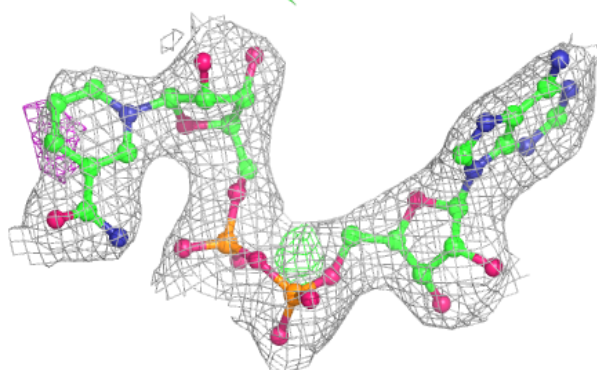
Electron density around NAD G 401:

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



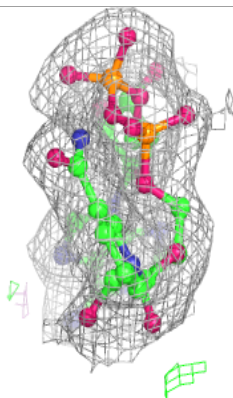
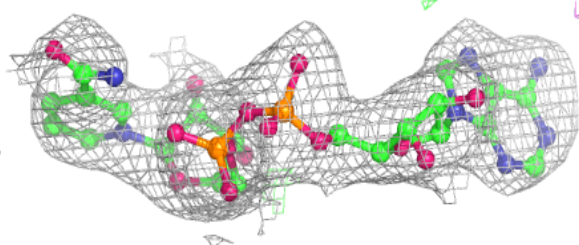
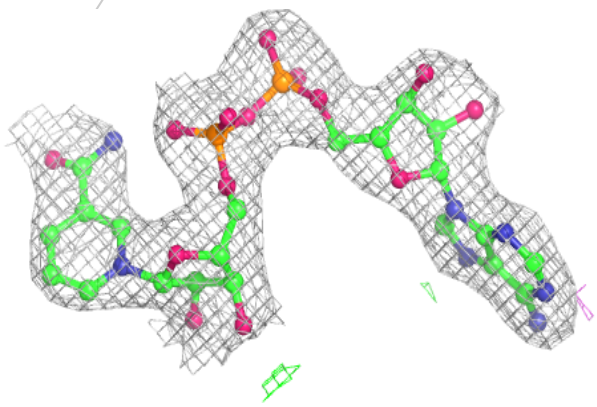
Electron density around NAD E 602:

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



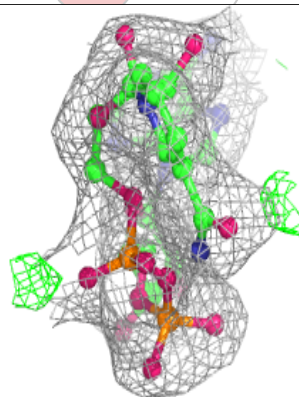
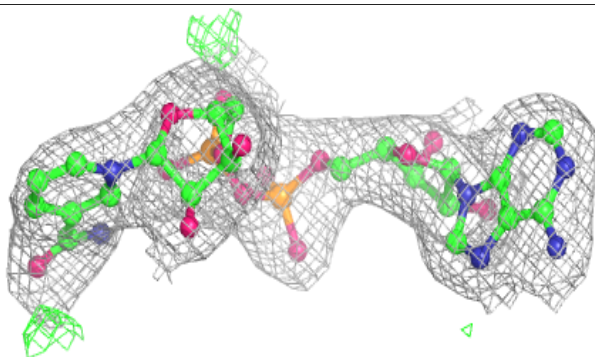
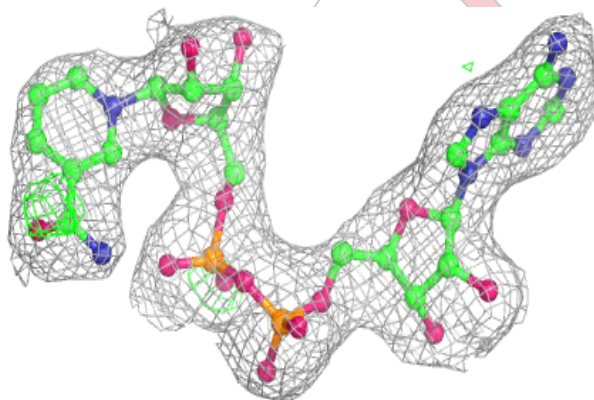
Electron density around NAD C 401:

