



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:12 PM EDT

PDB ID : 8G9V / pdb_00008g9v
Title : Crystal structures of 17-beta-hydroxysteroid dehydrogenase 13
Authors : Liu, S.
Deposited on : 2023-02-22
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

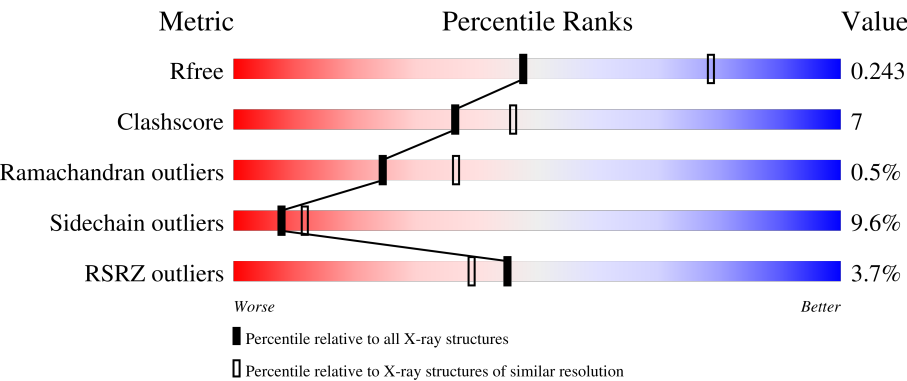
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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% 70% 17% • 10%
1	B	315	% 72% 16% •• 10%
1	C	315	% 68% 16% • 15%
1	D	315	5% 73% 13% • 11%
1	E	315	3% 71% 18% •• 7%

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Mol	Chain	Length	Quality of chain
1	F	315	5% 66% 16% 17%
1	G	315	5% 60% 20% 17%
1	H	315	4% 69% 20% 8%

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	-

2 Entry composition

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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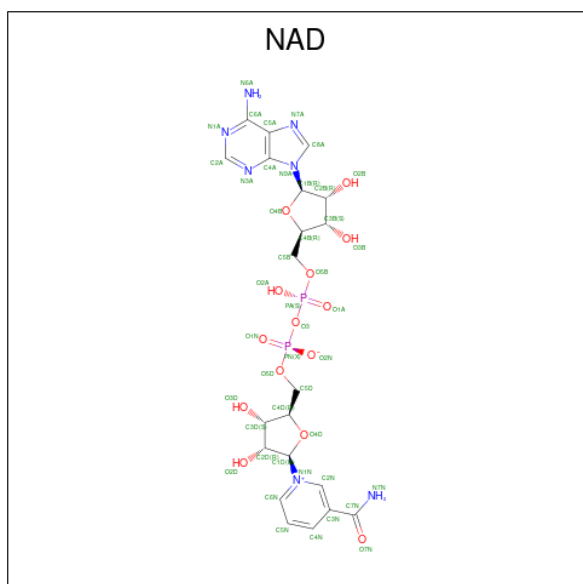
Chain	Residue	Modelled	Actual	Comment	Reference
E	312	HIS	-	expression tag	UNP Q7Z5P4
E	313	HIS	-	expression tag	UNP Q7Z5P4
E	314	HIS	-	expression tag	UNP Q7Z5P4
F	0	MET	-	initiating methionine	UNP Q7Z5P4
F	1	GLY	-	cloning artifact	UNP Q7Z5P4
F	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
F	62	ARG	ILE	engineered 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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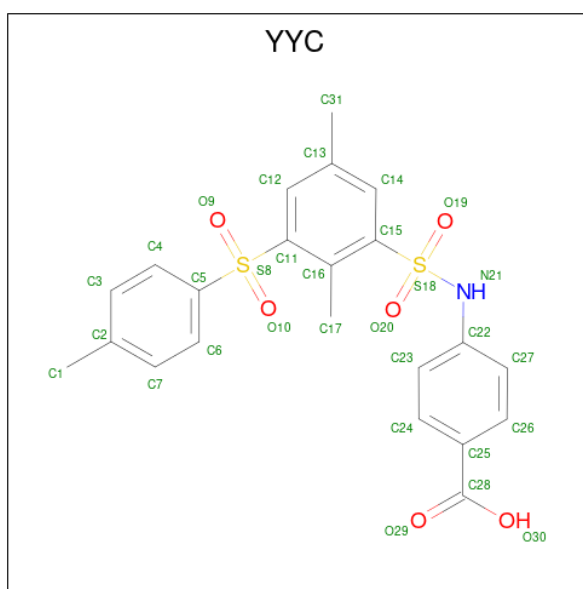
Chain	Residue	Modelled	Actual	Comment	Reference
G	315	HIS	-	expression tag	UNP Q7Z5P4
H	0	MET	-	initiating methionine	UNP Q7Z5P4
H	1	GLY	-	cloning artifact	UNP Q7Z5P4
H	60	LYS	GLN	engineered mutation	UNP Q7Z5P4
H	62	ARG	ILE	engineered mutation	UNP Q7Z5P4
H	71	HIS	ARG	engineered mutation	UNP Q7Z5P4
H	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

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 (CCD ID: YYC) (formula: C₂₂H₂₁NO₆S₂) (labeled as "Ligand of Interest" by depositor).



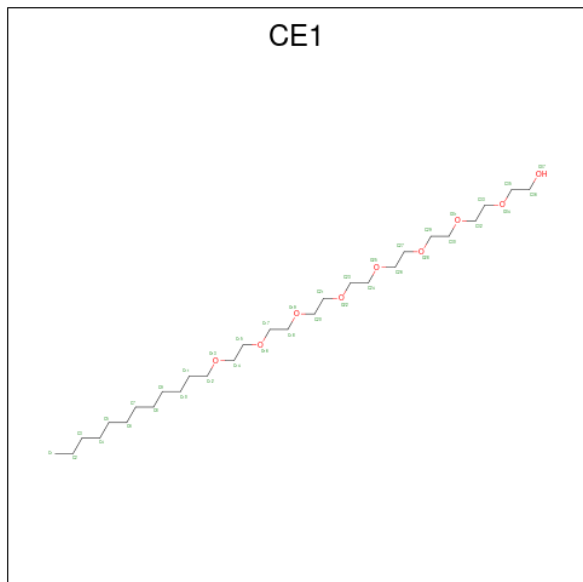
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	20	0
			51	22	20	1	6	2		
3	B	1	Total	C	H	N	O	S	21	0
			52	22	21	1	6	2		
3	C	1	Total	C	H	N	O	S	21	0
			52	22	21	1	6	2		

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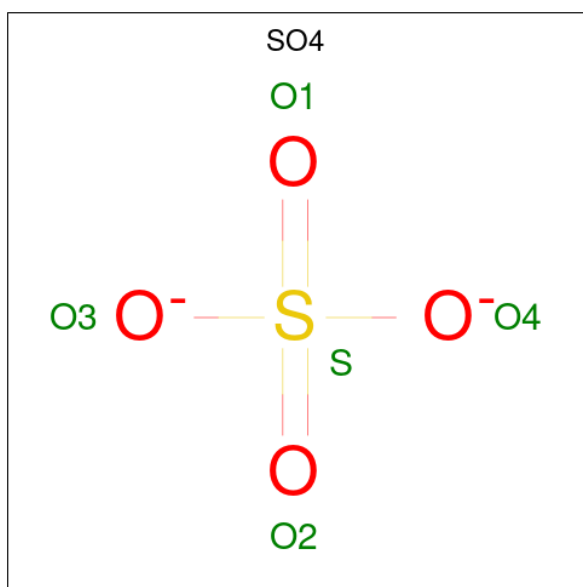
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	20	0
			51	22	20	1	6		
3	E	1	Total	C	H	N	O	21	0
			52	22	21	1	6		
3	F	1	Total	C	H	N	O	20	0
			51	22	20	1	6		
3	G	1	Total	C	H	N	O	21	0
			52	22	21	1	6		
3	H	1	Total	C	H	N	O	21	0
			52	22	21	1	6		

- Molecule 4 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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	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		

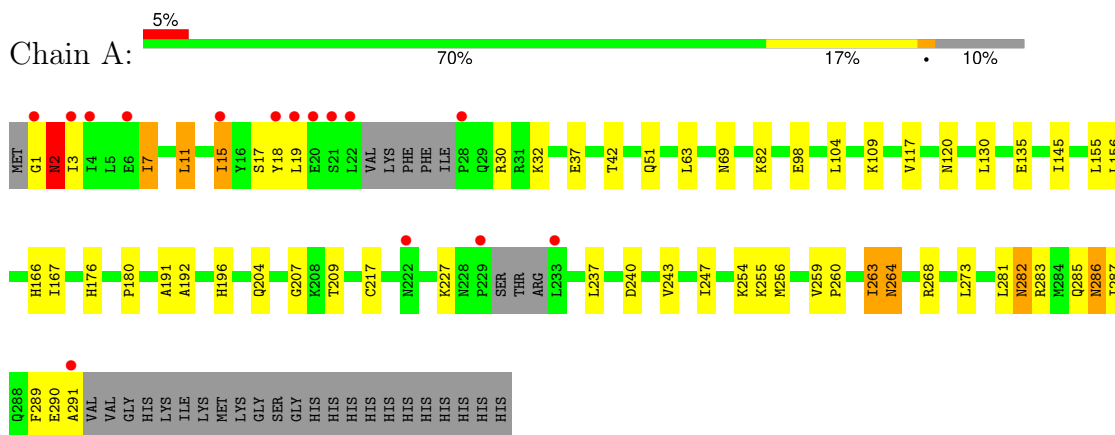
- Molecule 6 is water.

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		

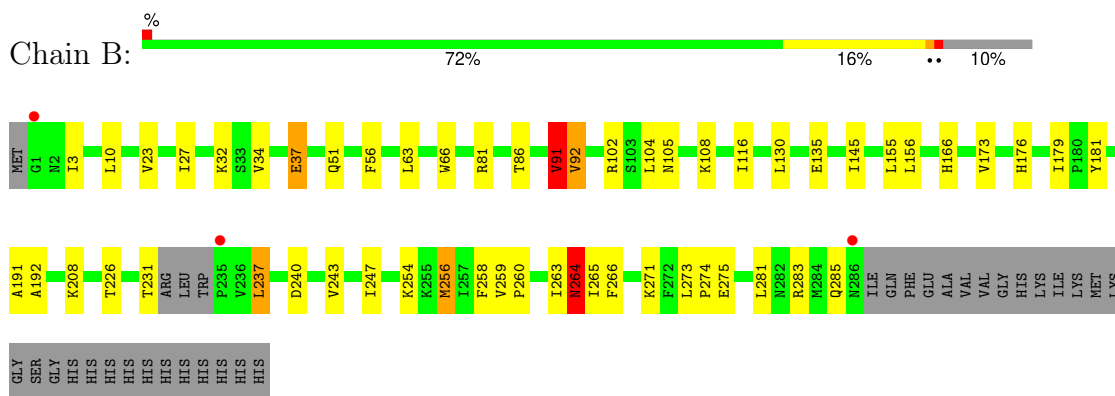
3 Residue-property plots [i](#)

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.

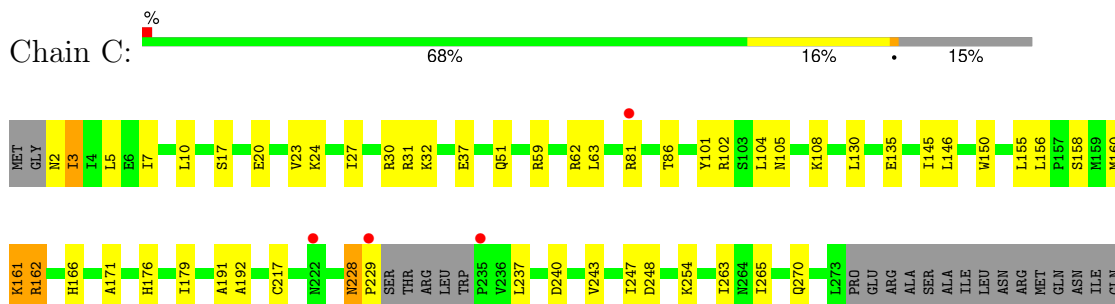
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



PHE
GLU
ALA
VAL
VAL
GLY
HIS
LYS
LYS
LYS
MET
LYS
LYS
GLY
SER
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain D: 

MET G1 N2 I3 I4 L5 E6 I7 L8 L9 L10 L11 L12 L13 L14 Y18 S21 L22 V23 LYS PHE LEU ILE PRO GLN R30 R31 K32 E37 Q51 N69 R81 T86 D93 L104 L130 I137 I145 L155 L156 H166 I167 A171 S172 V173

I179 P184 A191 A192 L199 L209 V219 N222 T226 K227 ASN PRO SER THR ARG LEU TRP PRO V236 L237 D240 V243 T247 D248 T252 R253 K254 V259 P260 L263 Q270 K271 L281 Q285 R286 Q287 Q288 F289 E290 A291 V292 G294

HIS
LYS
ILE
LYS
MET
LYS
GLY
SER
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain E: 

MET G1 I2 I3 I7 L10 L19 L22 V23 K24 I27 R31 K32 S33 V34 G165 A35 G36 I38 F39 V39 L40 L41 Q49 R50 Q51 T52 T53 R59 K60 S61 R62 L63 W66 T86 A87 H88 A89 Y90 V91 Y92 S95 Y101 L104 H105 K108 K109

E110 V111 T115 I116 E135 E142 V143 L146 W150 L155 L156 M160 H164 G165 H166 A171 S172 H176 A191 K208 C217 P218 V219 F220 T226 V236 D240 V243 L251 K254 P260 L263 N264 L265 L269 Q270 K271

E275 R276 I280 L281 N286 E290 A291 V292 V293 GLY HIS LYS ILE VAL MET LYS GLY SER GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain F: 

MET GLY N2 I3 I4 L5 E6 I7 L10 L20 S21 L22 V23 K24 I27 R30 R31 K32 E37 Q51 K60 L63 W66 N69 R81 G84 V85 V92 R96 E99 R102 S103 L104 T115 L130 K133 P134 E135 K139

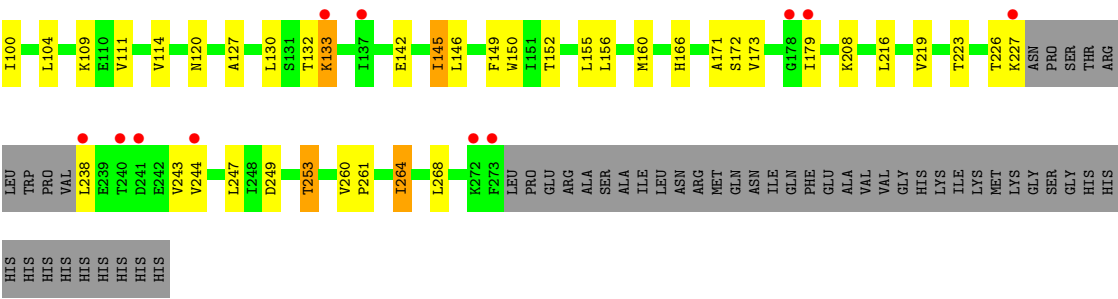
I145 L155 H166 I167 V173 I179 A191 A192 L199 K208 F220 T226 K227 P228 N228 PRO SER THR ARG LEU TRP P235 V236 L237 E238 T239 D240 V243 R244 S245 L246 I247 K254 V259 P260 L263 N264 L267 R268 L269 GLN LYS PHE LEU PRO ARG

