



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:01 PM JST

PDB ID : 7VF0  
Title : Crystal structure of Cyclosorus parasiticus chalcone synthase 1 (CpCHS1) complex with naringenin and CoA  
Authors : Li, J.X.; Cheng, A.X.  
Deposited on : 2021-09-10  
Resolution : 2.40 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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)  
Validation Pipeline (wwPDB-VP) : 2.36

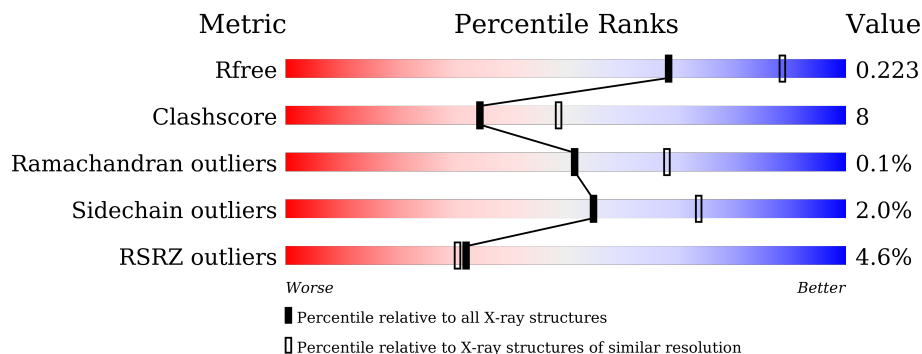
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	404	 4% (poor fit), 79% (0-1 outliers), 17% (2-3 outliers), .. (not modelled)
1	B	404	 4% (poor fit), 83% (0-1 outliers), 13% (2-3 outliers), .. (not modelled)
1	C	404	 6% (poor fit), 81% (0-1 outliers), 17% (2-3 outliers), . (not modelled)
1	D	404	 3% (poor fit), 79% (0-1 outliers), 18% (2-3 outliers), .. (not modelled)

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	C	502[A]	-	-	-	X
3	COA	C	502[B]	-	-	-	X
3	COA	D	502[A]	-	-	-	X
3	COA	D	502[B]	-	-	-	X

## 2 Entry composition [i](#)

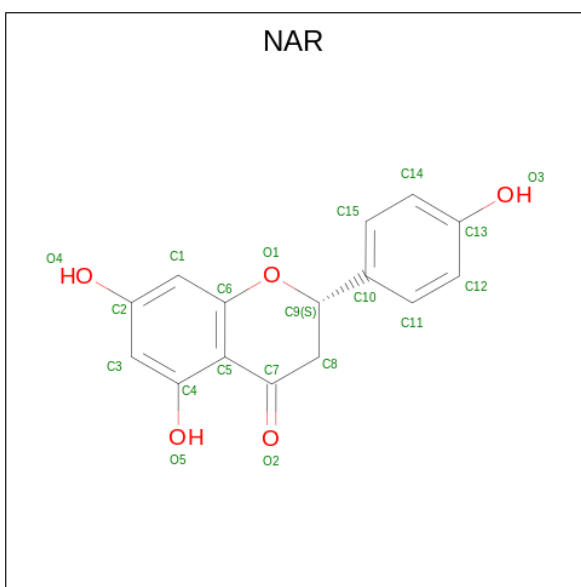
There are 4 unique types of molecules in this entry. The entry contains 12820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called chalcone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	Total 3010	C 1919	N 511	O 558	S 22	0	0	0
1	B	396	Total 3049	C 1940	N 517	O 570	S 22	0	0	0
1	C	396	Total 3049	C 1940	N 517	O 570	S 22	0	0	0
1	D	392	Total 3018	C 1923	N 513	O 560	S 22	0	0	0

- Molecule 2 is NARINGENIN (three-letter code: NAR) (formula: C<sub>15</sub>H<sub>12</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



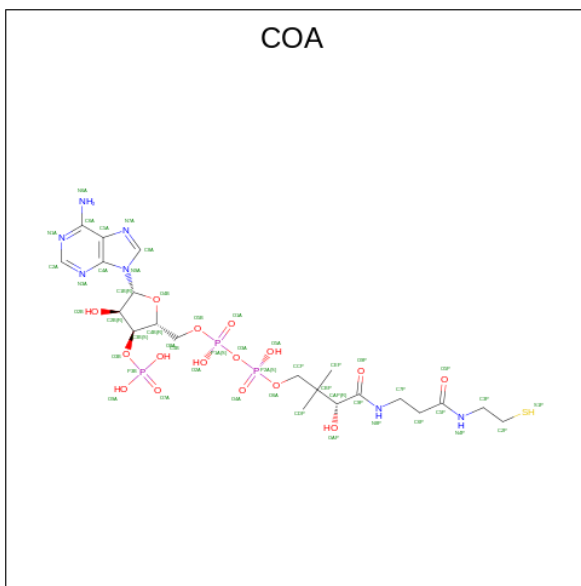
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 20	C 15	O 5	0	0
2	B	1	Total 20	C 15	O 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			20	15	5		
2	D	1	Total	C	O	0	0
			20	15	5		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	1
			49	21	7	16	3	2		
3	C	1	Total	C	N	O	P	S	0	1
			49	21	7	16	3	2		
3	D	1	Total	C	N	O	P	S	0	1
			49	21	7	16	3	2		

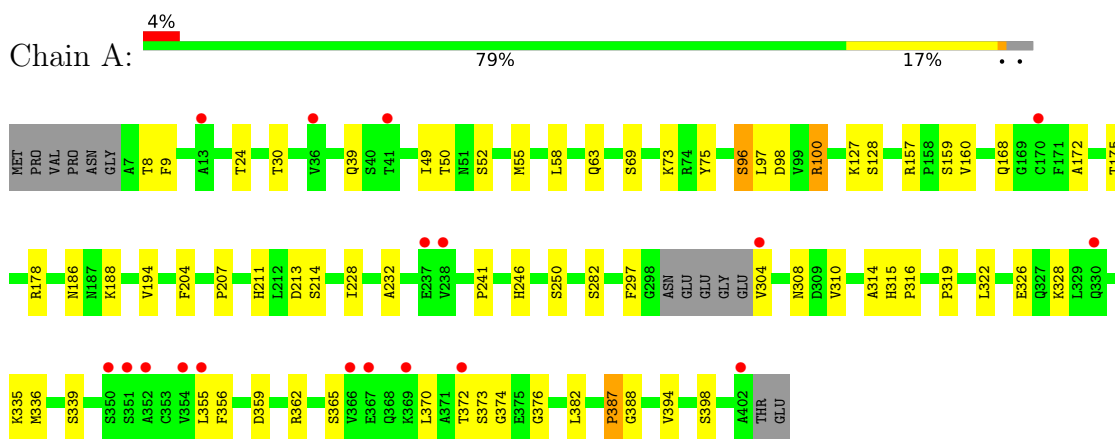
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	145	Total	O	0	0
			145	145		
4	C	124	Total	O	0	0
			124	124		
4	D	117	Total	O	0	0
			117	117		

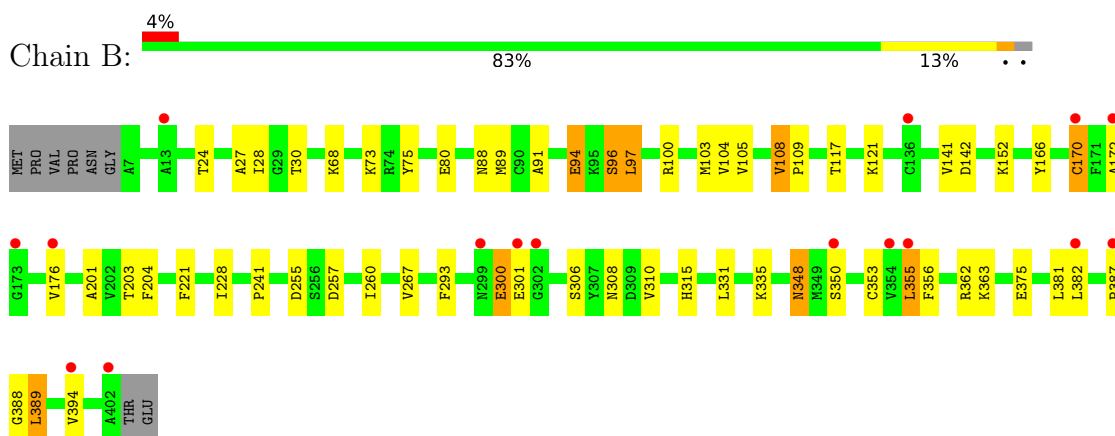
### 3 Residue-property plots [i](#)

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.