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



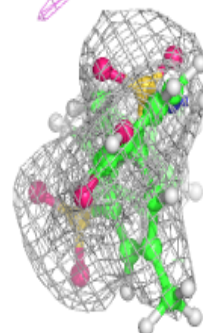
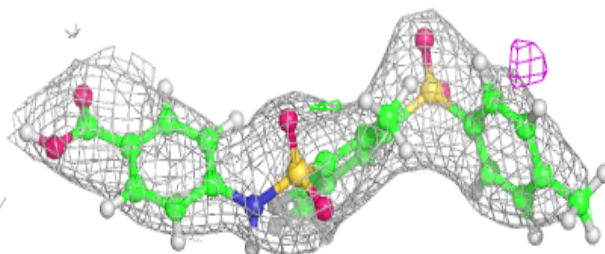
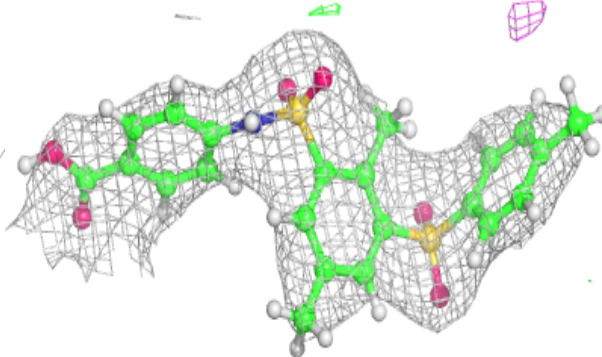
Electron density around NAD A 401:

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



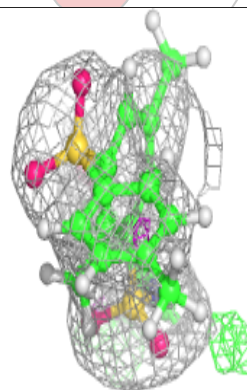
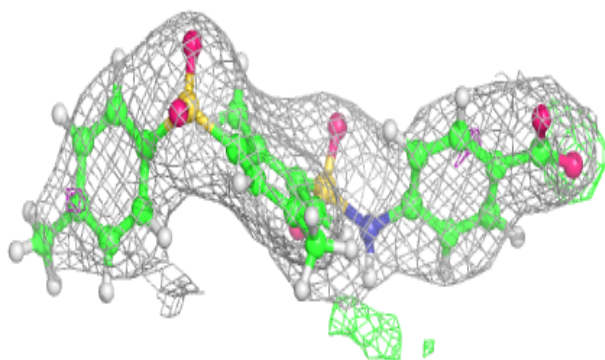
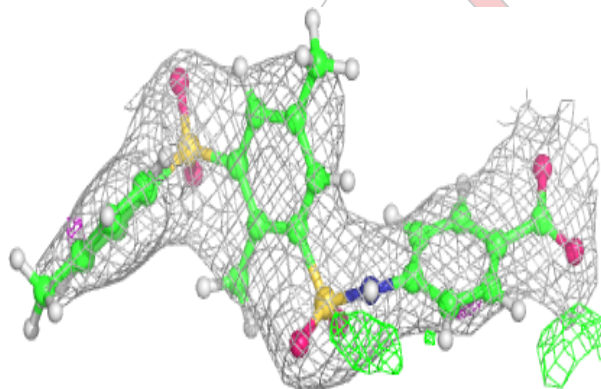
Electron density around YYC H 402:

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



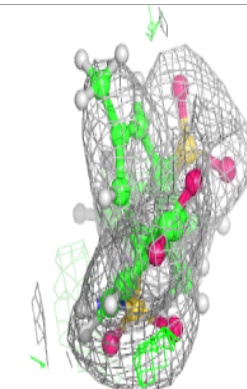
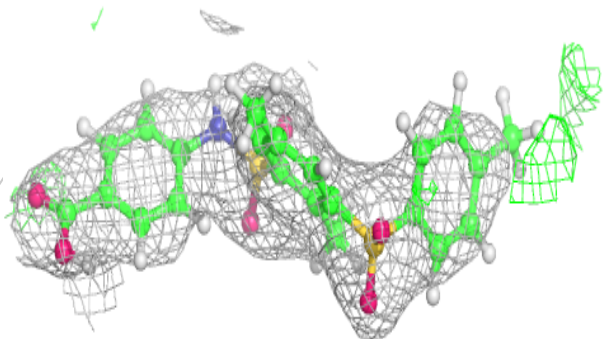
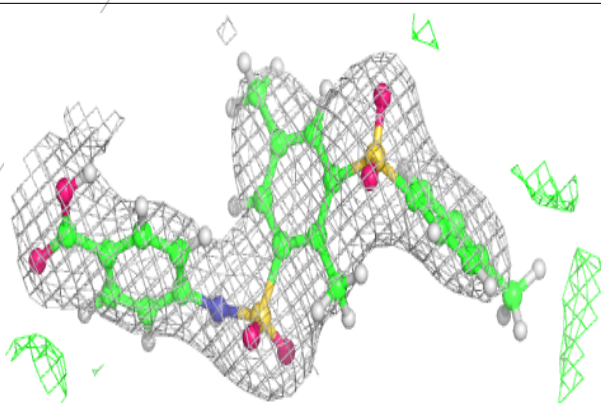
Electron density around YYC A 402:

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



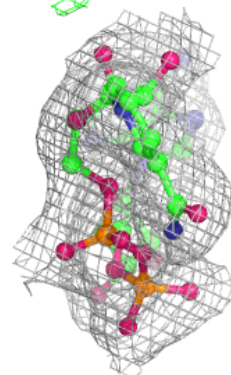
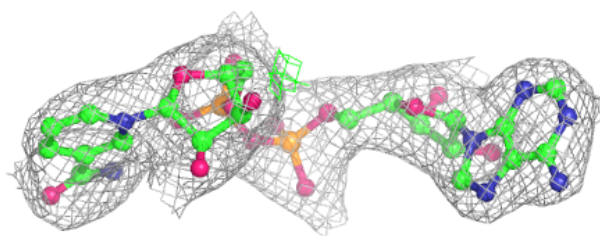
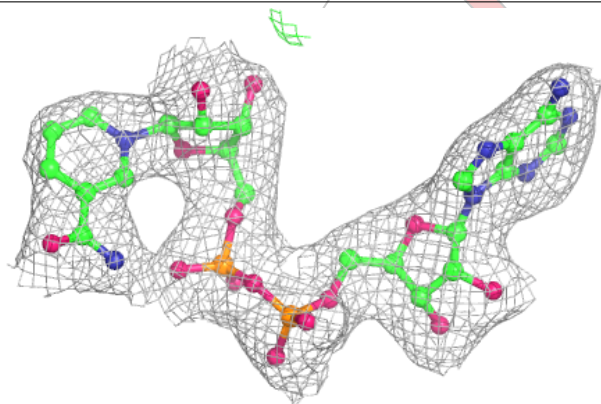
Electron density around YYC B 402:

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



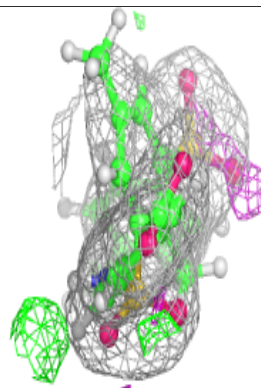
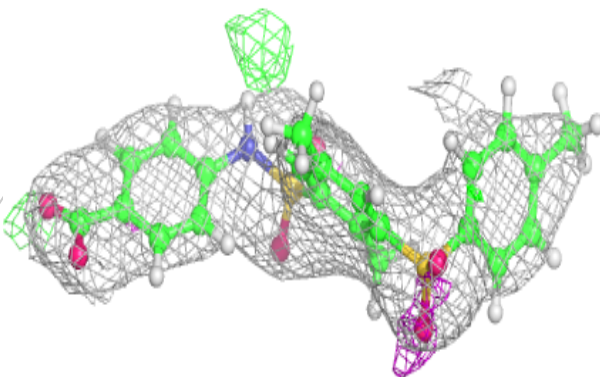
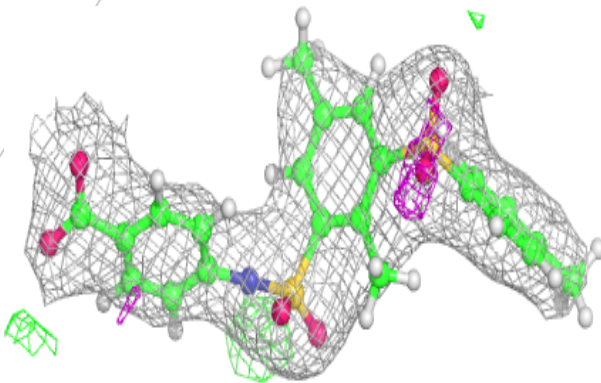
Electron density around NAD F 401:

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



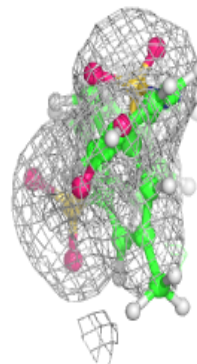
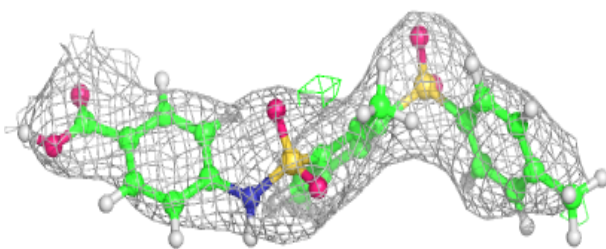
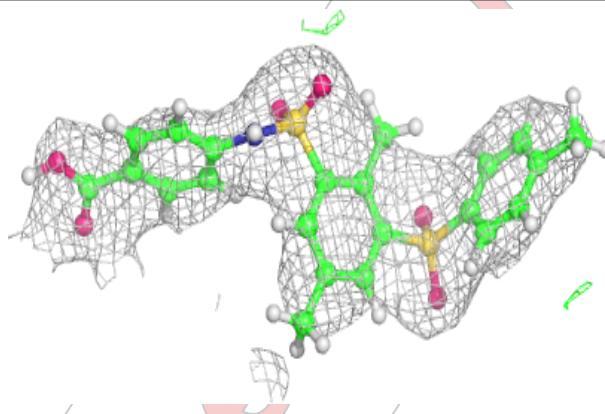
Electron density around YYC D 402:

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



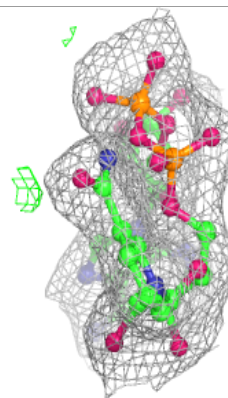
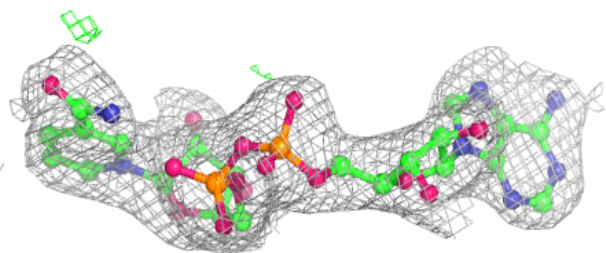
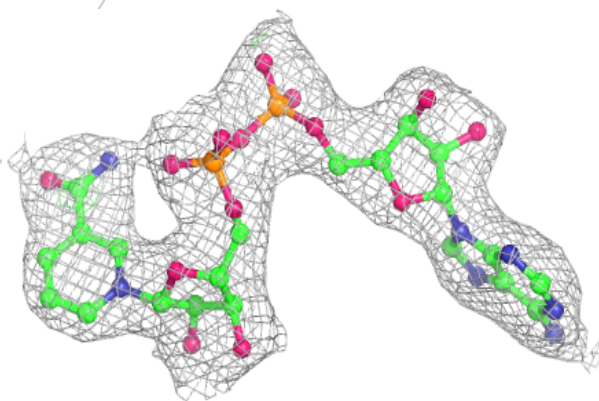
Electron density around YYC E 603:

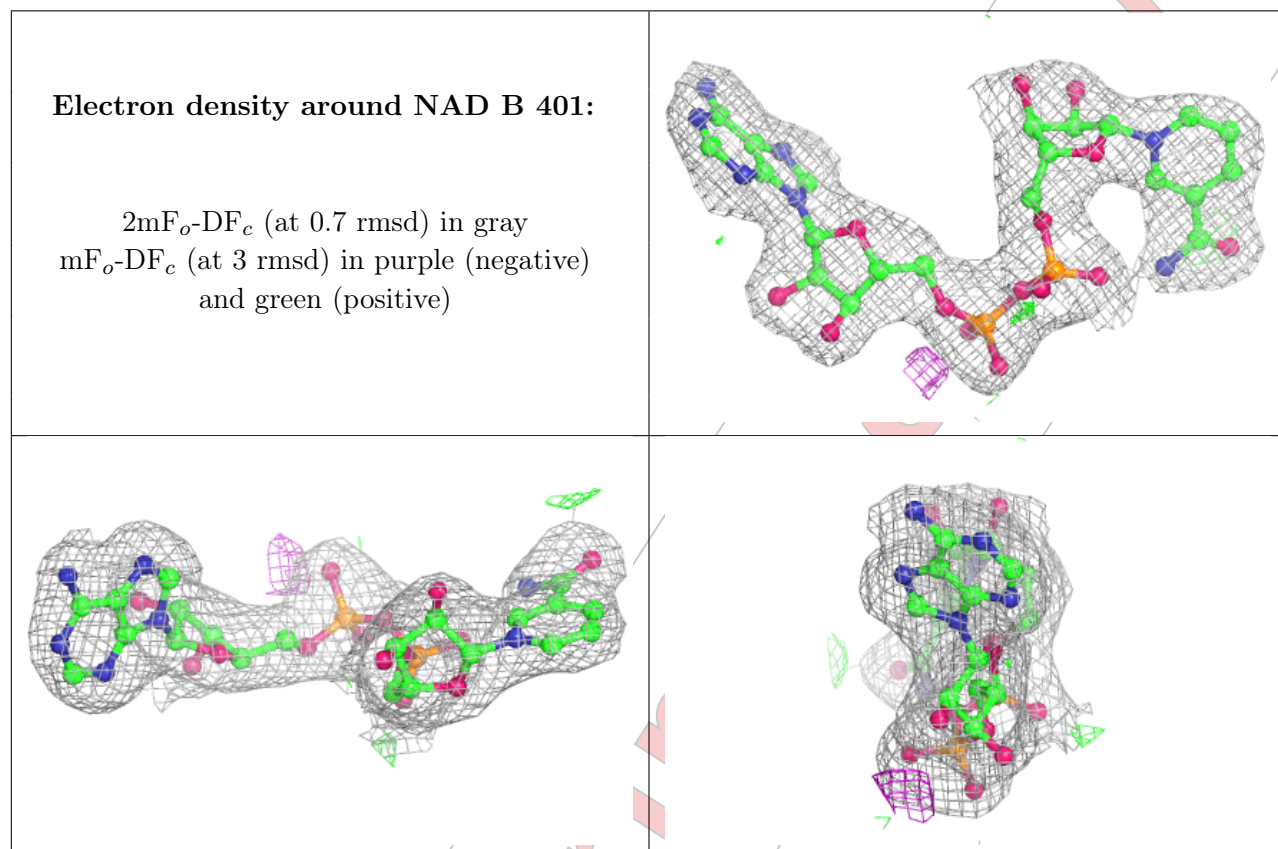
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



Electron density around NAD D 401:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.