ALA SER ALA ILE LEU ASN ARG MET GLN ASN ILE GLN PHE GLU ALA VAL VAL HIS LYS ILE LYS MET MET LYS GLY SER GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

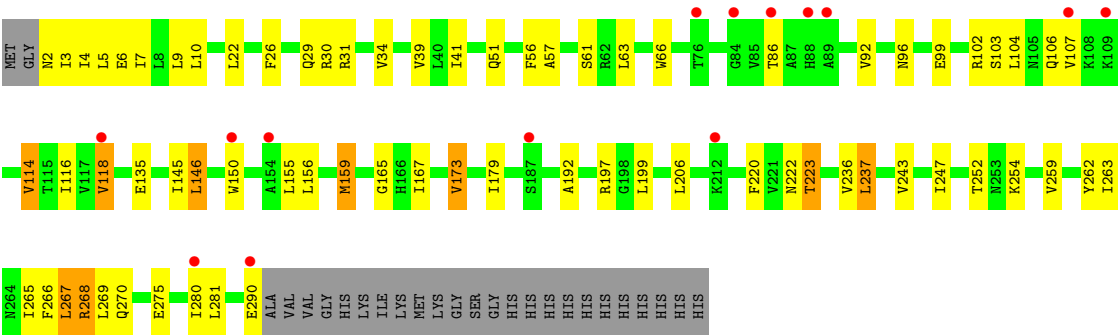
• Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13

Chain G: 

MET GLY N2 I3 I4 L5 E6 I9 L10 T13 L19 E20 S21 L22 V23 K24 I27 P28 Q29 Q30 R31 K32 V34 I41 T42 G45 H46 Q51 T52 T53 L65 W66 D67 I68 V73 E79 T86 A87 H88 A89 V92 D93 D94 S95 N96 E99



● Molecule 1: 17-beta-hydroxysteroid dehydrogenase 13



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 (3.81%)	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)	0.36 , 55.2	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YYC, CE1, SO4, 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	0.77	0/2265	1.15	6/3065 (0.2%)
1	B	0.77	1/2256 (0.0%)	1.16	5/3054 (0.2%)
1	C	0.74	1/2118 (0.0%)	1.14	5/2870 (0.2%)
1	D	0.78	1/2191 (0.0%)	1.14	3/2963 (0.1%)
1	E	0.76	1/2353 (0.0%)	1.21	10/3188 (0.3%)
1	F	0.73	0/2087	1.14	7/2826 (0.2%)
1	G	0.79	1/2065 (0.0%)	1.21	1/2797 (0.0%)
1	H	0.76	0/2316	1.19	4/3141 (0.1%)
All	All	0.76	5/17651 (0.0%)	1.17	41/23904 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	MET	SD-CE	-8.65	1.57	1.79
1	C	171	ALA	CA-C	5.75	1.60	1.52
1	G	171	ALA	CA-C	5.52	1.60	1.52
1	D	171	ALA	CA-C	5.22	1.59	1.52
1	E	171	ALA	CA-C	5.13	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	CA-CB-CG	7.64	120.24	112.60
1	E	63	LEU	N-CA-C	6.96	120.24	108.90
1	B	91	VAL	N-CA-CB	6.89	119.86	111.60
1	A	264	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	1	GLY	CA-C-N	6.48	133.92	121.54
1	A	1	GLY	C-N-CA	6.48	133.92	121.54
1	F	96	ASN	CA-C-N	6.06	128.73	120.54
1	F	96	ASN	C-N-CA	6.06	128.73	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	270	GLN	CA-C-N	5.91	128.52	120.54
1	E	270	GLN	C-N-CA	5.91	128.52	120.54
1	H	275	GLU	CB-CG-CD	5.88	122.61	112.60
1	B	264	ASN	CA-CB-CG	5.48	118.08	112.60
1	H	266	PHE	CA-C-N	5.47	127.55	120.44
1	H	266	PHE	C-N-CA	5.47	127.55	120.44
1	F	96	ASN	N-CA-C	5.46	117.59	107.99
1	D	69	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	63	LEU	N-CA-C	5.43	118.34	109.59
1	H	220	PHE	CA-CB-CG	5.43	119.23	113.80
1	C	101	TYR	CA-C-N	5.39	127.45	120.44
1	C	101	TYR	C-N-CA	5.39	127.45	120.44
1	E	101	TYR	CA-C-N	5.39	127.77	120.44
1	E	101	TYR	C-N-CA	5.39	127.77	120.44
1	B	63	LEU	N-CA-C	5.32	118.15	109.59
1	E	24	LYS	CA-C-N	5.26	127.59	120.44
1	E	24	LYS	C-N-CA	5.26	127.59	120.44
1	E	110	GLU	CA-C-N	5.19	127.20	120.56
1	E	110	GLU	C-N-CA	5.19	127.20	120.56
1	A	69	ASN	CA-CB-CG	5.16	117.76	112.60
1	G	73	VAL	N-CA-CB	5.14	117.54	110.54
1	F	227	LYS	N-CA-C	5.08	116.51	111.07
1	C	2	ASN	CA-C-N	5.08	131.11	121.97
1	C	2	ASN	C-N-CA	5.08	131.11	121.97
1	B	208	LYS	CA-C-N	5.08	127.33	120.38
1	B	208	LYS	C-N-CA	5.08	127.33	120.38
1	F	208	LYS	CA-C-N	5.05	127.30	120.38
1	F	208	LYS	C-N-CA	5.05	127.30	120.38
1	C	63	LEU	N-CA-C	5.05	117.72	109.59
1	E	226	THR	CB-CA-C	5.05	118.47	110.19
1	F	69	ASN	CA-CB-CG	5.03	117.63	112.60
1	D	5	LEU	CA-C-N	5.01	127.41	120.29
1	D	5	LEU	C-N-CA	5.01	127.41	120.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2298	35	0
1	B	2215	0	2291	38	0
1	C	2078	0	2138	29	0
1	D	2157	0	2210	26	0
1	E	2308	0	2393	45	0
1	F	2049	0	2120	26	0
1	G	2029	0	2087	49	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	1	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	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1	0	0	0	0
All	All	18131	268	18218	260	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 (260) 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: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: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:B:176:HIS:CE1	1:B:256:MET:HE3	2.22	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:H:51:GLN:HB2	1:H:243:VAL:HG21	1.73	0.71
1:F:32:LYS:HZ1	1:F:166:HIS:HD2	1.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:32:LYS:HZ1	1:G:166:HIS:HD2	1.36	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
1:A:32:LYS:NZ	1:A:166:HIS:HD2	1.92	0.68
1:D:137:ILE:HD12	1:D:184:PRO:CG	2.22	0.68
1:A:196:HIS:CD2	1:A:256:MET:HE2	2.29	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:E:88:HIS:CD2	1:E:111:VAL:HG22	2.32	0.64
1:A:32:LYS:HZ1	1:A:166:HIS:HD2	1.46	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:B:176:HIS:HE1	1:B:256:MET:HE3	1.62	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:G:88:HIS:CD2	1:G:111:VAL:HG22	2.36	0.60
1:D:32:LYS:HZ1	1:D:166:HIS:HD2	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:LYS:HZ1	1:B:166:HIS:HD2	1.48	0.59
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: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:C:32:LYS:HZ1	1:C:166:HIS:HD2	1.51	0.58
1:E:32:LYS:HZ1	1:E:166:HIS:HD2	1.52	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
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:H:57:ALA:HB2	1:H:63:LEU:HD21	1.88	0.55
1:C:160:MET:HE2	1:D:130:LEU:HD22	1.88	0.55
1:G:146:LEU:HB3	1:G:150:TRP:CH2	2.42	0.55
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:32:LYS:NZ	1:E:166:HIS:HD2	2.05	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:31:ARG:HH22	1:C:248:ASP:CG	2.18	0.52
1:H:104:LEU:HD22	1:H:155:LEU:HD21	1.92	0.52
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:A:196:HIS:NE2	1:A:256:MET:HE2	2.25	0.51
1:F:237:LEU:HD21	1:F:259:VAL:HG12	1.92	0.51
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: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:G:160:MET:HE3	1:G:208:LYS:HG3	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:109:LYS:HZ1	1:G:109:LYS:HE2	1.78	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:C:32:LYS:HZ3	1:C:166:HIS:CD2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:292:VAL:O	1:E:292:VAL:HG13	2.13	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:H:159:MET:CG	1:H:165:GLY:HA3	2.45	0.47
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:A:289:PHE:C	1:A:291:ALA:H	2.25	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:G:223:THR:OG1	2:G:401:NAD:O2N	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:109:LYS:HZ3	1:G:109:LYS:NZ	2.16	0.44
1:F:66:TRP:CG	1:F:92:VAL:CG1	3.00	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: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: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
1:G:53:THR:HG21	1:G:65:LEU:HD23	1.99	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:B:32:LYS:HZ3	1:B:166:HIS:CD2	2.36	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:F:37:GLU:HG3	1:F:115:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:HIS:HE1	1:B:256:MET:CE	2.32	0.41
1:B:258:PHE:CD2	1:B:264:ASN:HB3	2.55	0.41
1:H:22:LEU:HD22	1:H:26:PHE:HE2	1.86	0.41
1:D:32:LYS:HZ3	1:D:166:HIS:CD2	2.39	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: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
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%)	11 16
1	B	279/315 (89%)	268 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	263/315 (84%)	252 (96%)	9 (3%)	2 (1%)	16	24
1	D	274/315 (87%)	268 (98%)	6 (2%)	0	100	100
1	E	291/315 (92%)	274 (94%)	14 (5%)	3 (1%)	12	18
1	F	258/315 (82%)	251 (97%)	7 (3%)	0	100	100
1	G	258/315 (82%)	242 (94%)	13 (5%)	3 (1%)	10	15
1	H	287/315 (91%)	275 (96%)	12 (4%)	0	100	100
All	All	2187/2520 (87%)	2095 (96%)	81 (4%)	11 (0%)	24	36

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%)	224 (91%)	22 (9%)	9	14
1	B	246/275 (90%)	224 (91%)	22 (9%)	9	14
1	C	228/275 (83%)	210 (92%)	18 (8%)	11	18
1	D	232/275 (84%)	209 (90%)	23 (10%)	7	10
1	E	256/275 (93%)	231 (90%)	25 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	228/275 (83%)	204 (90%)	24 (10%)	6	9
1	G	223/275 (81%)	202 (91%)	21 (9%)	8	12
1	H	250/275 (91%)	221 (88%)	29 (12%)	5	7
All	All	1909/2200 (87%)	1725 (90%)	184 (10%)	8	12

All (184) 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
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	209	THR
1	A	227	LYS
1	A	240	ASP
1	A	247	ILE
1	A	254	LYS
1	A	263	ILE
1	A	264	ASN
1	A	268	ARG
1	A	283	ARG
1	A	286	ASN
1	A	287	ILE
1	B	3	ILE
1	B	10	LEU
1	B	37	GLU
1	B	81	ARG
1	B	86	THR
1	B	91	VAL
1	B	92	VAL
1	B	135	GLU
1	B	173	VAL
1	B	179	ILE
1	B	226	THR

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Mol	Chain	Res	Type
1	B	231	THR
1	B	237	LEU
1	B	240	ASP
1	B	247	ILE
1	B	254	LYS
1	B	264	ASN
1	B	265	ILE
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	27	ILE
1	C	37	GLU
1	C	81	ARG
1	C	86	THR
1	C	102	ARG
1	C	135	GLU
1	C	158	SER
1	C	161	LYS
1	C	162	ARG
1	C	179	ILE
1	C	237	LEU
1	C	240	ASP
1	C	247	ILE
1	C	254	LYS
1	C	263	ILE
1	C	270	GLN
1	D	4	ILE
1	D	5	LEU
1	D	10	LEU
1	D	37	GLU
1	D	81	ARG
1	D	86	THR
1	D	173	VAL
1	D	179	ILE
1	D	226	THR
1	D	227	LYS
1	D	236	VAL
1	D	237	LEU
1	D	240	ASP

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Mol	Chain	Res	Type
1	D	247	ILE
1	D	252	THR
1	D	254	LYS
1	D	263	ILE
1	D	271	LYS
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	27	ILE
1	E	37	GLU
1	E	86	THR
1	E	92	VAL
1	E	110	GLU
1	E	115	THR
1	E	116	ILE
1	E	135	GLU
1	E	160	MET
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	290	GLU
1	E	292	VAL
1	F	4	ILE
1	F	5	LEU
1	F	10	LEU
1	F	20	GLU
1	F	22	LEU
1	F	27	ILE
1	F	30	ARG

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Mol	Chain	Res	Type
1	F	81	ARG
1	F	92	VAL
1	F	96	ASN
1	F	102	ARG
1	F	133	LYS
1	F	135	GLU
1	F	139	LYS
1	F	173	VAL
1	F	179	ILE
1	F	226	THR
1	F	237	LEU
1	F	238	GLU
1	F	240	ASP
1	F	245	SER
1	F	247	ILE
1	F	254	LYS
1	F	263	ILE
1	G	4	ILE
1	G	6	GLU
1	G	10	LEU
1	G	19	LEU
1	G	20	GLU
1	G	27	ILE
1	G	29	GLN
1	G	30	ARG
1	G	65	LEU
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	173	VAL
1	G	179	ILE
1	G	253	THR
1	G	264	ILE
1	G	268	LEU
1	H	4	ILE
1	H	9	LEU
1	H	10	LEU
1	H	30	ARG

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Mol	Chain	Res	Type
1	H	31	ARG
1	H	61	SER
1	H	86	THR
1	H	102	ARG
1	H	103	SER
1	H	106	GLN
1	H	107	VAL
1	H	114	VAL
1	H	118	VAL
1	H	135	GLU
1	H	146	LEU
1	H	159	MET
1	H	173	VAL
1	H	179	ILE
1	H	206	LEU
1	H	223	THR
1	H	237	LEU
1	H	247	ILE
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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	164	HIS
1	A	166	HIS
1	A	176	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	270	GLN
1	C	166	HIS
1	C	176	HIS