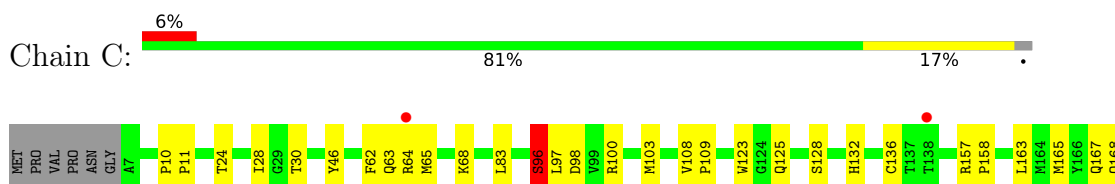
- Molecule 1: chalcone synthase

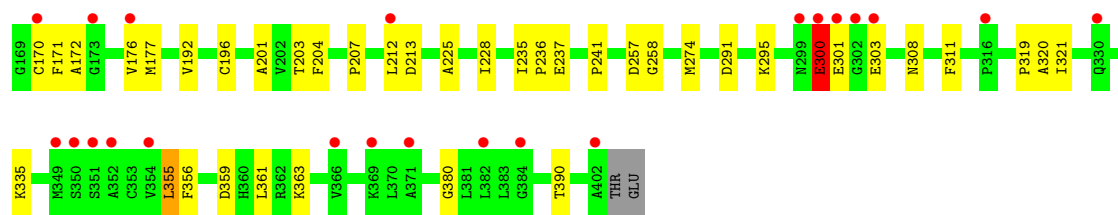


- Molecule 1: chalcone synthase

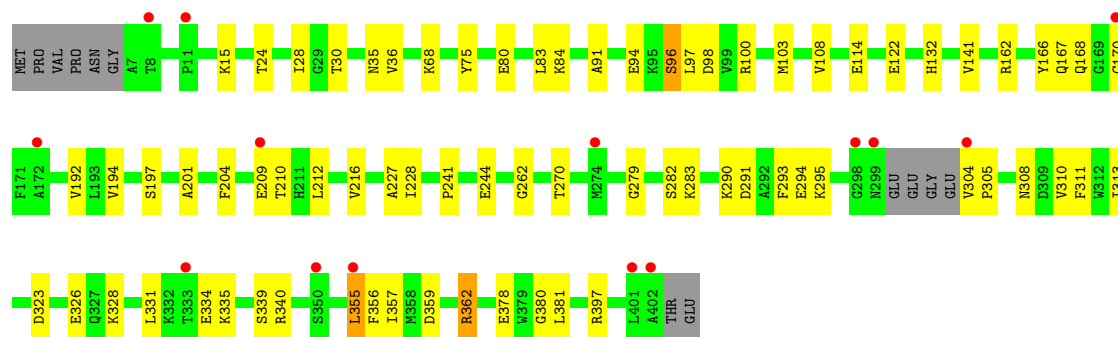
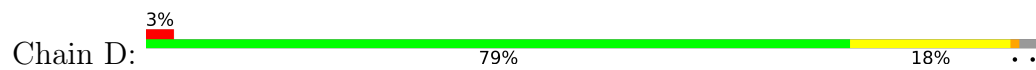


- Molecule 1: chalcone synthase





● Molecule 1: chalcone synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.66Å 82.89Å 143.16Å 90.00° 103.34° 90.00°	Depositor
Resolution (Å)	32.48 – 2.40 32.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (32.48-2.40) 95.3 (32.48-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.12 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.179 , 0.225 0.179 , 0.223	Depositor DCC
$R_{free}$ test set	2003 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.55	0/3076	0.66	3/4168 (0.1%)
1	B	0.66	1/3116 (0.0%)	0.67	5/4223 (0.1%)
1	C	0.66	0/3116	0.66	2/4223 (0.0%)
1	D	0.60	0/3084	0.64	2/4179 (0.0%)
All	All	0.62	1/12392 (0.0%)	0.66	12/16793 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	CYS	CB-SG	-5.09	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	SER	CB-CA-C	11.53	132.00	110.10
1	A	96	SER	CB-CA-C	10.73	130.49	110.10
1	D	96	SER	CB-CA-C	8.92	127.04	110.10
1	B	389	LEU	CA-CB-CG	7.39	132.29	115.30
1	B	96	SER	CB-CA-C	6.88	123.17	110.10
1	B	388	GLY	N-CA-C	6.52	129.41	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	355	LEU	CB-CG-CD1	6.52	122.09	111.00
1	A	388	GLY	N-CA-C	6.18	128.56	113.10
1	A	100	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	B	355	LEU	CB-CG-CD1	5.44	120.25	111.00
1	B	170	CYS	CA-CB-SG	5.10	123.18	114.00
1	C	355	LEU	CB-CG-CD1	5.04	119.56	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	GLU	Peptide
1	C	300	GLU	Peptide
1	C	96	SER	Peptide

## 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	3010	0	3024	49	0
1	B	3049	0	3052	40	0
1	C	3049	0	3052	48	0
1	D	3018	0	3029	52	0
2	A	20	0	9	1	0
2	B	20	0	9	1	0
2	C	20	0	9	1	0
2	D	20	0	9	0	0
3	B	49	0	6	1	0
3	C	49	0	6	0	0
3	D	49	0	6	1	0
4	A	81	0	0	9	0
4	B	145	0	0	5	0
4	C	124	0	0	5	0
4	D	117	0	0	8	0
All	All	12820	0	12211	189	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 8.

All (189) 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:D:100:ARG:NH1	1:D:204:PHE:O	1.78	1.15
1:C:100:ARG:NH1	1:C:204:PHE:O	1.86	1.07
1:A:359:ASP:OD2	1:A:362:ARG:NH1	1.91	1.03
1:B:96:SER:OG	1:B:100:ARG:NH2	1.99	0.96
1:A:128:SER:O	1:A:157:ARG:NH2	1.98	0.95
1:D:326:GLU:OE1	4:D:601:HOH:O	1.84	0.95
1:A:100:ARG:NH1	1:A:204:PHE:O	2.05	0.89
1:C:128:SER:O	1:C:157:ARG:NH2	2.07	0.87
1:C:165:MET:HB3	1:C:168:GLN:HE21	1.41	0.83
1:C:308:ASN:HA	1:C:335:LYS:HD2	1.58	0.82
1:A:373:SER:OG	1:A:398:SER:HB2	1.85	0.77
1:D:308:ASN:HA	1:D:335:LYS:HD2	1.67	0.76
1:A:63:GLN:OE1	4:A:602:HOH:O	2.03	0.75
1:A:96:SER:O	1:A:98:ASP:N	2.20	0.75
1:A:308:ASN:HA	1:A:335:LYS:HD2	1.69	0.73
1:A:387:PRO:O	4:A:603:HOH:O	2.07	0.73
1:C:257:ASP:OD2	4:C:601:HOH:O	2.07	0.72
1:B:308:ASN:HA	1:B:335:LYS:HD2	1.69	0.72
1:B:375:GLU:OE1	4:B:601:HOH:O	2.07	0.72
1:D:310:VAL:O	1:D:335:LYS:NZ	2.22	0.72
1:A:186:ASN:O	4:A:604:HOH:O	2.10	0.70
1:C:167:GLN:O	4:C:602:HOH:O	2.10	0.69
1:D:122:GLU:OE1	1:D:362:ARG:NH2	2.22	0.69
1:D:166:TYR:O	1:D:168:GLN:NE2	2.24	0.69
1:B:91:ALA:HB3	1:B:94:GLU:HG3	1.75	0.69
1:A:24:THR:HG21	1:A:241:PRO:HB3	1.75	0.69
1:A:232:ALA:O	4:A:606:HOH:O	2.11	0.68
1:A:326:GLU:OE2	4:A:605:HOH:O	2.11	0.68
1:B:100:ARG:NH1	1:B:204:PHE:O	2.28	0.67
1:C:62:PHE:HA	1:C:65:MET:HE3	1.76	0.67
1:A:159:SER:O	4:A:607:HOH:O	2.11	0.67
1:D:209:GLU:HG3	1:D:210:THR:HG23	1.76	0.67
1:C:63:GLN:OE1	4:C:603:HOH:O	2.13	0.66
1:B:100:ARG:NH2	1:B:267:VAL:O	2.29	0.66
1:D:114:GLU:OE1	4:D:602:HOH:O	2.14	0.65
1:B:310:VAL:O	1:B:335:LYS:NZ	2.29	0.64
1:D:304:VAL:N	4:D:609:HOH:O	2.29	0.64
1:C:158:PRO:HD2	4:C:697:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:MET:HE3	1:D:201:ALA:HB1	1.81	0.63
1:A:8:THR:HG22	1:A:9:PHE:O	1.97	0.63
1:D:24:THR:HG21	1:D:241:PRO:HB3	1.81	0.62
1:D:334:GLU:OE1	1:D:334:GLU:N	2.25	0.62
1:A:372:THR:HG23	1:A:374:GLY:H	1.65	0.62
1:A:194:VAL:HB	1:A:228:ILE:HG12	1.82	0.61
1:D:291:ASP:OD1	1:D:295:LYS:NZ	2.33	0.61
1:B:104:VAL:O	1:B:108:VAL:HG13	2.00	0.60
1:C:291:ASP:OD2	1:C:295:LYS:NZ	2.31	0.60
1:C:103:MET:HE1	1:C:201:ALA:HB1	1.83	0.60
1:B:24:THR:HG21	1:B:241:PRO:HB3	1.83	0.59
1:C:363:LYS:NZ	4:C:608:HOH:O	2.35	0.59
1:B:260:ILE:HB	1:B:387:PRO:HA	1.86	0.58
1:D:162:ARG:NH2	4:D:617:HOH:O	2.35	0.58
1:B:108:VAL:HG22	1:B:109:PRO:HD3	1.85	0.57
1:A:211:HIS:HD2	1:A:213:ASP:OD1	1.87	0.57
1:D:167:GLN:NE2	4:D:615:HOH:O	2.34	0.56
1:D:170:CYS:SG	3:D:502[A]:COA:S1P	3.00	0.56
1:A:314:ALA:HB3	1:A:336:MET:HE1	1.87	0.56
1:A:322:LEU:HD22	1:A:336:MET:HE1	1.87	0.56
1:D:279:GLY:O	1:D:283:LYS:HG2	2.05	0.56
1:A:213:ASP:OD1	1:A:213:ASP:N	2.33	0.55
1:D:80:GLU:HG2	1:D:84:LYS:HE3	1.88	0.55
1:A:372:THR:HG22	1:A:376:GLY:H	1.73	0.54
1:D:100:ARG:HA	1:D:103:MET:CE	2.38	0.53
1:D:290:LYS:NZ	1:D:294:GLU:OE2	2.32	0.53
1:C:136:CYS:HB2	1:C:165:MET:HE2	1.91	0.53
1:B:255:ASP:OD1	4:B:602:HOH:O	2.19	0.52
1:D:244:GLU:OE2	4:D:604:HOH:O	2.19	0.52
1:D:282:SER:OG	1:D:328:LYS:NZ	2.41	0.52
1:D:35:ASN:ND2	4:D:608:HOH:O	2.27	0.51
1:B:363:LYS:NZ	4:B:614:HOH:O	2.43	0.51
1:C:30:THR:HB	1:C:356:PHE:CZ	2.46	0.51
1:A:157:ARG:O	1:A:160:VAL:HG13	2.11	0.51
1:B:293:PHE:HE1	1:B:381:LEU:HD21	1.77	0.50
1:C:108:VAL:HG22	1:C:109:PRO:HD3	1.93	0.50
1:D:132:HIS:HB2	1:D:192:VAL:HG22	1.94	0.50
1:B:348:ASN:ND2	1:B:350:SER:H	2.09	0.50
1:A:310:VAL:O	1:A:335:LYS:NZ	2.38	0.49
1:A:211:HIS:CE1	1:A:214:SER:HB2	2.45	0.49
1:B:105:VAL:HG22	1:B:142:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LEU:HB3	1:B:394:VAL:HB	1.93	0.49
1:A:50:THR:O	4:A:608:HOH:O	2.18	0.49
1:D:100:ARG:HA	1:D:103:MET:HE2	1.94	0.49
1:B:362:ARG:HG3	1:B:363:LYS:N	2.27	0.49
1:D:359:ASP:OD1	1:D:362:ARG:HD3	2.13	0.49
1:D:28:ILE:HG12	1:D:228:ILE:HG22	1.95	0.49
1:B:301:GLU:HG2	1:B:301:GLU:O	2.13	0.48
1:A:168:GLN:HB3	1:A:172:ALA:HB2	1.95	0.48
1:D:96:SER:O	1:D:98:ASP:N	2.46	0.48
1:B:28:ILE:HG12	1:B:228:ILE:HG22	1.95	0.48
1:B:88:ASN:OD1	1:B:88:ASN:N	2.46	0.48
1:B:141:VAL:HA	1:B:166:TYR:CE1	2.49	0.47
1:C:168:GLN:HA	1:C:168:GLN:OE1	2.14	0.47
1:C:177:MET:HE1	1:C:228:ILE:HD11	1.97	0.47
1:C:132:HIS:HB2	1:C:192:VAL:HG22	1.96	0.47
1:C:28:ILE:HG21	1:C:359:ASP:HB2	1.95	0.47
1:B:170:CYS:HB3	1:B:315:HIS:CE1	2.49	0.47
1:C:170:CYS:SG	2:C:501:NAR:H11	2.55	0.47
1:D:141:VAL:HG12	1:D:166:TYR:CG	2.49	0.47
1:B:170:CYS:HB3	1:B:315:HIS:NE2	2.30	0.47
1:C:96:SER:O	1:C:98:ASP:N	2.48	0.47
1:A:69:SER:O	1:A:319:PRO:HG3	2.16	0.46
1:B:73:LYS:HE2	1:B:75:TYR:OH	2.16	0.46
1:B:335:LYS:HE2	4:B:637:HOH:O	2.15	0.46
1:B:30:THR:HB	1:B:356:PHE:CZ	2.50	0.46
1:C:103:MET:HE3	1:C:103:MET:HB2	1.74	0.46
1:C:24:THR:HG21	1:C:241:PRO:HB3	1.97	0.46
1:B:331:LEU:HB3	1:B:335:LYS:HG3	1.98	0.46
1:D:339:SER:HA	1:D:357:ILE:HD13	1.97	0.46
1:B:152:LYS:NZ	4:B:606:HOH:O	2.35	0.46
1:C:213:ASP:N	1:C:213:ASP:OD1	2.48	0.46
1:D:340:ARG:NE	4:D:610:HOH:O	2.29	0.45
1:B:221:PHE:CD1	2:B:501:NAR:H111	2.50	0.45
1:C:28:ILE:HG12	1:C:228:ILE:HG22	1.96	0.45
1:A:282:SER:O	1:A:328:LYS:HG2	2.16	0.45
1:B:117:THR:O	1:B:121:LYS:HG2	2.17	0.45
1:D:293:PHE:HE1	1:D:381:LEU:HD21	1.82	0.45
1:C:176:VAL:HG23	1:C:177:MET:HE3	1.98	0.45
1:A:316:PRO:HB3	1:A:322:LEU:HD11	1.97	0.45
1:D:91:ALA:HB3	1:D:94:GLU:HG3	1.99	0.45
1:A:322:LEU:HD22	1:A:336:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PHE:HB2	1:A:304:VAL:HG12	2.00	0.44
1:B:103:MET:CE	1:B:201:ALA:HB1	2.47	0.44
1:D:335:LYS:HA	1:D:335:LYS:HE2	1.97	0.44
1:C:235:ILE:HA	1:C:236:PRO:HD3	1.80	0.44
1:A:382:LEU:HB3	1:A:394:VAL:HB	2.00	0.44
1:D:331:LEU:HB3	1:D:335:LYS:HG3	2.00	0.44
1:A:372:THR:HG23	1:A:374:GLY:N	2.31	0.44
1:C:10:PRO:HA	1:C:11:PRO:HD3	1.86	0.44
1:D:313:ILE:HG23	1:D:357:ILE:HB	1.98	0.44
1:A:365:SER:HA	1:A:370:LEU:HD12	2.00	0.44
1:D:108:VAL:HG13	1:D:197:SER:HB3	2.00	0.43
1:A:246:HIS:HB3	1:D:15:LYS:HG3	2.01	0.43
1:C:100:ARG:HA	1:C:103:MET:HE2	1.99	0.43
1:C:171:PHE:CD2	1:C:390:THR:HB	2.53	0.43
1:A:175:THR:HG23	1:A:178:ARG:NH2	2.33	0.43
1:A:127:LYS:HB2	1:A:127:LYS:HE2	1.70	0.43
1:D:310:VAL:HB	1:D:380:GLY:HA2	2.00	0.43
1:B:103:MET:HE1	1:B:201:ALA:HB1	1.99	0.43
1:D:36:VAL:HG22	1:D:75:TYR:CE1	2.53	0.43
1:D:311:PHE:CE1	1:D:380:GLY:HA3	2.53	0.43
1:D:323:ASP:OD1	1:D:340:ARG:NH2	2.52	0.43
1:A:315:HIS:HA	1:A:316:PRO:HD3	1.80	0.43
1:A:39:GLN:OE1	4:A:609:HOH:O	2.21	0.42
1:B:121:LYS:HA	1:B:121:LYS:HD3	1.84	0.42
1:D:194:VAL:HB	1:D:228:ILE:HG13	2.01	0.42
1:D:378:GLU:O	1:D:397:ARG:HG3	2.19	0.42
1:C:103:MET:CE	1:C:201:ALA:HB1	2.49	0.42
1:C:258:GLY:O	1:C:274:MET:HB2	2.20	0.42
1:C:123:TRP:CD2	1:C:125:GLN:HB2	2.53	0.42
1:A:319:PRO:HD2	4:A:661:HOH:O	2.18	0.42
1:D:30:THR:HB	1:D:356:PHE:CZ	2.55	0.42
1:D:194:VAL:O	1:D:227:ALA:HA	2.19	0.42
2:A:501:NAR:O2	2:A:501:NAR:O5	2.34	0.42
1:C:64:ARG:HG3	1:C:68:LYS:HD3	2.01	0.42
1:B:172:ALA:O	1:B:176:VAL:HG13	2.19	0.41
1:C:62:PHE:HD1	1:C:65:MET:CE	2.32	0.41
1:D:97:LEU:O	1:D:97:LEU:HG	2.19	0.41
1:D:212:LEU:O	1:D:216:VAL:HG23	2.20	0.41
1:C:300:GLU:OE2	1:C:300:GLU:N	2.48	0.41
1:C:311:PHE:CE1	1:C:380:GLY:HA3	2.55	0.41
1:D:304:VAL:HA	1:D:305:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:CYS:SG	3:B:502[B]:COA:S1P	3.19	0.41
1:B:301:GLU:O	1:B:301:GLU:CG	2.69	0.41
1:D:311:PHE:CD1	1:D:380:GLY:HA3	2.54	0.41
1:B:89:MET:SD	1:B:103:MET:HE2	2.60	0.41
1:A:30:THR:HB	1:A:356:PHE:CZ	2.56	0.41
1:C:335:LYS:HA	1:C:335:LYS:HE2	2.03	0.41
1:A:322:LEU:HB3	1:A:336:MET:HE2	2.02	0.41
1:A:336:MET:HE3	1:A:339:SER:HB2	2.02	0.41
1:C:196:CYS:O	1:C:225:ALA:HA	2.21	0.41
1:A:52:SER:O	1:A:55:MET:HG3	2.20	0.41
1:A:194:VAL:HB	1:A:228:ILE:CG1	2.49	0.41
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.82	0.41
1:C:46:TYR:CE2	1:C:207:PRO:HG3	2.56	0.41
1:D:262:GLY:HA2	1:D:270:THR:O	2.21	0.41
1:A:58:LEU:HD23	1:A:207:PRO:HB2	2.03	0.40
1:C:64:ARG:HG3	1:C:68:LYS:NZ	2.37	0.40
1:A:73:LYS:HE2	1:A:75:TYR:OH	2.22	0.40
1:A:228:ILE:HG21	1:A:355:LEU:HD22	2.03	0.40
1:B:27:ALA:O	1:B:228:ILE:HA	2.21	0.40
1:A:49:ILE:HD12	1:A:49:ILE:HA	1.92	0.40
1:C:168:GLN:HB3	1:C:172:ALA:HB2	2.03	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	387/404 (96%)	372 (96%)	14 (4%)	1 (0%)	41 55
1	B	394/404 (98%)	382 (97%)	11 (3%)	1 (0%)	41 55
1	C	394/404 (98%)	384 (98%)	10 (2%)	0	100 100
1	D	388/404 (96%)	375 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1563/1616 (97%)	1513 (97%)	48 (3%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	B	97	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	327/338 (97%)	324 (99%)	3 (1%)	78 90
1	B	331/338 (98%)	320 (97%)	11 (3%)	38 57
1	C	331/338 (98%)	322 (97%)	9 (3%)	44 65
1	D	328/338 (97%)	325 (99%)	3 (1%)	78 90
All	All	1317/1352 (97%)	1291 (98%)	26 (2%)	55 74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	250	SER
1	A	387	PRO
1	B	80	GLU
1	B	94	GLU
1	B	97	LEU
1	B	108	VAL
1	B	203	THR
1	B	257	ASP
1	B	300	GLU
1	B	306	SER
1	B	348	ASN
1	B	355	LEU