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Mol	Chain	Res	Type
1	D	2	ASN
1	D	148	HIS
1	D	166	HIS
1	D	285	GLN
1	E	166	HIS
1	E	176	HIS
1	E	264	ASN
1	F	164	HIS
1	F	166	HIS
1	F	228	ASN
1	F	264	ASN
1	G	2	ASN
1	G	96	ASN
1	G	166	HIS
1	H	51	GLN
1	H	96	ASN
1	H	106	GLN
1	H	119	ASN
1	H	228	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 oligosaccharides 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	$\# Z > 2$
4	CE1	D	403	-	30,30,36	0.33	0	29,29,35	0.22	0
5	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.35	0
5	SO4	C	404	-	4,4,4	0.44	0	6,6,6	0.18	0
5	SO4	H	403	-	4,4,4	0.30	0	6,6,6	0.17	0
3	YYC	C	402	-	33,33,33	0.24	0	48,50,50	0.40	0
3	YYC	A	402	-	33,33,33	0.21	0	48,50,50	0.34	0
5	SO4	E	604	-	4,4,4	0.24	0	6,6,6	0.18	0
2	NAD	G	401	-	46,48,48	0.43	0	64,73,73	0.50	0
2	NAD	D	401	-	46,48,48	0.41	0	64,73,73	0.64	1 (1%)
3	YYC	B	402	-	33,33,33	0.25	0	48,50,50	0.55	0
5	SO4	G	403	-	4,4,4	0.25	0	6,6,6	0.28	0
5	SO4	F	405	-	4,4,4	0.20	0	6,6,6	0.33	0
4	CE1	C	403	-	11,11,36	0.45	0	10,10,35	0.29	0
2	NAD	A	401	-	46,48,48	0.41	0	64,73,73	0.47	0
3	YYC	G	402	-	33,33,33	0.21	0	48,50,50	0.37	0
3	YYC	E	603	-	33,33,33	0.19	0	48,50,50	0.35	0
5	SO4	H	404	-	4,4,4	0.23	0	6,6,6	0.23	0
5	SO4	C	407	-	4,4,4	0.21	0	6,6,6	0.12	0
5	SO4	H	405	-	4,4,4	0.24	0	6,6,6	0.16	0
4	CE1	A	403	-	36,36,36	0.40	0	35,35,35	0.22	0
5	SO4	A	405	-	4,4,4	0.28	0	6,6,6	0.30	0
3	YYC	D	402	-	33,33,33	0.25	0	48,50,50	0.43	0
2	NAD	B	401	-	46,48,48	0.40	0	64,73,73	0.52	0
5	SO4	C	405	-	4,4,4	0.32	0	6,6,6	0.18	0
3	YYC	F	402	-	33,33,33	0.20	0	48,50,50	0.33	0
5	SO4	B	404	-	4,4,4	0.22	0	6,6,6	0.28	0
2	NAD	H	401	-	46,48,48	0.39	0	64,73,73	0.46	0
5	SO4	G	404	-	4,4,4	0.27	0	6,6,6	0.20	0
5	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.19	0
5	SO4	F	403	-	4,4,4	0.24	0	6,6,6	0.36	0
2	NAD	C	401	-	46,48,48	0.37	0	64,73,73	0.46	0
5	SO4	A	404	-	4,4,4	0.37	0	6,6,6	0.12	0
2	NAD	F	401	-	46,48,48	0.37	0	64,73,73	0.47	0
2	NAD	E	602	-	46,48,48	0.39	0	64,73,73	0.46	0
5	SO4	F	404	-	4,4,4	0.15	0	6,6,6	0.09	0
4	CE1	E	601	-	11,11,36	0.25	0	10,10,35	0.18	0
3	YYC	H	402	-	33,33,33	0.21	0	48,50,50	0.45	0

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
4	CE1	D	403	-	-	9/28/28/34	-
3	YYC	C	402	-	-	11/27/27/27	0/3/3/3
3	YYC	A	402	-	-	12/27/27/27	0/3/3/3
2	NAD	G	401	-	-	6/30/62/62	0/5/5/5
2	NAD	D	401	-	-	5/30/62/62	0/5/5/5
3	YYC	B	402	-	-	6/27/27/27	0/3/3/3
4	CE1	C	403	-	-	3/9/9/34	-
2	NAD	A	401	-	-	8/30/62/62	0/5/5/5
3	YYC	G	402	-	-	11/27/27/27	0/3/3/3
3	YYC	E	603	-	-	6/27/27/27	0/3/3/3
4	CE1	A	403	-	-	13/34/34/34	-
3	YYC	D	402	-	-	10/27/27/27	0/3/3/3
2	NAD	B	401	-	-	7/30/62/62	0/5/5/5
3	YYC	F	402	-	-	11/27/27/27	0/3/3/3
2	NAD	H	401	-	-	7/30/62/62	0/5/5/5
2	NAD	C	401	-	-	7/30/62/62	0/5/5/5
2	NAD	F	401	-	-	8/30/62/62	0/5/5/5
2	NAD	E	602	-	-	7/30/62/62	0/5/5/5
4	CE1	E	601	-	-	2/9/9/34	-
3	YYC	H	402	-	-	6/27/27/27	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	C4D-O4D-C1D	-3.07	107.12	109.92

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	401	NAD	C5D-O5D-PN-O3
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-O3
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-O3
2	E	602	NAD	C5D-O5D-PN-O1N
2	E	602	NAD	C5D-O5D-PN-O2N
2	E	602	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	C5D-O5D-PN-O3
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-O3
2	G	401	NAD	C5D-O5D-PN-O1N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	C5D-O5D-PN-O3
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	D	403	CE1	O19-C20-C21-O22
4	A	403	CE1	O19-C20-C21-O22
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	A	403	CE1	O16-C17-C18-O19
4	D	403	CE1	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
4	A	403	CE1	O34-C35-C36-O37
4	D	403	CE1	O34-C35-C36-O37
4	E	601	CE1	C6-C7-C8-C9
4	A	403	CE1	C3-C4-C5-C6
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	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	A	402	YYC	C22-N21-S18-O19
3	A	402	YYC	C22-N21-S18-O20
4	A	403	CE1	C1-C2-C3-C4
3	A	402	YYC	C4-C5-S8-O9
3	G	402	YYC	C6-C5-S8-O9
3	D	402	YYC	C6-C5-S8-O9
3	F	402	YYC	C6-C5-S8-O9
3	A	402	YYC	C6-C5-S8-O9
3	C	402	YYC	C6-C5-S8-O9
4	A	403	CE1	C2-C3-C4-C5
3	F	402	YYC	C4-C5-S8-O9
3	G	402	YYC	C4-C5-S8-O9
2	D	401	NAD	PN-O3-PA-O5B
4	A	403	CE1	C20-C21-O22-C23
3	C	402	YYC	C4-C5-S8-O9
3	D	402	YYC	C4-C5-S8-O9
4	D	403	CE1	C20-C21-O22-C23
3	C	402	YYC	C22-N21-S18-C15
3	D	402	YYC	C22-N21-S18-C15
3	F	402	YYC	C22-N21-S18-C15

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Mol	Chain	Res	Type	Atoms
3	G	402	YYC	C22-N21-S18-C15
4	A	403	CE1	C23-C24-O25-C26
4	D	403	CE1	C23-C24-O25-C26
3	H	402	YYC	C22-N21-S18-O20
4	D	403	CE1	C21-C20-O19-C18
4	A	403	CE1	C21-C20-O19-C18
4	A	403	CE1	C18-C17-O16-C15
3	A	402	YYC	C22-N21-S18-C15
4	D	403	CE1	C18-C17-O16-C15
3	B	402	YYC	C16-C15-S18-O20
3	D	402	YYC	C16-C15-S18-O19
2	G	401	NAD	C5D-O5D-PN-O2N
3	E	603	YYC	C22-N21-S18-C15
3	B	402	YYC	C4-C5-S8-O9
3	B	402	YYC	C6-C5-S8-O9
3	H	402	YYC	C16-C15-S18-O19
4	C	403	CE1	C3-C4-C5-C6
2	F	401	NAD	C2D-C1D-N1N-C6N
3	A	402	YYC	C16-C15-S18-O20
3	C	402	YYC	C16-C15-S18-O19
3	E	603	YYC	C16-C15-S18-O19
3	A	402	YYC	C4-C5-S8-C11
3	H	402	YYC	C22-N21-S18-O19
4	E	601	CE1	C5-C6-C7-C8
3	F	402	YYC	C16-C15-S18-O19
3	G	402	YYC	C16-C15-S18-O19
3	F	402	YYC	C6-C5-S8-C11
3	G	402	YYC	C6-C5-S8-C11
2	A	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	E	602	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	H	401	NAD	O4D-C1D-N1N-C6N
3	D	402	YYC	C6-C5-S8-C11
2	B	401	NAD	PA-O3-PN-O1N
2	F	401	NAD	PA-O3-PN-O1N
2	H	401	NAD	PA-O3-PN-O1N
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	F	402	YYC	C16-C15-S18-O20
4	D	403	CE1	C24-C23-O22-C21

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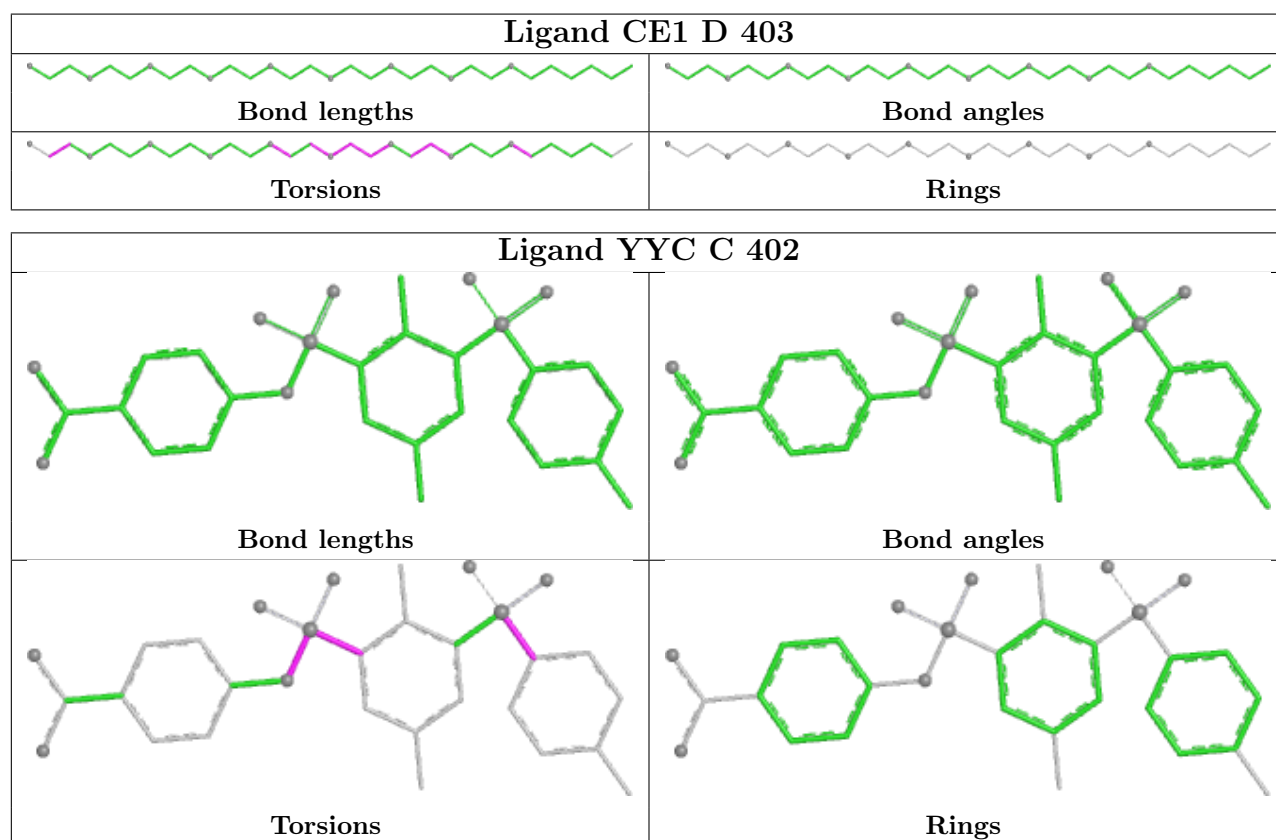
Mol	Chain	Res	Type	Atoms
4	C	403	CE1	C11-C10-C9-C8
3	G	402	YYC	C4-C5-S8-C11
3	H	402	YYC	C22-N21-S18-C15
3	A	402	YYC	C16-C15-S18-O19
3	C	402	YYC	C16-C15-S18-O20
3	G	402	YYC	C16-C15-S18-O20
4	D	403	CE1	C11-C12-O13-C14
3	C	402	YYC	C4-C5-S8-C11
3	D	402	YYC	C4-C5-S8-C11
4	A	403	CE1	C24-C23-O22-C21
2	C	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PA-O3-PN-O1N
2	E	602	NAD	PA-O3-PN-O1N
2	G	401	NAD	O4B-C4B-C5B-O5B
2	H	401	NAD	O4B-C4B-C5B-O5B
3	A	402	YYC	C26-C25-C28-O29
4	C	403	CE1	C1-C2-C3-C4
4	A	403	CE1	C11-C12-O13-C14
3	B	402	YYC	C14-C15-S18-O20
2	A	401	NAD	PA-O3-PN-O2N
2	B	401	NAD	PA-O3-PN-O2N
2	C	401	NAD	PA-O3-PN-O2N
2	E	602	NAD	PA-O3-PN-O2N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B

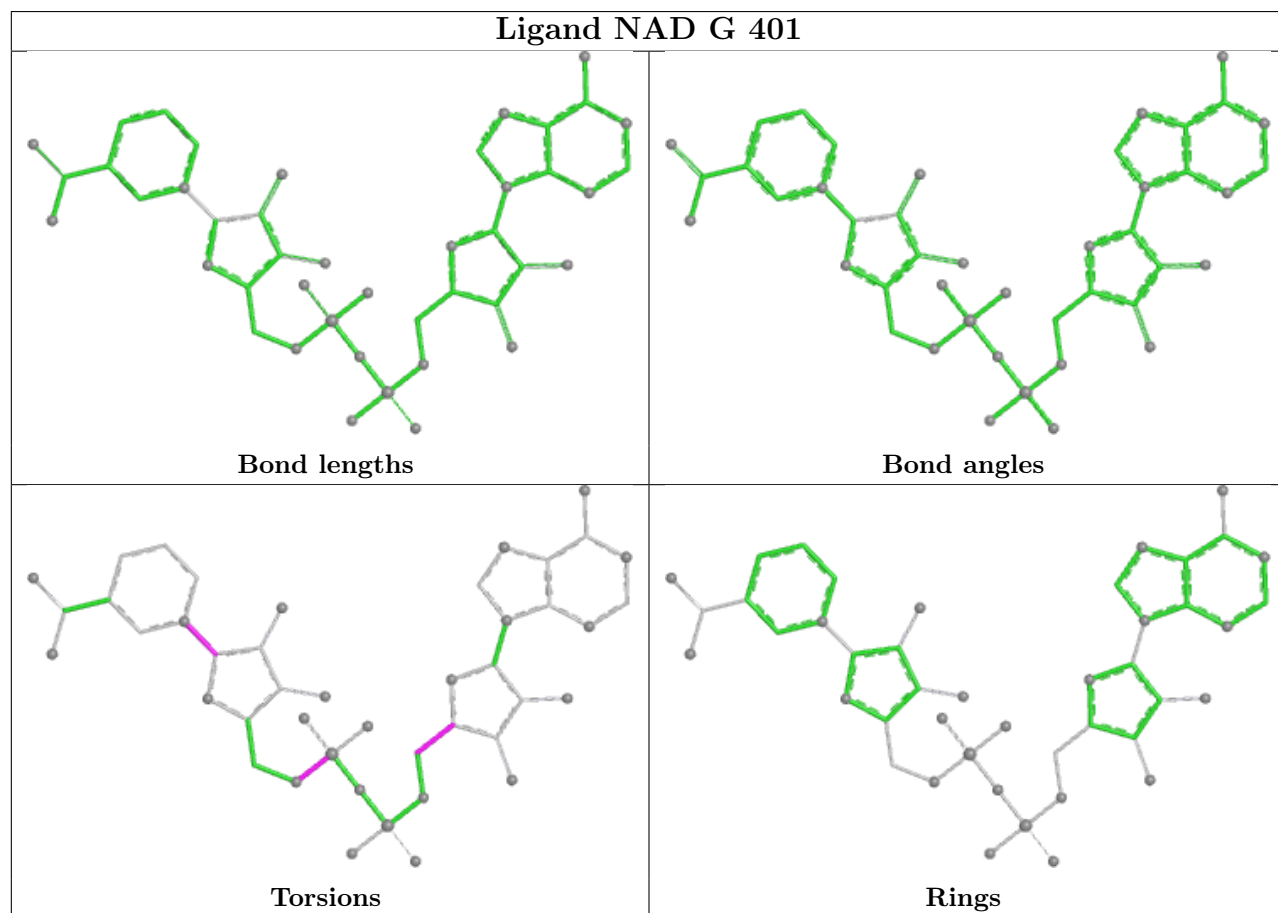
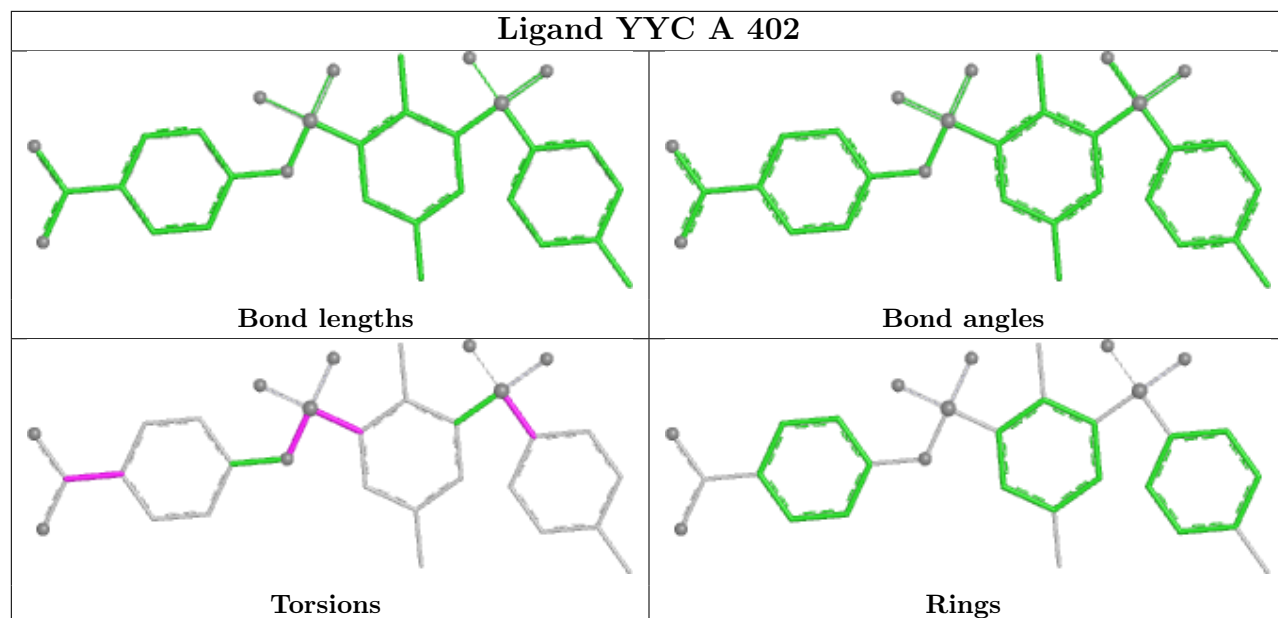
There are no ring outliers.