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Mol	Chain	Res	Type
1	B	389	LEU
1	C	83	LEU
1	C	97	LEU
1	C	203	THR
1	C	237	GLU
1	C	300	GLU
1	C	301	GLU
1	C	303	GLU
1	C	355	LEU
1	C	361	LEU
1	D	83	LEU
1	D	355	LEU
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	B	348	ASN
1	B	360	HIS
1	D	32	ASN
1	D	86	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

10 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	NAR	A	501	-	22,22,22	1.71	6 (27%)	32,32,32	2.02	9 (28%)
2	NAR	B	501	-	22,22,22	1.96	7 (31%)	32,32,32	1.78	8 (25%)
3	COA	D	502[A]	-	41,50,50	1.03	3 (7%)	52,75,75	1.72	10 (19%)
3	COA	B	502[B]	-	41,50,50	1.31	7 (17%)	52,75,75	1.70	13 (25%)
3	COA	C	502[B]	-	41,50,50	0.99	1 (2%)	52,75,75	1.61	11 (21%)
2	NAR	D	501	-	22,22,22	1.36	4 (18%)	32,32,32	1.86	10 (31%)
2	NAR	C	501	-	22,22,22	1.69	9 (40%)	32,32,32	2.07	11 (34%)
3	COA	B	502[A]	-	41,50,50	1.32	7 (17%)	52,75,75	1.70	13 (25%)
3	COA	C	502[A]	-	41,50,50	0.99	1 (2%)	52,75,75	1.61	11 (21%)
3	COA	D	502[B]	-	41,50,50	1.03	3 (7%)	52,75,75	1.72	10 (19%)

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	NAR	A	501	-	-	0/4/16/16	0/3/3/3
2	NAR	B	501	-	-	0/4/16/16	0/3/3/3
3	COA	D	502[A]	-	-	13/44/64/64	0/3/3/3
3	COA	B	502[B]	-	-	12/44/64/64	0/3/3/3
3	COA	C	502[B]	-	-	23/44/64/64	0/3/3/3
2	NAR	D	501	-	-	0/4/16/16	0/3/3/3
2	NAR	C	501	-	-	0/4/16/16	0/3/3/3
3	COA	B	502[A]	-	-	12/44/64/64	0/3/3/3
3	COA	C	502[A]	-	-	22/44/64/64	0/3/3/3
3	COA	D	502[B]	-	-	13/44/64/64	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAR	O1-C6	-4.34	1.32	1.38
2	B	501	NAR	O1-C6	-3.96	1.32	1.38
2	B	501	NAR	C10-C9	-3.49	1.45	1.51
3	B	502[A]	COA	C4A-N3A	-3.06	1.31	1.35
3	B	502[B]	COA	C4A-N3A	-3.06	1.31	1.35
2	C	501	NAR	C5-C6	2.96	1.45	1.40
2	C	501	NAR	C10-C9	-2.86	1.46	1.51
2	A	501	NAR	C5-C4	2.83	1.46	1.41
2	C	501	NAR	O1-C6	-2.73	1.34	1.38
2	B	501	NAR	C5-C4	2.73	1.45	1.41
2	D	501	NAR	C5-C6	2.71	1.45	1.40
2	B	501	NAR	O3-C13	-2.67	1.30	1.37
2	D	501	NAR	C10-C9	-2.67	1.46	1.51
2	D	501	NAR	C5-C4	2.62	1.45	1.41
2	B	501	NAR	C5-C6	2.59	1.45	1.40
2	B	501	NAR	C3-C4	-2.54	1.35	1.38
3	D	502[A]	COA	O4B-C1B	2.50	1.44	1.41
3	D	502[B]	COA	O4B-C1B	2.50	1.44	1.41
3	D	502[A]	COA	O5P-C5P	-2.41	1.18	1.23
3	D	502[B]	COA	O5P-C5P	-2.41	1.18	1.23
3	B	502[A]	COA	C2B-C1B	-2.40	1.50	1.53
3	B	502[B]	COA	C2B-C1B	-2.40	1.50	1.53
3	D	502[A]	COA	C2B-C1B	-2.40	1.50	1.53
3	D	502[B]	COA	C2B-C1B	-2.40	1.50	1.53
2	A	501	NAR	C10-C9	-2.38	1.47	1.51
3	B	502[A]	COA	C5A-N7A	-2.38	1.31	1.39
3	B	502[B]	COA	C5A-N7A	-2.38	1.31	1.39
3	B	502[A]	COA	OAP-CAP	2.37	1.46	1.42
3	B	502[B]	COA	OAP-CAP	2.37	1.46	1.42
2	C	501	NAR	O4-C2	-2.35	1.31	1.37
3	B	502[A]	COA	P3B-O3B	2.35	1.63	1.59
3	B	502[B]	COA	P3B-O3B	2.35	1.63	1.59
2	C	501	NAR	O3-C13	-2.35	1.31	1.37
2	C	501	NAR	O2-C7	-2.32	1.18	1.22
2	C	501	NAR	C5-C4	2.30	1.45	1.41
3	C	502[A]	COA	C5A-C4A	2.28	1.46	1.40
3	C	502[B]	COA	C5A-C4A	2.28	1.46	1.40
2	C	501	NAR	C15-C10	-2.20	1.35	1.39
2	B	501	NAR	O2-C7	-2.20	1.18	1.22
2	A	501	NAR	C12-C11	-2.16	1.34	1.38
2	A	501	NAR	O1-C9	-2.15	1.39	1.44
3	B	502[A]	COA	O5P-C5P	-2.06	1.19	1.23
3	B	502[B]	COA	O5P-C5P	-2.06	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAR	O3-C13	-2.04	1.32	1.37
2	C	501	NAR	C12-C11	-2.03	1.35	1.38
3	B	502[A]	COA	O9P-C9P	-2.03	1.19	1.23
3	B	502[B]	COA	O9P-C9P	-2.03	1.19	1.23
2	D	501	NAR	O1-C9	-2.02	1.39	1.44

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502[A]	COA	P2A-O3A-P1A	-5.65	113.44	132.83
3	D	502[B]	COA	P2A-O3A-P1A	-5.65	113.44	132.83
2	A	501	NAR	O2-C7-C5	-4.81	114.77	122.38
2	A	501	NAR	O1-C6-C1	4.48	123.42	116.38
3	D	502[A]	COA	CDP-CBP-CCP	4.38	115.38	108.23
3	D	502[B]	COA	CDP-CBP-CCP	4.38	115.38	108.23
2	D	501	NAR	C3-C4-C5	-4.29	115.95	120.93
3	B	502[A]	COA	P2A-O3A-P1A	-4.26	118.20	132.83
3	B	502[B]	COA	P2A-O3A-P1A	-4.26	118.20	132.83
2	C	501	NAR	C4-C5-C6	4.23	121.65	117.35
2	B	501	NAR	O2-C7-C8	3.96	126.36	120.79
2	A	501	NAR	O2-C7-C8	3.96	126.35	120.79
2	B	501	NAR	O2-C7-C5	-3.89	116.22	122.38
2	D	501	NAR	C4-C5-C6	3.84	121.25	117.35
2	C	501	NAR	C3-C4-C5	-3.84	116.48	120.93
3	B	502[A]	COA	O3B-P3B-O7A	-3.78	94.81	109.39
3	B	502[B]	COA	O3B-P3B-O7A	-3.78	94.81	109.39
2	C	501	NAR	C6-O1-C9	3.78	121.85	115.50
2	C	501	NAR	O1-C6-C1	3.73	122.25	116.38
2	D	501	NAR	O2-C7-C8	3.70	125.99	120.79
3	B	502[A]	COA	N3A-C2A-N1A	-3.58	123.09	128.68
3	B	502[B]	COA	N3A-C2A-N1A	-3.58	123.09	128.68
2	D	501	NAR	O1-C6-C1	3.53	121.93	116.38
2	A	501	NAR	O1-C6-C5	-3.52	117.93	121.56
2	B	501	NAR	C3-C4-C5	-3.51	116.86	120.93
3	D	502[A]	COA	C4A-C5A-N7A	-3.49	105.76	109.40
3	D	502[B]	COA	C4A-C5A-N7A	-3.49	105.76	109.40
3	C	502[A]	COA	C4A-C5A-N7A	-3.45	105.81	109.40
3	C	502[B]	COA	C4A-C5A-N7A	-3.45	105.81	109.40
3	D	502[A]	COA	O6A-CCP-CBP	3.37	115.96	110.55
3	D	502[B]	COA	O6A-CCP-CBP	3.37	115.96	110.55
3	C	502[A]	COA	C6P-C7P-N8P	-3.36	105.11	111.90
3	C	502[B]	COA	C6P-C7P-N8P	-3.36	105.11	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502[A]	COA	CEP-CBP-CAP	3.29	114.52	108.82
3	C	502[B]	COA	CEP-CBP-CAP	3.29	114.52	108.82
2	C	501	NAR	C14-C15-C10	-3.29	117.89	121.20
3	C	502[A]	COA	C3P-N4P-C5P	3.27	128.91	122.84
3	C	502[B]	COA	C3P-N4P-C5P	3.27	128.91	122.84
3	B	502[A]	COA	O4B-C1B-C2B	-3.19	102.27	106.93
3	B	502[B]	COA	O4B-C1B-C2B	-3.19	102.27	106.93
2	C	501	NAR	C3-C2-C1	3.18	124.83	120.43
2	D	501	NAR	O2-C7-C5	-3.16	117.38	122.38
2	B	501	NAR	C4-C5-C6	3.13	120.53	117.35
2	C	501	NAR	O2-C7-C5	-3.12	117.44	122.38
3	C	502[A]	COA	C3B-C2B-C1B	3.03	106.59	99.89
3	C	502[B]	COA	C3B-C2B-C1B	3.03	106.59	99.89
3	D	502[A]	COA	O9A-P3B-O8A	2.98	119.01	107.64
3	D	502[B]	COA	O9A-P3B-O8A	2.98	119.01	107.64
3	C	502[A]	COA	P2A-O3A-P1A	-2.88	122.95	132.83
3	C	502[B]	COA	P2A-O3A-P1A	-2.88	122.95	132.83
2	C	501	NAR	C11-C12-C13	-2.88	116.72	119.88
3	D	502[A]	COA	N3A-C2A-N1A	-2.88	124.18	128.68
3	D	502[B]	COA	N3A-C2A-N1A	-2.88	124.18	128.68
2	A	501	NAR	C6-O1-C9	2.78	120.17	115.50
2	A	501	NAR	C4-C5-C6	2.74	120.14	117.35
3	D	502[A]	COA	C6P-C5P-N4P	2.70	120.96	116.42
3	D	502[B]	COA	C6P-C5P-N4P	2.70	120.96	116.42
3	C	502[A]	COA	CEP-CBP-CDP	-2.69	103.67	109.17
3	C	502[B]	COA	CEP-CBP-CDP	-2.69	103.67	109.17
3	B	502[A]	COA	O5P-C5P-C6P	-2.68	117.11	122.02
3	B	502[B]	COA	O5P-C5P-C6P	-2.68	117.11	122.02
2	B	501	NAR	C3-C2-C1	2.59	124.01	120.43
2	A	501	NAR	C3-C4-C5	-2.56	117.97	120.93
3	B	502[A]	COA	C6P-C7P-N8P	2.52	116.98	111.90
3	B	502[B]	COA	C6P-C7P-N8P	2.52	116.98	111.90
2	B	501	NAR	O1-C6-C1	2.48	120.29	116.38
3	B	502[A]	COA	O3B-C3B-C2B	2.48	120.67	111.68
3	B	502[B]	COA	O3B-C3B-C2B	2.48	120.67	111.68
2	A	501	NAR	O5-C4-C5	-2.44	116.57	121.14
3	B	502[A]	COA	OAP-CAP-CBP	-2.41	104.58	110.25
3	B	502[B]	COA	OAP-CAP-CBP	-2.41	104.58	110.25
3	B	502[A]	COA	C7P-N8P-C9P	2.40	126.86	122.59
3	B	502[B]	COA	C7P-N8P-C9P	2.40	126.86	122.59
2	C	501	NAR	O5-C4-C3	2.39	125.85	119.46
3	C	502[A]	COA	C5A-C6A-N6A	2.37	123.95	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502[B]	COA	C5A-C6A-N6A	2.37	123.95	120.35
3	B	502[A]	COA	CEP-CBP-CCP	2.34	112.04	108.23
3	B	502[B]	COA	CEP-CBP-CCP	2.34	112.04	108.23
2	D	501	NAR	O1-C6-C5	-2.33	119.16	121.56
2	C	501	NAR	O1-C6-C5	-2.33	119.16	121.56
3	B	502[A]	COA	O6A-P2A-O4A	-2.32	100.02	109.07
3	B	502[B]	COA	O6A-P2A-O4A	-2.32	100.02	109.07
3	C	502[A]	COA	C7P-N8P-C9P	-2.31	118.47	122.59
3	C	502[B]	COA	C7P-N8P-C9P	-2.31	118.47	122.59
2	D	501	NAR	C4-C3-C2	2.26	121.74	119.70
2	D	501	NAR	C3-C2-C1	2.25	123.54	120.43
2	A	501	NAR	O5-C4-C3	2.24	125.46	119.46
3	D	502[A]	COA	CEP-CBP-CDP	-2.19	104.70	109.17
3	D	502[B]	COA	CEP-CBP-CDP	-2.19	104.70	109.17
2	D	501	NAR	O5-C4-C3	2.19	125.32	119.46
3	B	502[A]	COA	O5A-P2A-O4A	2.15	122.86	112.24
3	B	502[B]	COA	O5A-P2A-O4A	2.15	122.86	112.24
2	B	501	NAR	C15-C10-C11	2.14	120.96	118.29
3	D	502[A]	COA	O5P-C5P-C6P	-2.12	118.14	122.02
3	D	502[B]	COA	O5P-C5P-C6P	-2.12	118.14	122.02
3	C	502[A]	COA	CDP-CBP-CAP	2.11	112.47	108.82
3	C	502[B]	COA	CDP-CBP-CAP	2.11	112.47	108.82
2	C	501	NAR	C15-C10-C11	2.08	120.89	118.29
3	B	502[A]	COA	C6P-C5P-N4P	2.07	119.91	116.42
3	B	502[B]	COA	C6P-C5P-N4P	2.07	119.91	116.42
2	B	501	NAR	C1-C6-C5	-2.06	118.23	121.86
3	D	502[A]	COA	C6P-C7P-N8P	2.05	116.03	111.90
3	D	502[B]	COA	C6P-C7P-N8P	2.05	116.03	111.90
3	C	502[A]	COA	N3A-C2A-N1A	-2.03	125.50	128.68
3	C	502[B]	COA	N3A-C2A-N1A	-2.03	125.50	128.68
2	D	501	NAR	C15-C10-C11	2.01	120.80	118.29