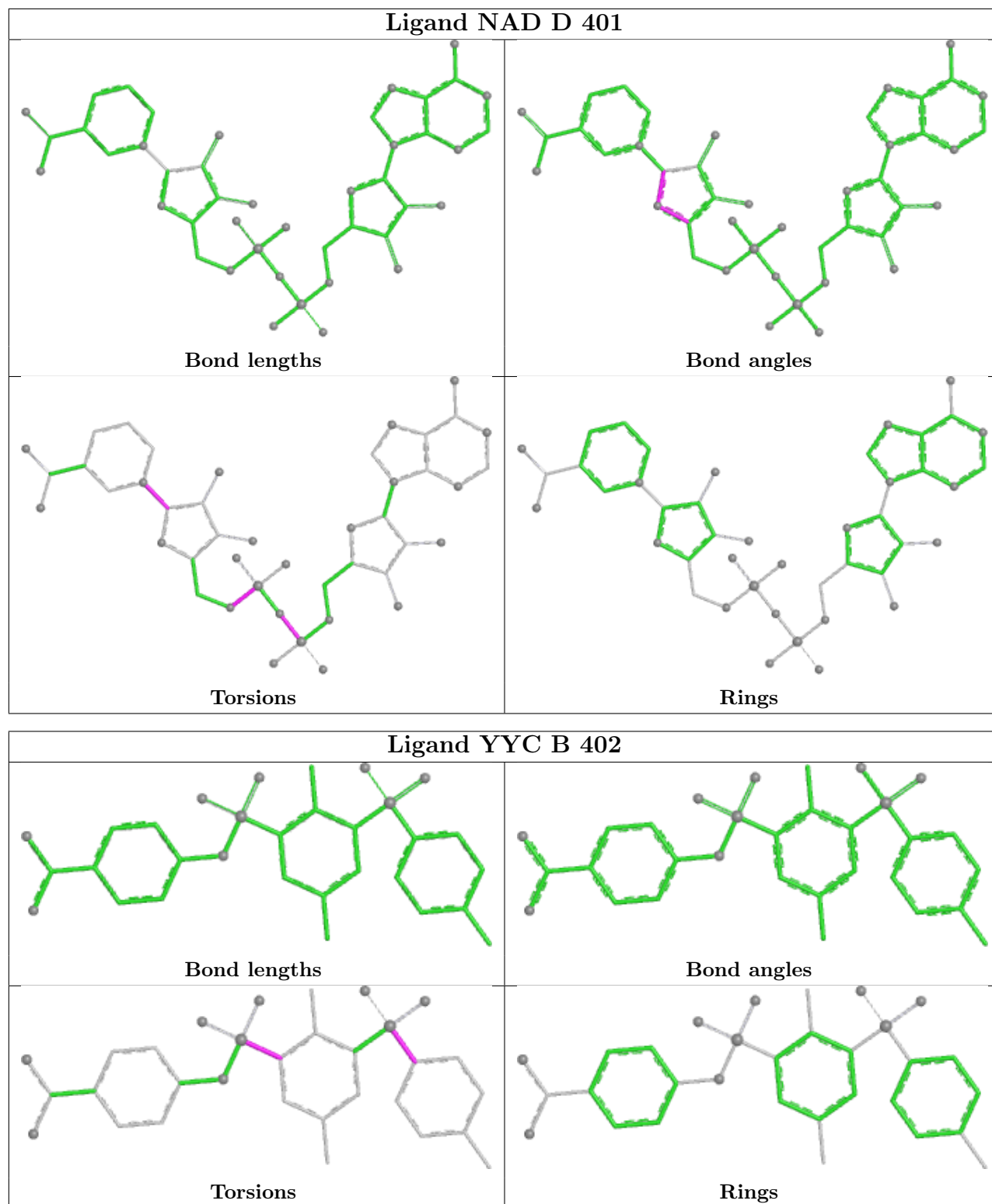
12 monomers are involved in 21 short contacts:

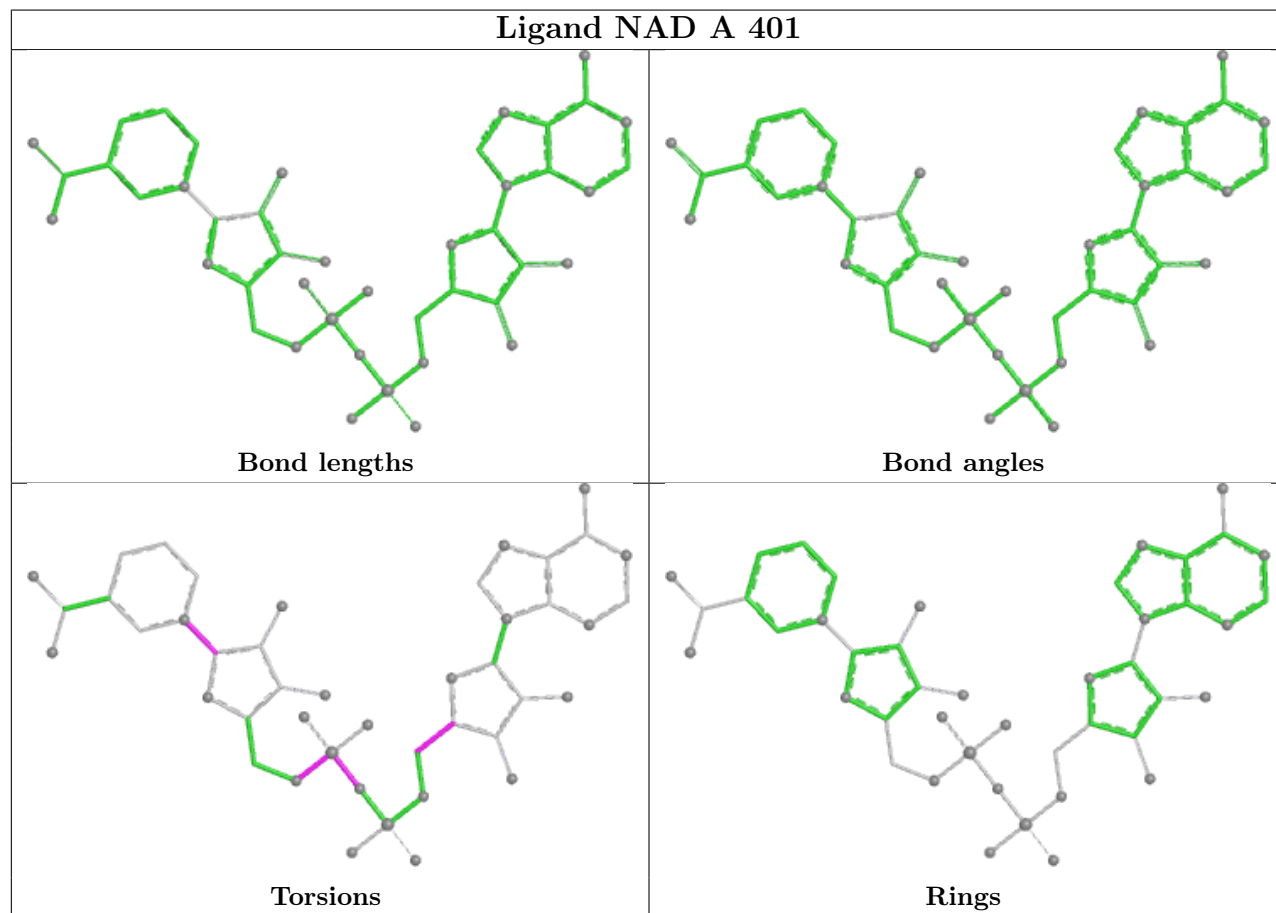
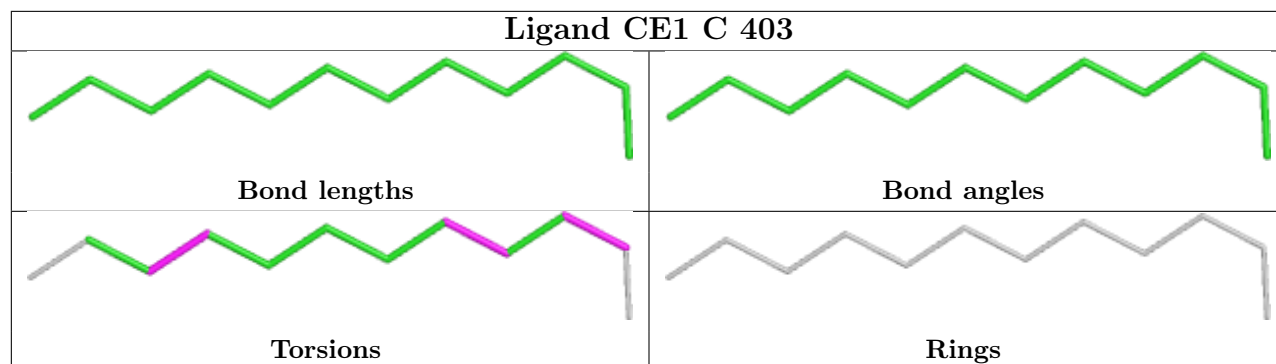
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	CE1	4	0
5	C	406	SO4	1	0
5	C	404	SO4	2	0
2	G	401	NAD	1	0
2	D	401	NAD	1	0
4	C	403	CE1	2	0
5	C	407	SO4	1	0
5	H	405	SO4	1	0
4	A	403	CE1	2	0
2	H	401	NAD	2	0
5	G	404	SO4	1	0
4	E	601	CE1	3	0

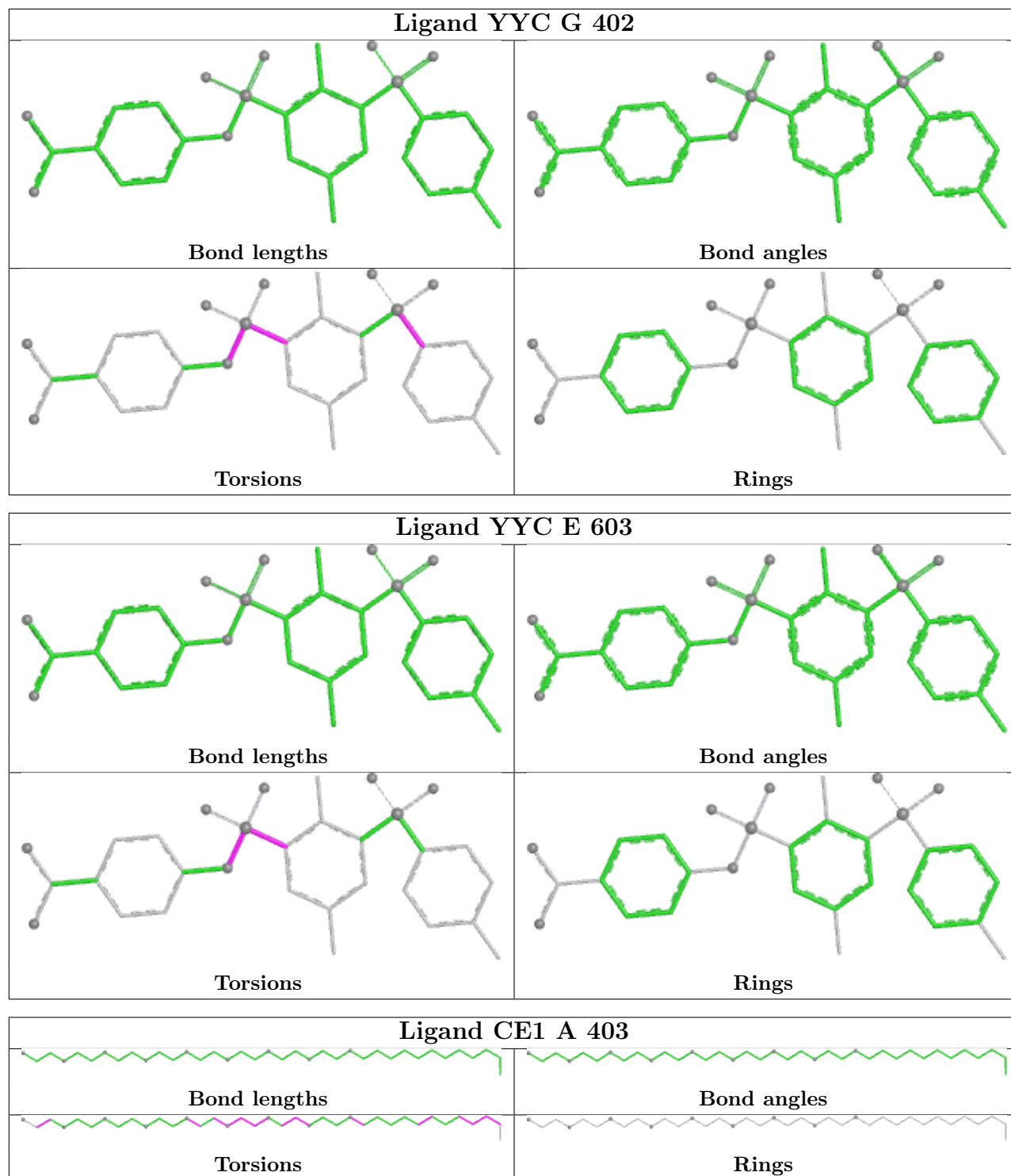
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

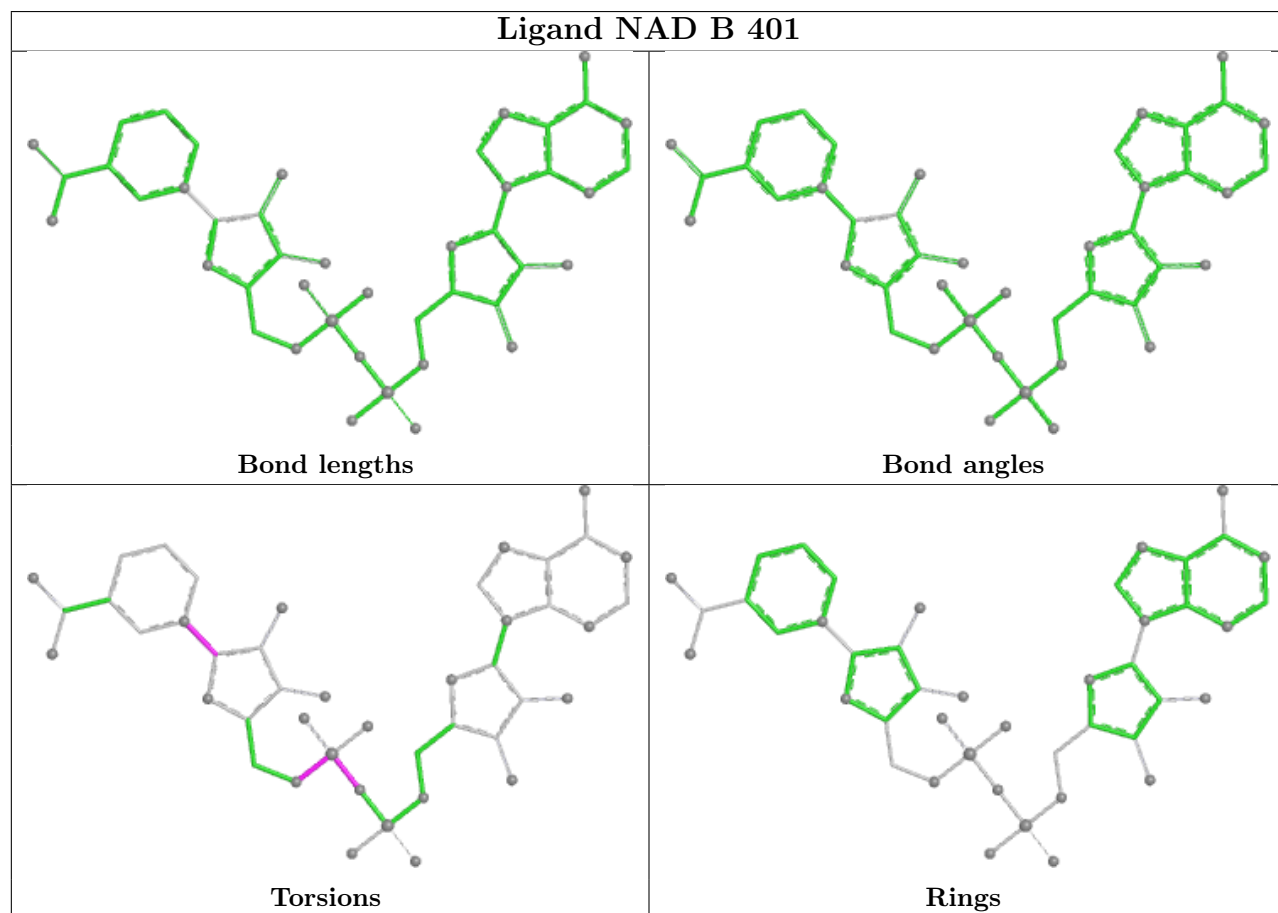
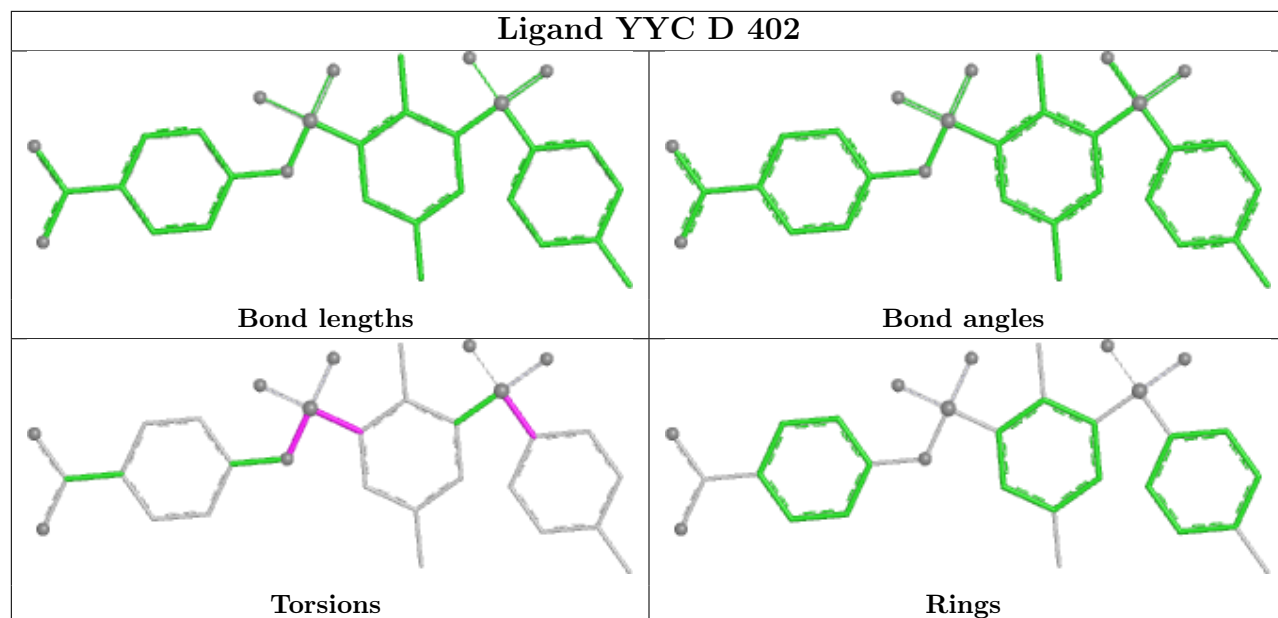


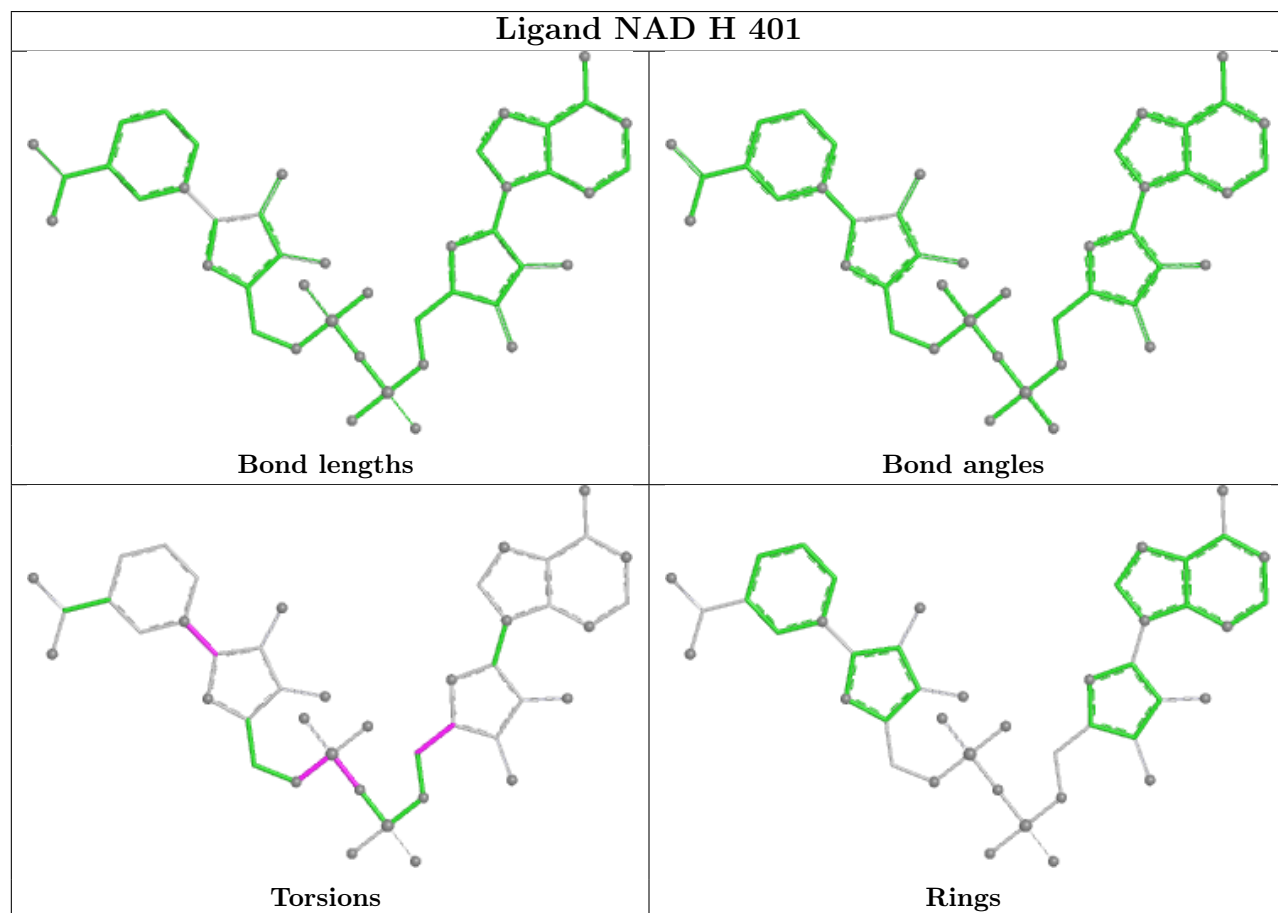
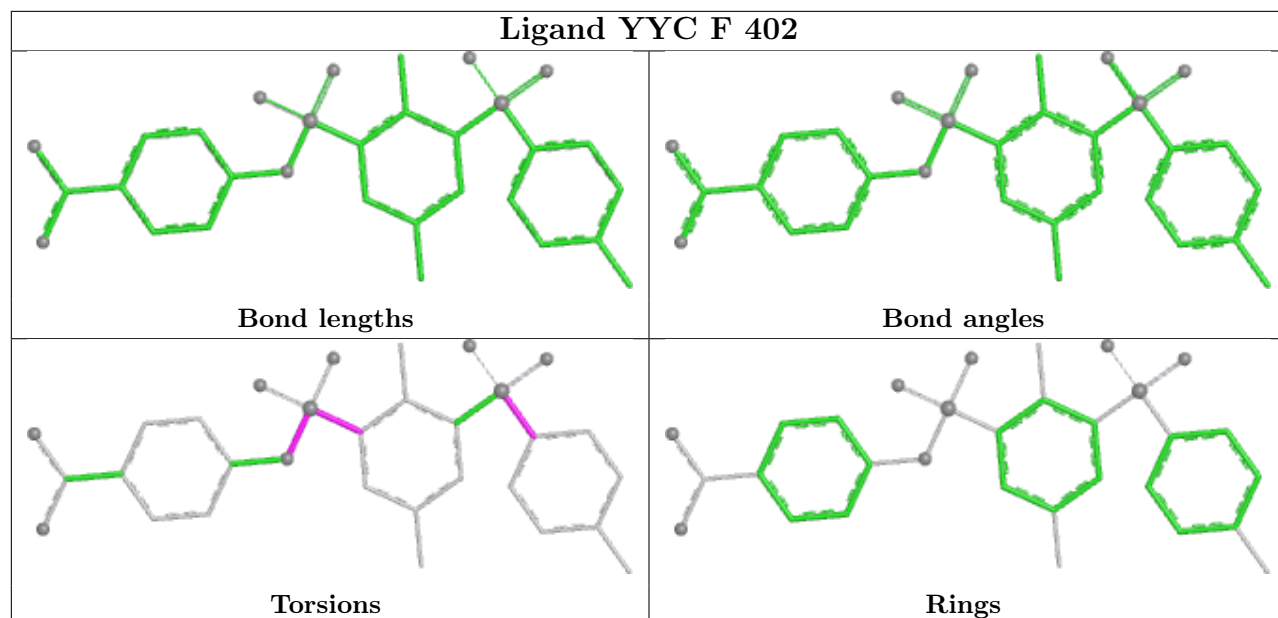