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[A]	COA	C5B-O5B-P1A-O1A
3	B	502[A]	COA	C5B-O5B-P1A-O2A
3	B	502[A]	COA	CCP-O6A-P2A-O3A
3	B	502[A]	COA	CCP-O6A-P2A-O5A
3	B	502[A]	COA	O9P-C9P-CAP-CBP
3	B	502[A]	COA	N8P-C9P-CAP-CBP

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Mol	Chain	Res	Type	Atoms
3	B	502[A]	COA	N8P-C9P-CAP-OAP
3	B	502[A]	COA	C6P-C5P-N4P-C3P
3	B	502[A]	COA	O5P-C5P-N4P-C3P
3	B	502[B]	COA	C5B-O5B-P1A-O1A
3	B	502[B]	COA	C5B-O5B-P1A-O2A
3	B	502[B]	COA	CCP-O6A-P2A-O3A
3	B	502[B]	COA	CCP-O6A-P2A-O5A
3	B	502[B]	COA	O9P-C9P-CAP-CBP
3	B	502[B]	COA	N8P-C9P-CAP-CBP
3	B	502[B]	COA	N8P-C9P-CAP-OAP
3	B	502[B]	COA	C6P-C5P-N4P-C3P
3	B	502[B]	COA	O5P-C5P-N4P-C3P
3	C	502[A]	COA	C3B-C4B-C5B-O5B
3	C	502[A]	COA	O4B-C4B-C5B-O5B
3	C	502[A]	COA	C5B-O5B-P1A-O3A
3	C	502[A]	COA	CAP-C9P-N8P-C7P
3	C	502[A]	COA	C5P-C6P-C7P-N8P
3	C	502[A]	COA	C2P-C3P-N4P-C5P
3	C	502[B]	COA	C3B-C4B-C5B-O5B
3	C	502[B]	COA	O4B-C4B-C5B-O5B
3	C	502[B]	COA	C5B-O5B-P1A-O3A
3	C	502[B]	COA	CAP-C9P-N8P-C7P
3	C	502[B]	COA	C5P-C6P-C7P-N8P
3	C	502[B]	COA	C2P-C3P-N4P-C5P
3	D	502[A]	COA	C5B-O5B-P1A-O1A
3	D	502[A]	COA	CBP-CCP-O6A-P2A
3	D	502[A]	COA	O9P-C9P-CAP-CBP
3	D	502[A]	COA	N8P-C9P-CAP-CBP
3	D	502[B]	COA	C5B-O5B-P1A-O1A
3	D	502[B]	COA	CBP-CCP-O6A-P2A
3	D	502[B]	COA	O9P-C9P-CAP-CBP
3	D	502[B]	COA	N8P-C9P-CAP-CBP
3	D	502[A]	COA	C6P-C7P-N8P-C9P
3	D	502[B]	COA	C6P-C7P-N8P-C9P
3	C	502[A]	COA	O5P-C5P-N4P-C3P
3	C	502[B]	COA	O5P-C5P-N4P-C3P
3	C	502[A]	COA	C2B-C3B-O3B-P3B
3	C	502[B]	COA	C2B-C3B-O3B-P3B
3	D	502[A]	COA	C2B-C3B-O3B-P3B
3	D	502[B]	COA	C2B-C3B-O3B-P3B
3	C	502[A]	COA	C6P-C5P-N4P-C3P
3	C	502[B]	COA	C6P-C5P-N4P-C3P