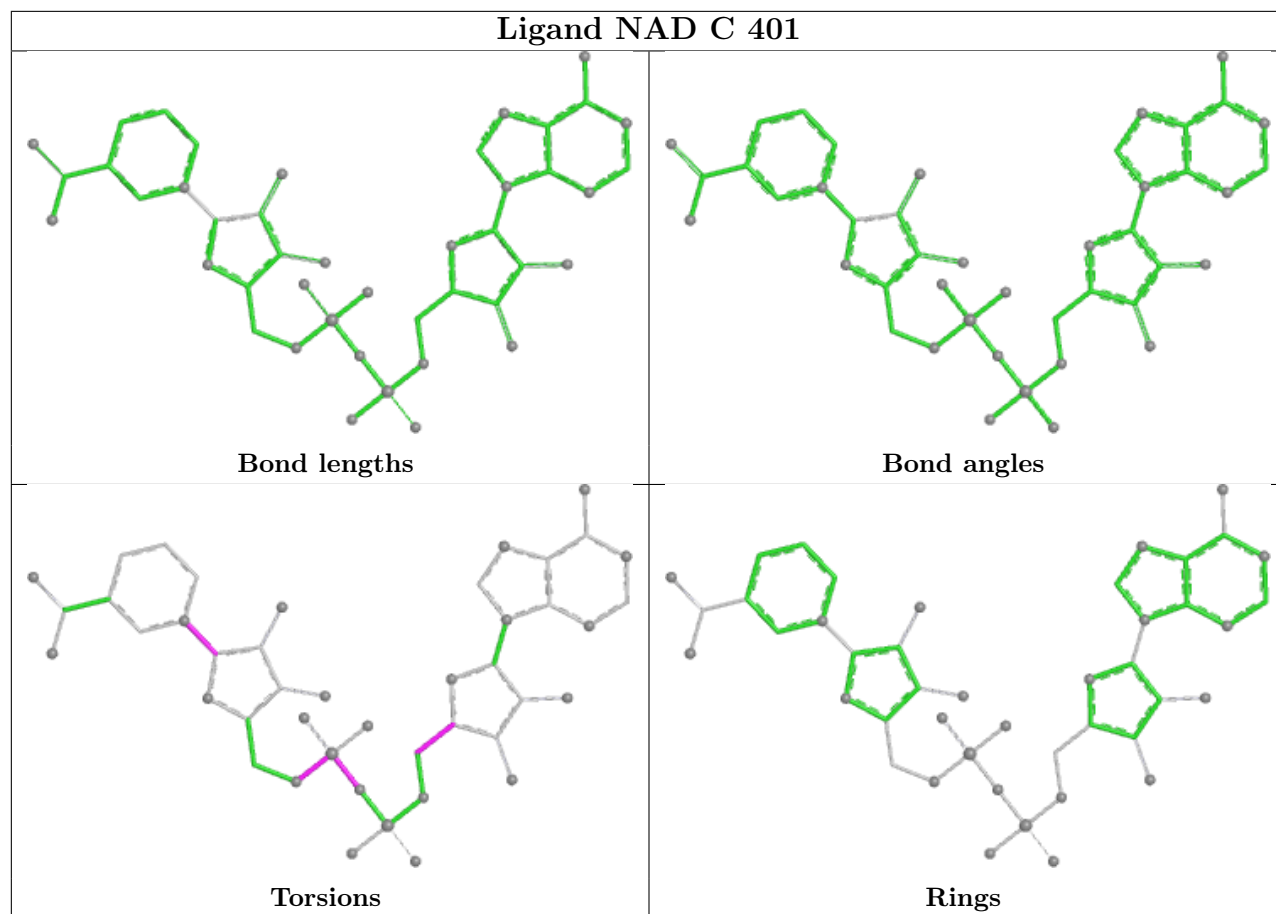


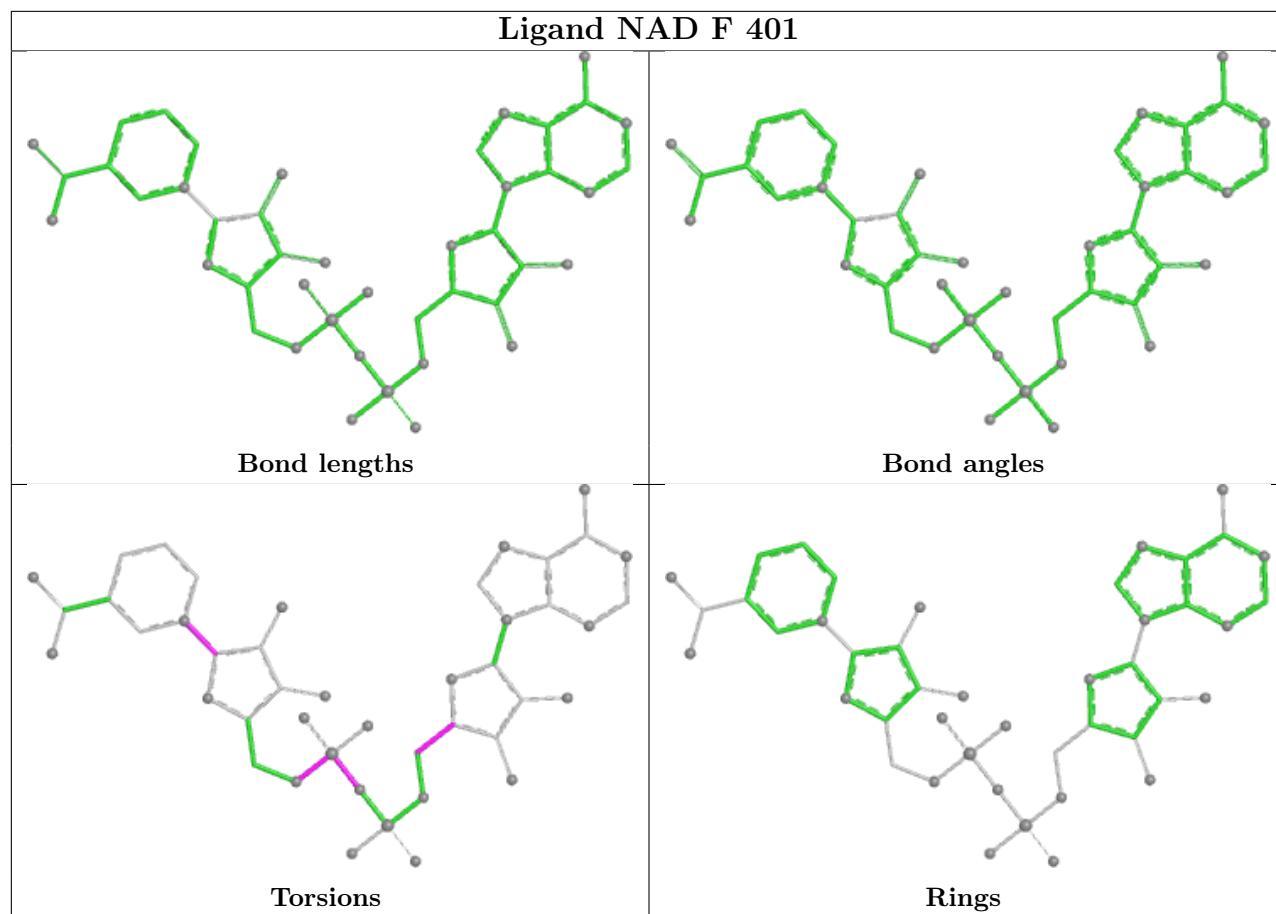


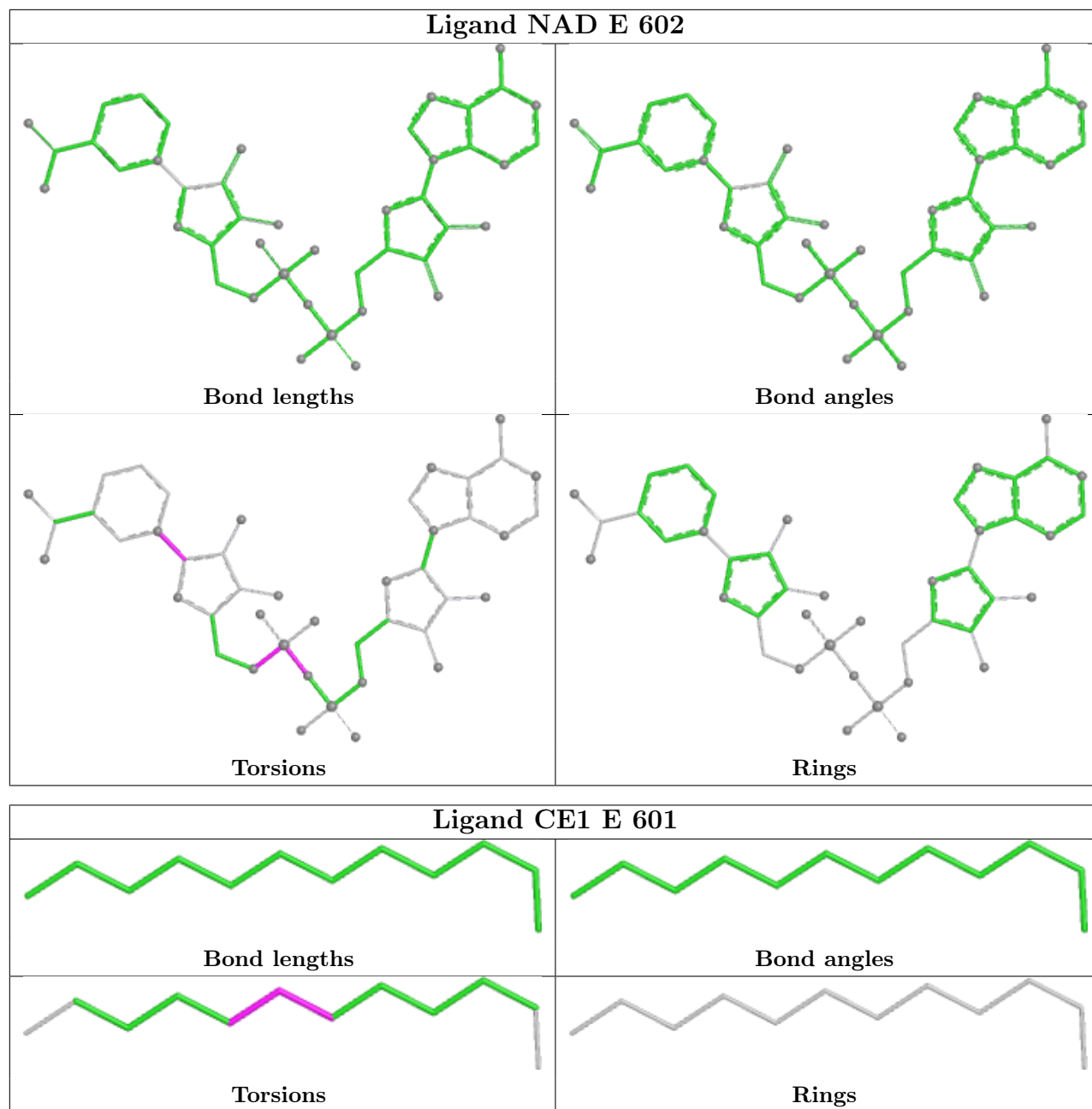


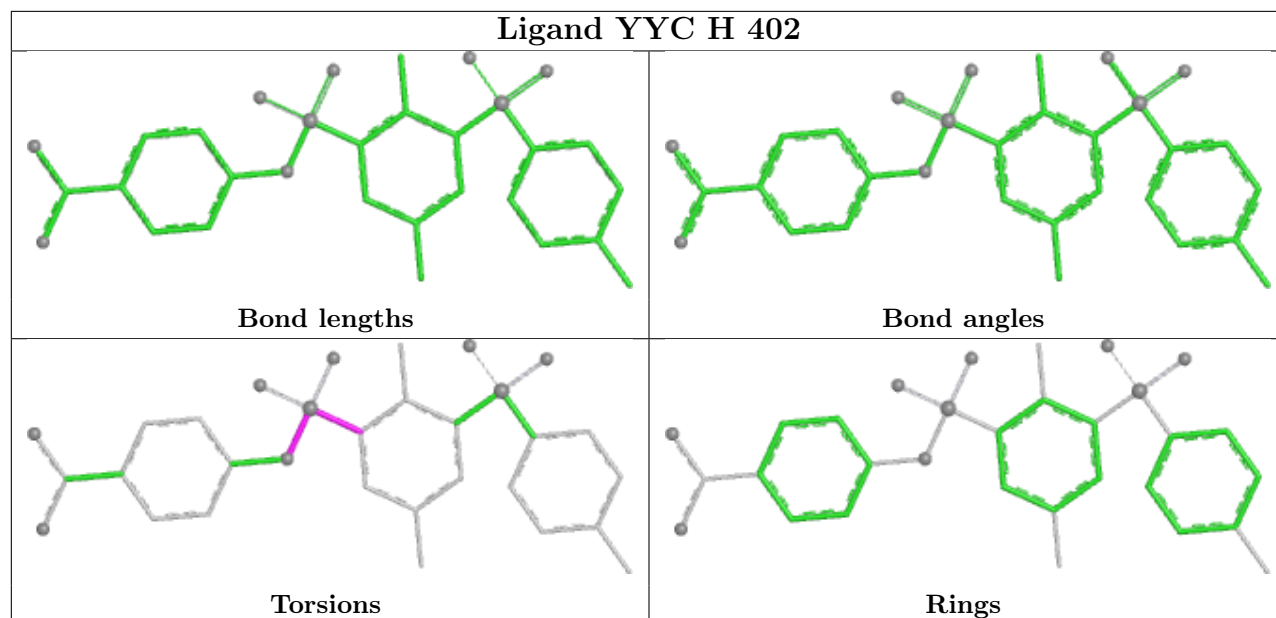












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	283/315 (89%)	0.19	15 (5%)	32 26	37, 53, 83, 110	0
1	B	283/315 (89%)	0.03	3 (1%)	78 75	37, 51, 69, 84	0
1	C	267/315 (84%)	0.11	4 (1%)	72 69	38, 54, 75, 89	0
1	D	280/315 (88%)	0.25	16 (5%)	29 24	39, 54, 105, 117	0
1	E	293/315 (93%)	0.43	10 (3%)	48 42	44, 66, 89, 101	0
1	F	262/315 (83%)	0.18	3 (1%)	78 75	42, 55, 78, 88	0
1	G	262/315 (83%)	0.53	17 (6%)	25 21	50, 69, 93, 104	0
1	H	289/315 (91%)	0.58	14 (4%)	35 29	43, 70, 99, 109	0
All	All	2219/2520 (88%)	0.29	82 (3%)	45 39	37, 58, 90, 117	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	235	PRO	5.5
1	G	240	THR	4.6
1	D	23	VAL	4.5
1	C	229	PRO	4.4
1	D	3	ILE	4.2
1	D	4	ILE	4.1
1	A	22	LEU	4.0
1	E	116	ILE	3.9
1	E	90	TYR	3.8
1	A	6	GLU	3.7
1	A	19	LEU	3.5
1	A	21	SER	3.4
1	G	241	ASP	3.4
1	A	233	LEU	3.4
1	H	107	VAL	3.3
1	A	28	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	235	PRO	3.3
1	G	86	THR	3.2
1	A	3	ILE	3.2
1	D	18	TYR	3.1
1	C	222	ASN	3.1
1	E	36	GLY	3.1
1	A	18	TYR	3.0
1	D	6	GLU	2.8
1	D	14	ILE	2.8
1	B	286	ASN	2.8
1	D	13	THR	2.8
1	D	1	GLY	2.8
1	H	154	ALA	2.7
1	G	244	VAL	2.7
1	B	235	PRO	2.7
1	A	4	ILE	2.6
1	A	222	ASN	2.6
1	F	24	LYS	2.6
1	G	238	LEU	2.6
1	E	89	ALA	2.6
1	A	291	ALA	2.6
1	D	209	THR	2.5
1	H	76	THR	2.5
1	D	5	LEU	2.5
1	E	34	VAL	2.5
1	F	23	VAL	2.5
1	D	21	SER	2.5
1	D	11	LEU	2.5
1	H	280	ILE	2.5
1	G	79	GLU	2.5
1	G	272	LYS	2.4
1	G	273	PHE	2.4
1	G	137	ILE	2.3
1	H	187	SER	2.3
1	G	28	PRO	2.3
1	E	108	LYS	2.3
1	A	1	GLY	2.3
1	H	86	THR	2.3
1	G	179	ILE	2.3
1	H	89	ALA	2.3
1	H	118	VAL	2.3
1	H	290	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	34	VAL	2.2
1	A	229	PRO	2.2
1	D	22	LEU	2.2
1	H	150	TRP	2.2
1	C	81	ARG	2.2
1	A	20	GLU	2.1
1	B	1	GLY	2.1
1	E	91	VAL	2.1
1	G	30	ARG	2.1
1	E	52	THR	2.1
1	G	133	LYS	2.1
1	D	8	LEU	2.1
1	D	10	LEU	2.1
1	G	2	ASN	2.1
1	H	88	HIS	2.1
1	E	293	VAL	2.1
1	G	227	LYS	2.1
1	D	2	ASN	2.1
1	A	15	ILE	2.1
1	E	61	SER	2.0
1	H	84	GLY	2.0
1	H	109	LYS	2.0
1	H	212	LYS	2.0
1	G	178	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

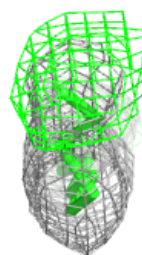
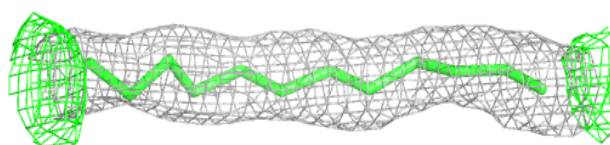
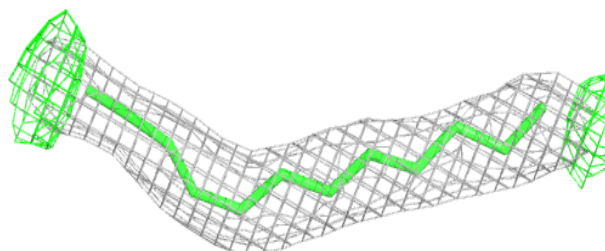
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	407	5/5	0.74	0.16	157,157,157,157	0
4	CE1	C	403	12/37	0.83	0.15	47,47,48,48	0
5	SO4	E	604	5/5	0.84	0.15	100,100,101,101	0
5	SO4	G	404	5/5	0.85	0.11	132,132,132,132	0
5	SO4	A	405	5/5	0.86	0.11	93,93,94,94	0
5	SO4	H	405	5/5	0.88	0.09	130,130,130,130	0
4	CE1	A	403	37/37	0.90	0.13	51,60,62,63	58
5	SO4	F	405	5/5	0.90	0.11	82,83,83,83	0
5	SO4	H	404	5/5	0.91	0.08	80,80,80,80	0
5	SO4	H	403	5/5	0.91	0.08	107,107,107,107	0
3	YYC	C	402	31/31	0.92	0.14	77,86,97,98	21
5	SO4	B	403	5/5	0.92	0.09	93,93,93,93	0
5	SO4	C	405	5/5	0.92	0.08	96,97,97,97	0
3	YYC	G	402	31/31	0.92	0.13	89,91,100,102	21
4	CE1	D	403	31/37	0.92	0.11	51,55,59,60	45
3	YYC	F	402	31/31	0.93	0.12	74,76,84,85	20
4	CE1	E	601	12/37	0.93	0.11	46,47,49,49	0
5	SO4	B	404	5/5	0.93	0.10	103,103,103,104	0
5	SO4	C	404	5/5	0.93	0.10	75,75,75,75	0
2	NAD	H	401	44/44	0.94	0.10	60,70,75,76	0
2	NAD	E	602	44/44	0.95	0.10	61,69,72,72	0
2	NAD	G	401	44/44	0.95	0.09	73,76,81,81	0
5	SO4	A	404	5/5	0.95	0.07	83,83,83,83	0
5	SO4	F	403	5/5	0.96	0.07	64,64,64,64	0
2	NAD	C	401	44/44	0.96	0.07	52,59,62,63	0
5	SO4	G	403	5/5	0.96	0.06	64,65,65,65	0
3	YYC	D	402	31/31	0.96	0.08	48,49,53,54	20
5	SO4	C	406	5/5	0.96	0.07	78,78,78,79	0
2	NAD	A	401	44/44	0.96	0.07	45,48,51,51	0
3	YYC	A	402	31/31	0.96	0.08	49,52,54,55	20
3	YYC	H	402	31/31	0.97	0.07	55,60,64,64	21
2	NAD	B	401	44/44	0.97	0.06	37,41,44,44	0
3	YYC	E	603	31/31	0.97	0.07	48,54,57,57	21
3	YYC	B	402	31/31	0.97	0.07	46,49,51,53	21
2	NAD	F	401	44/44	0.97	0.07	52,53,56,56	0
5	SO4	F	404	5/5	0.97	0.07	55,55,56,56	0
2	NAD	D	401	44/44	0.98	0.06	43,45,46,47	0

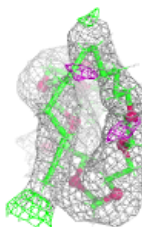
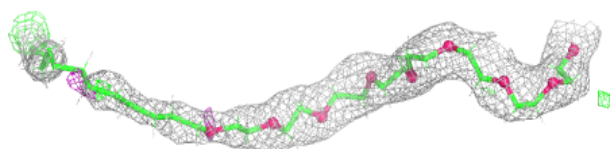
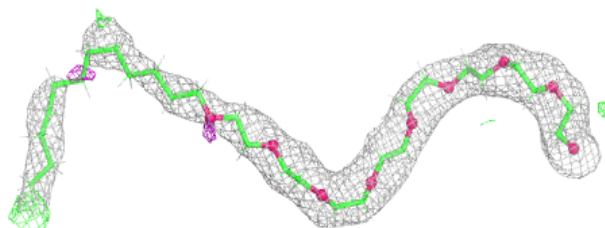
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CE1 C 403:

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

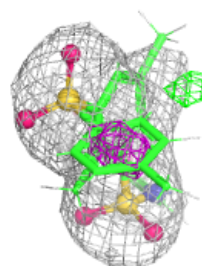
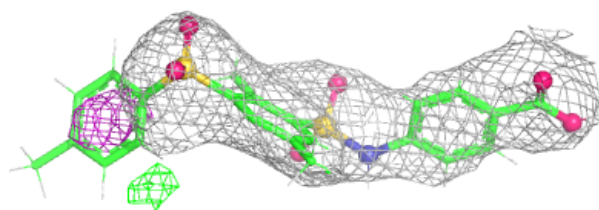
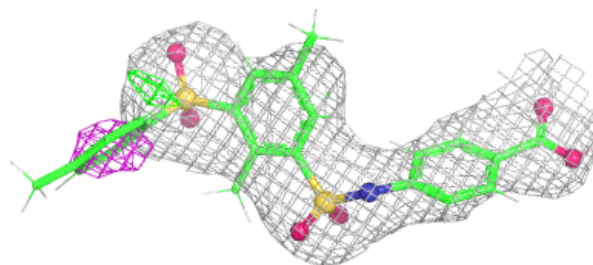
**Electron density around CE1 A 403:**

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

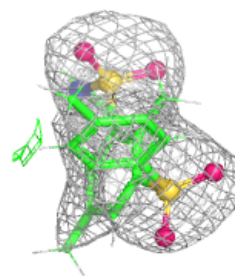
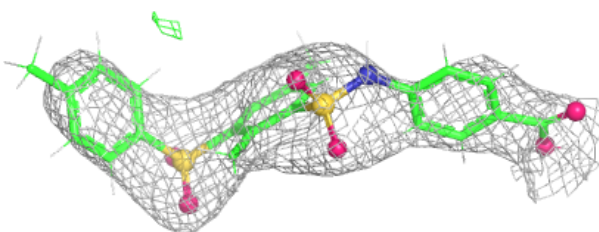
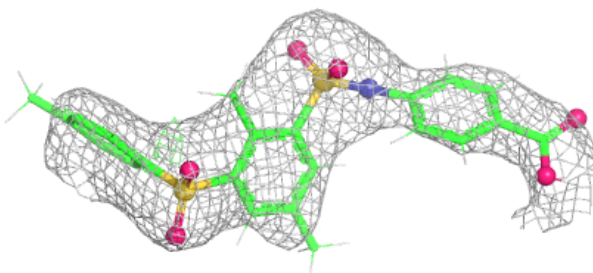


Electron density around YYC C 402:

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

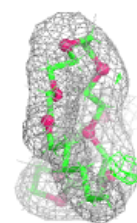
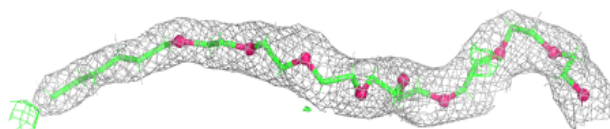
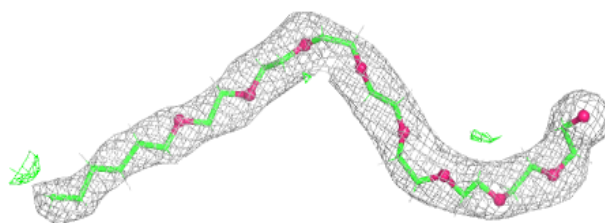
**Electron density around YYC G 402:**

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

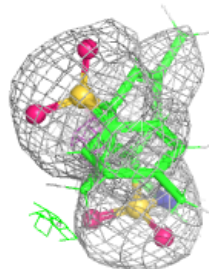
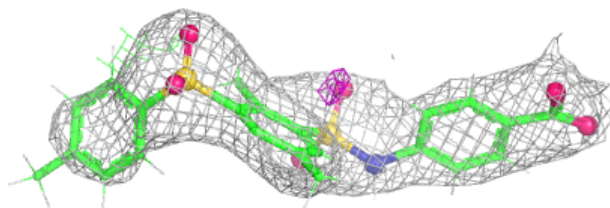
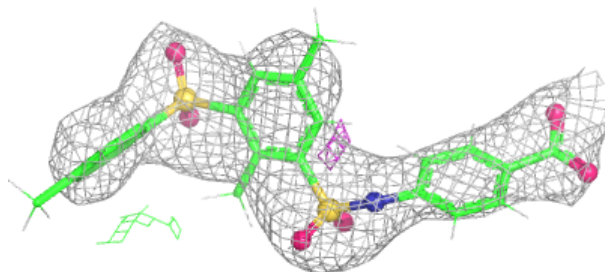


Electron density around CE1 D 403:

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

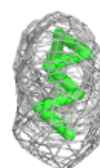
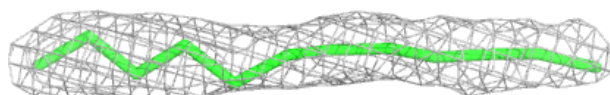
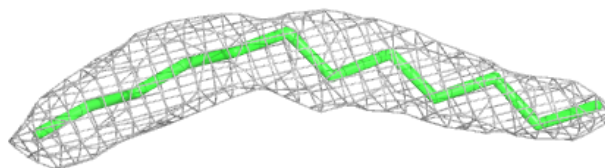
**Electron density around YYC F 402:**

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

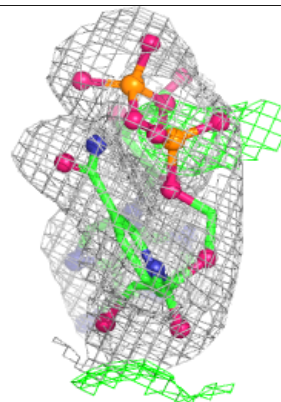
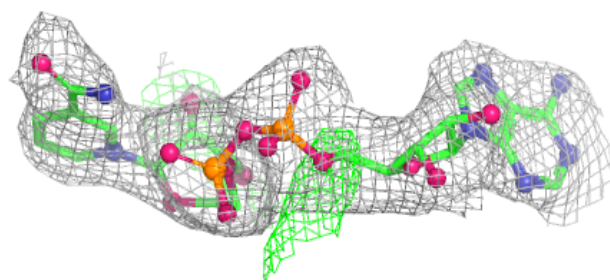
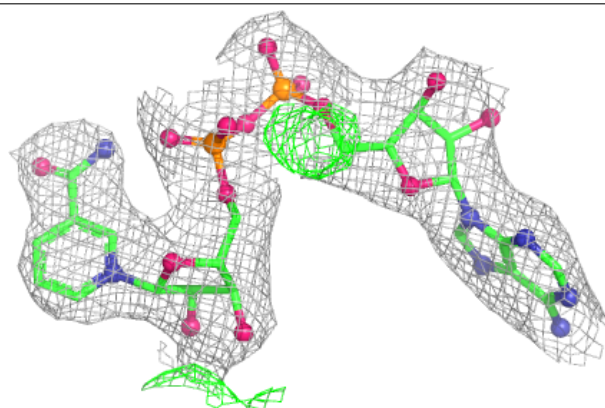


Electron density around CE1 E 601:

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

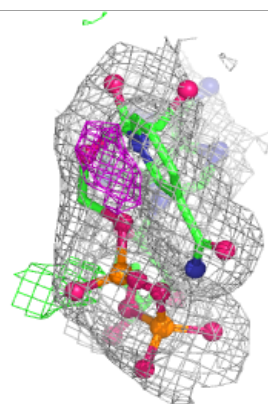
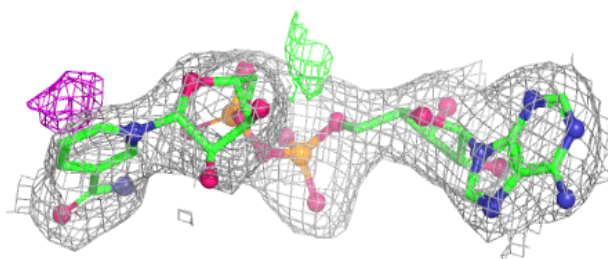
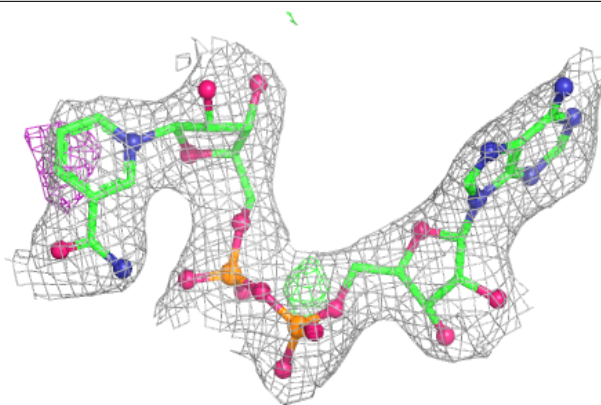
**Electron density around NAD H 401:**

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

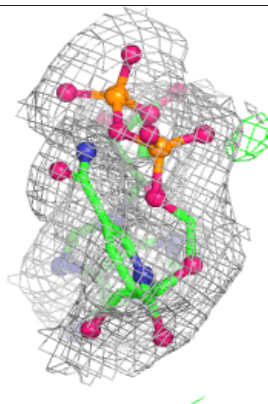
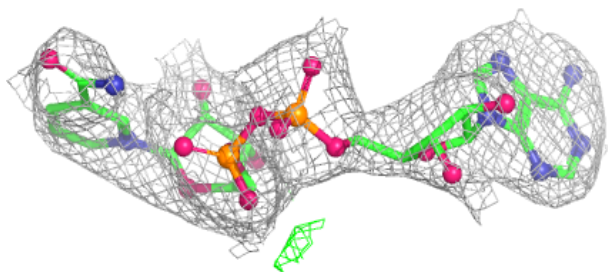
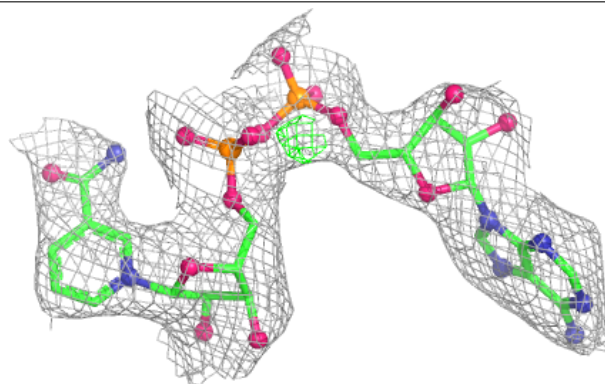