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Mol	Chain	Res	Type	Atoms
3	C	502[A]	COA	O9P-C9P-N8P-C7P
3	C	502[B]	COA	O9P-C9P-N8P-C7P
3	C	502[A]	COA	C6P-C7P-N8P-C9P
3	C	502[B]	COA	C6P-C7P-N8P-C9P
3	D	502[A]	COA	C4B-C3B-O3B-P3B
3	D	502[B]	COA	C4B-C3B-O3B-P3B
3	B	502[A]	COA	C5P-C6P-C7P-N8P
3	B	502[B]	COA	C5P-C6P-C7P-N8P
3	D	502[A]	COA	C5P-C6P-C7P-N8P
3	D	502[B]	COA	C5P-C6P-C7P-N8P
3	B	502[A]	COA	O9P-C9P-CAP-OAP
3	B	502[B]	COA	O9P-C9P-CAP-OAP
3	C	502[A]	COA	CDP-CBP-CCP-O6A
3	C	502[B]	COA	CDP-CBP-CCP-O6A
3	C	502[A]	COA	C3B-O3B-P3B-O7A
3	C	502[B]	COA	C3B-O3B-P3B-O7A
3	C	502[A]	COA	C9P-CAP-CBP-CDP
3	C	502[A]	COA	C9P-CAP-CBP-CEP
3	C	502[B]	COA	C9P-CAP-CBP-CDP
3	C	502[B]	COA	C9P-CAP-CBP-CEP
3	D	502[A]	COA	C5B-O5B-P1A-O3A
3	D	502[B]	COA	C5B-O5B-P1A-O3A
3	D	502[A]	COA	C3B-C4B-C5B-O5B
3	D	502[B]	COA	C3B-C4B-C5B-O5B
3	C	502[A]	COA	C5B-O5B-P1A-O1A
3	C	502[B]	COA	C5B-O5B-P1A-O1A
3	D	502[A]	COA	C5B-O5B-P1A-O2A
3	D	502[B]	COA	C5B-O5B-P1A-O2A
3	C	502[A]	COA	OAP-CAP-CBP-CEP
3	C	502[B]	COA	OAP-CAP-CBP-CEP
3	C	502[A]	COA	O9P-C9P-CAP-CBP
3	C	502[B]	COA	O9P-C9P-CAP-CBP
3	C	502[A]	COA	CEP-CBP-CCP-O6A
3	C	502[B]	COA	CEP-CBP-CCP-O6A
3	D	502[A]	COA	CEP-CBP-CCP-O6A
3	D	502[B]	COA	CEP-CBP-CCP-O6A
3	C	502[A]	COA	N8P-C9P-CAP-CBP
3	C	502[B]	COA	N8P-C9P-CAP-CBP
3	C	502[A]	COA	C4B-C3B-O3B-P3B
3	C	502[B]	COA	C4B-C3B-O3B-P3B
3	C	502[B]	COA	S1P-C2P-C3P-N4P
3	D	502[A]	COA	CDP-CBP-CCP-O6A

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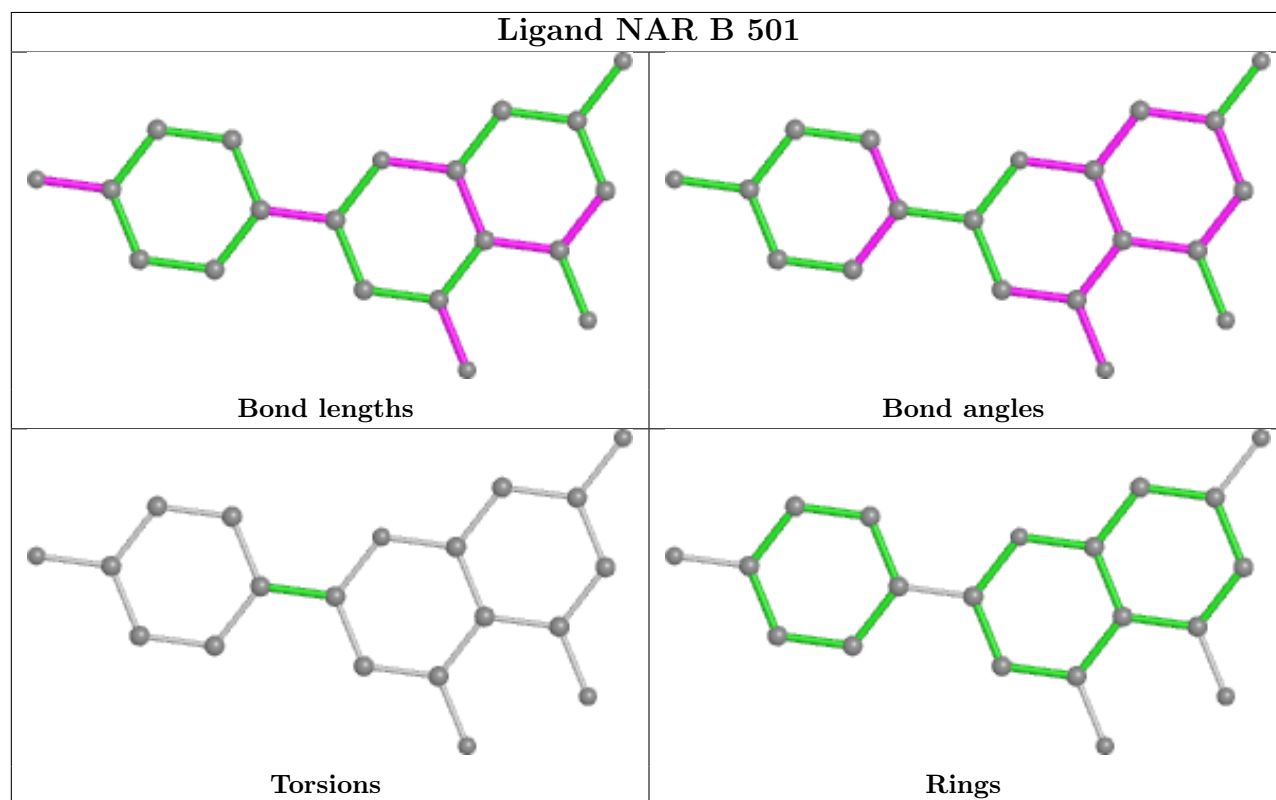
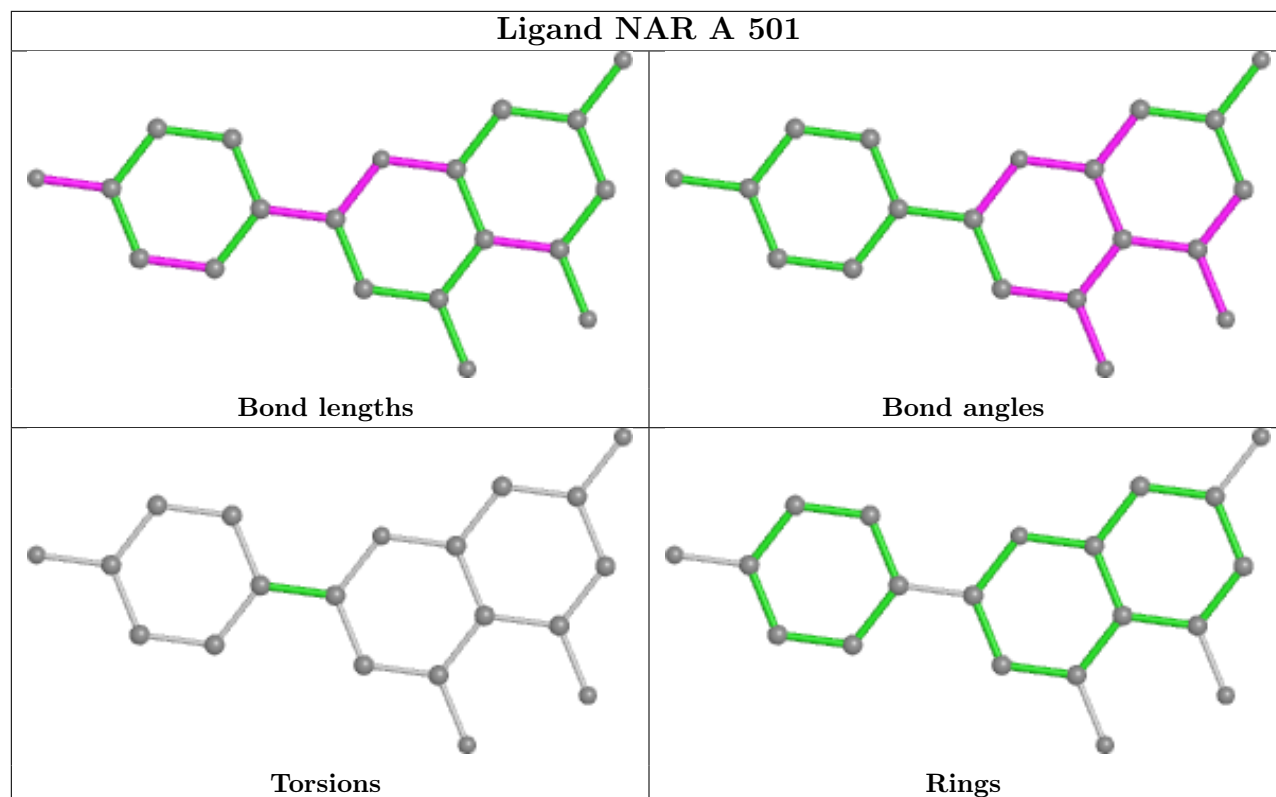
Mol	Chain	Res	Type	Atoms
3	D	502[B]	COA	CDP-CBP-CCP-O6A
3	B	502[A]	COA	C5B-O5B-P1A-O3A
3	B	502[B]	COA	C5B-O5B-P1A-O3A
3	C	502[A]	COA	C9P-CAP-CBP-CCP
3	C	502[B]	COA	C9P-CAP-CBP-CCP