Electron density around NAD E 602:

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

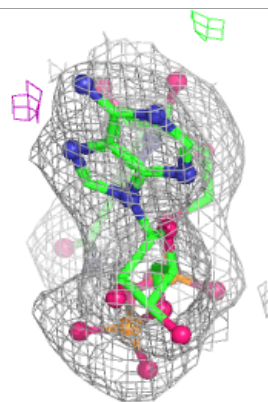
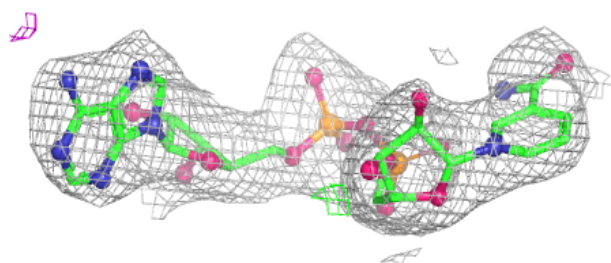
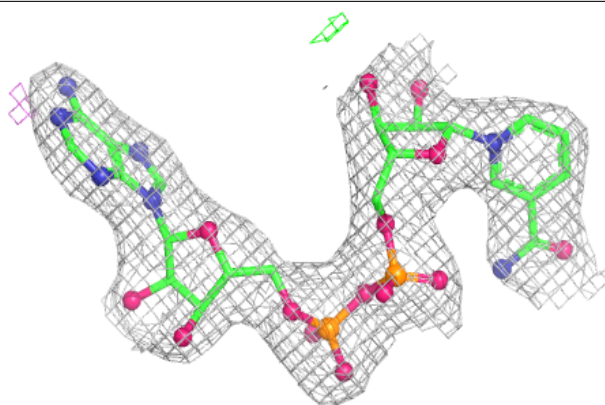
**Electron density around NAD G 401:**

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

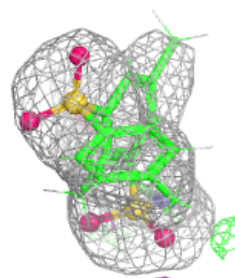
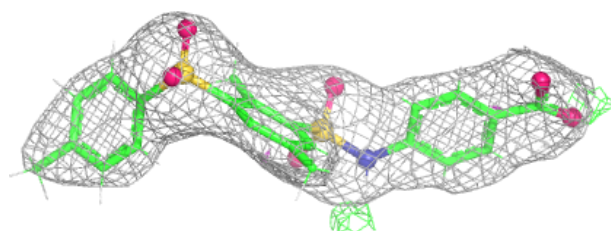
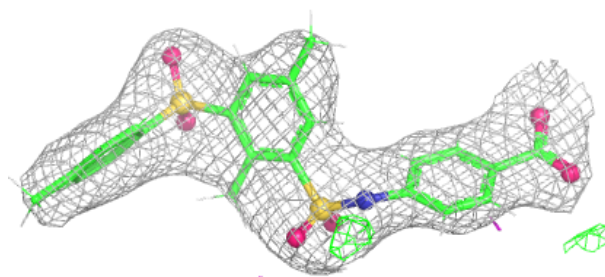


Electron density around NAD C 401:

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

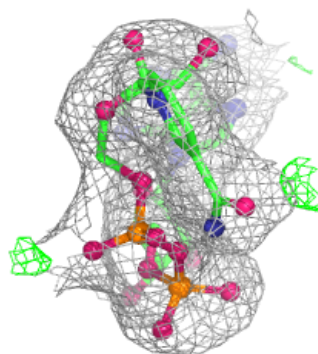
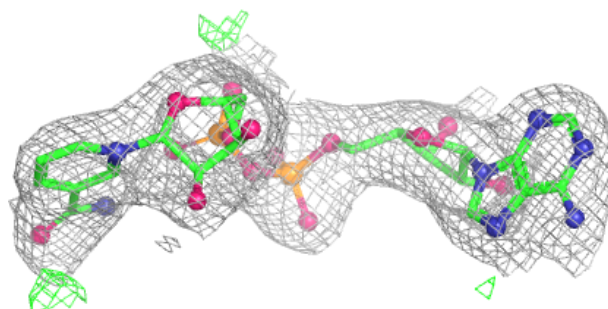
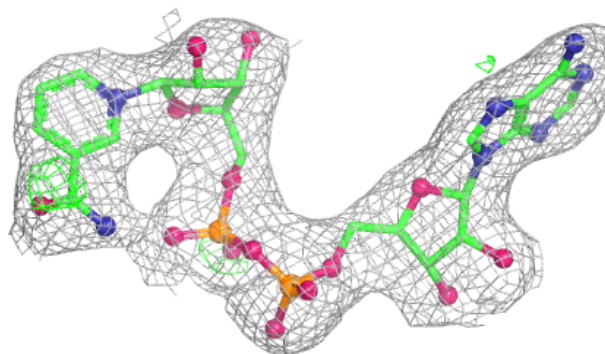
**Electron density around YYC D 402:**

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

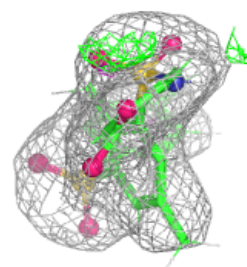
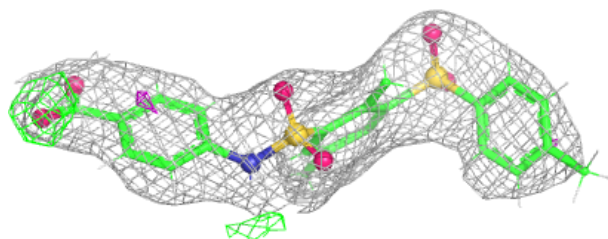
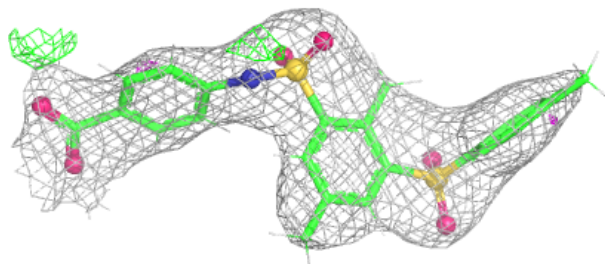


Electron density around NAD A 401:

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

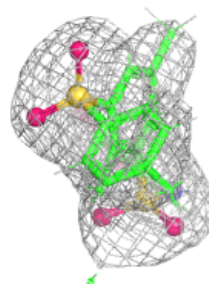
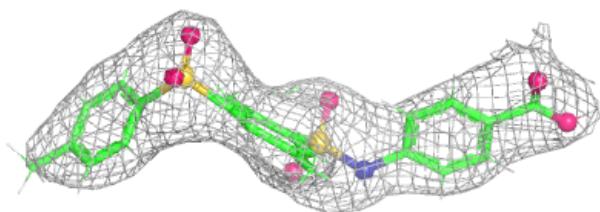
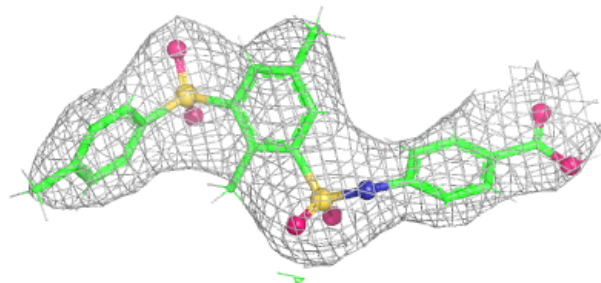
**Electron density around YYC A 402:**

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

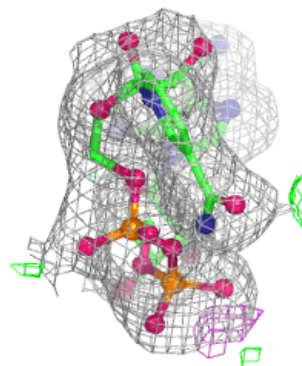
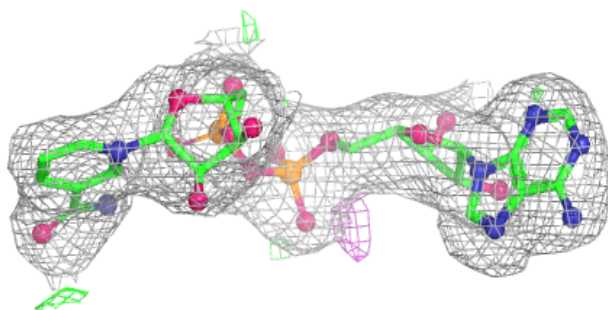
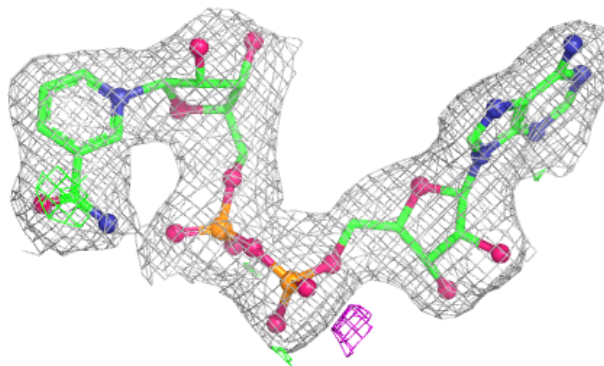


Electron density around YYC H 402:

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

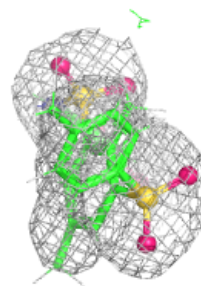
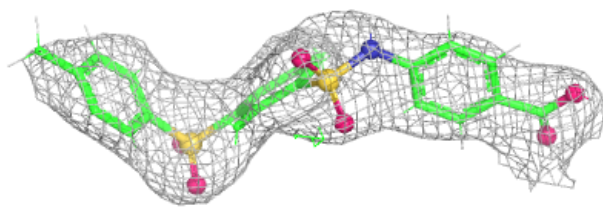
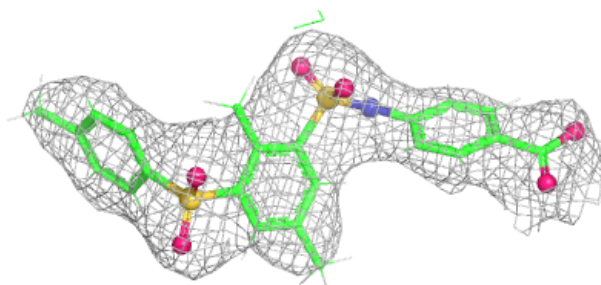
**Electron density around NAD B 401:**

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

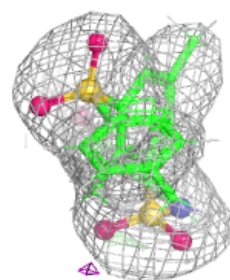
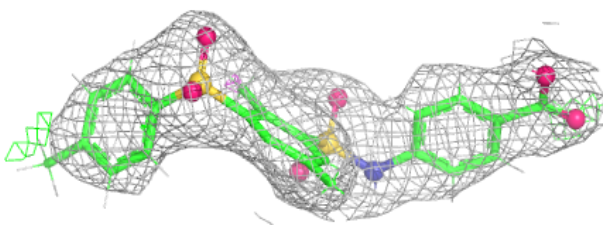
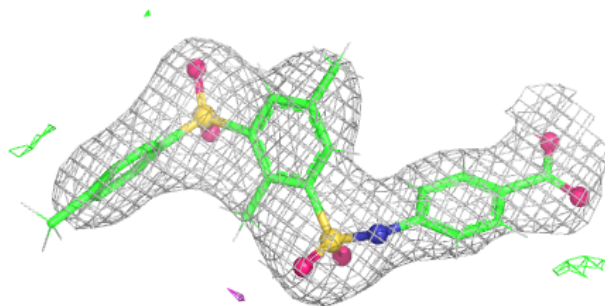


Electron density around YYC E 603:

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

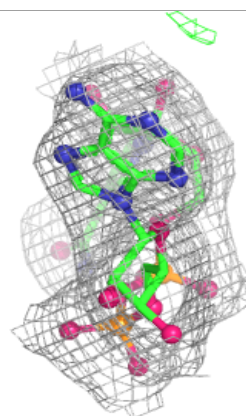
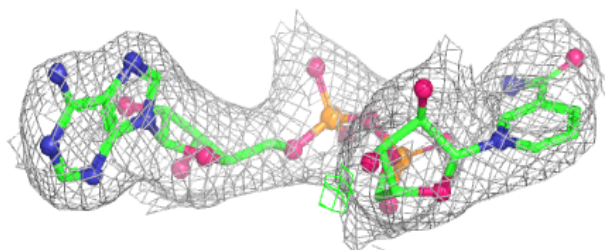
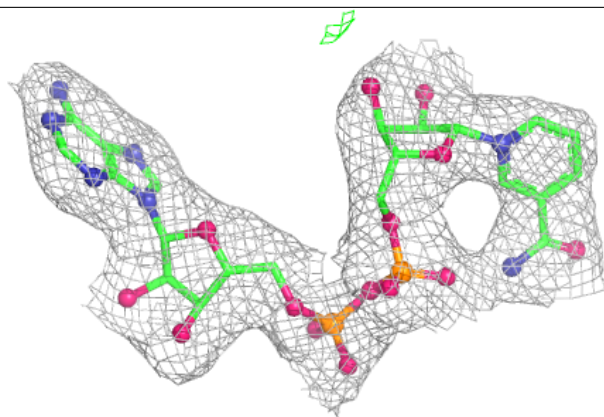
**Electron density around YYC B 402:**

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

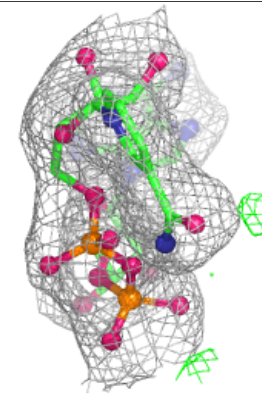
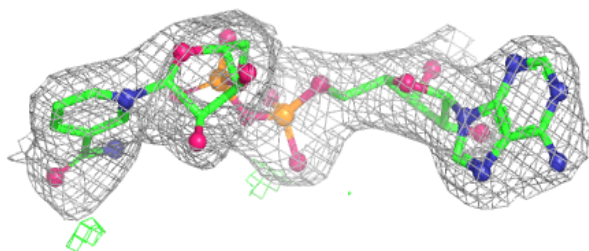
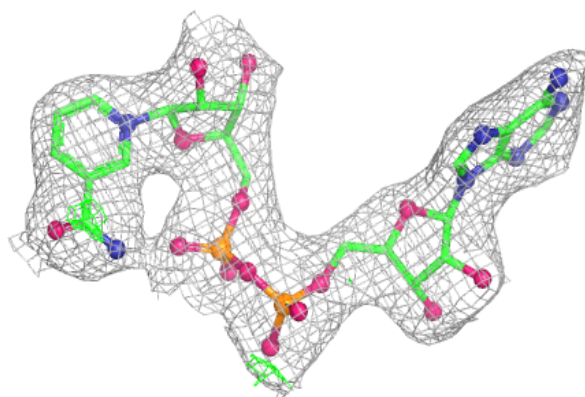


Electron density around NAD F 401:

$2mF_o-DF_c$ (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.