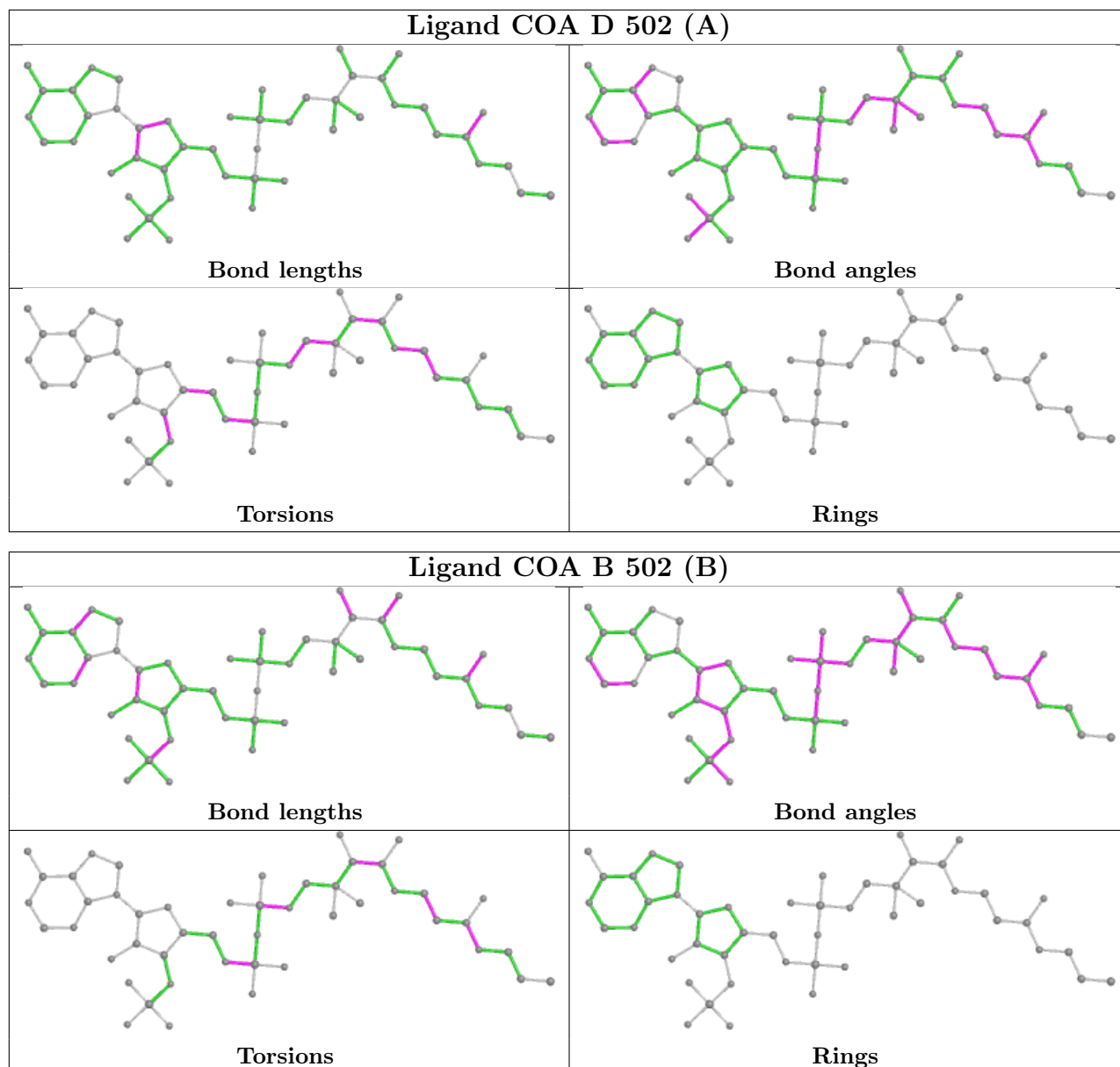
There are no ring outliers.

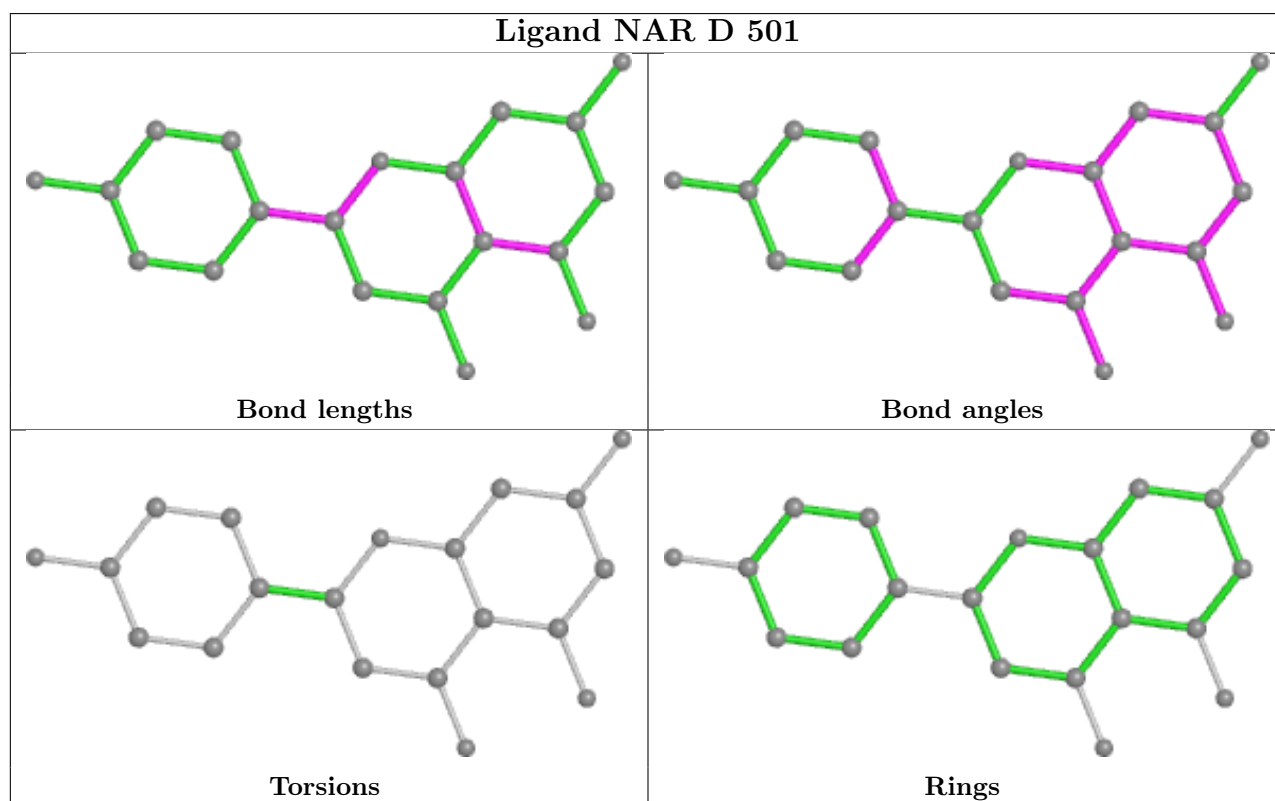
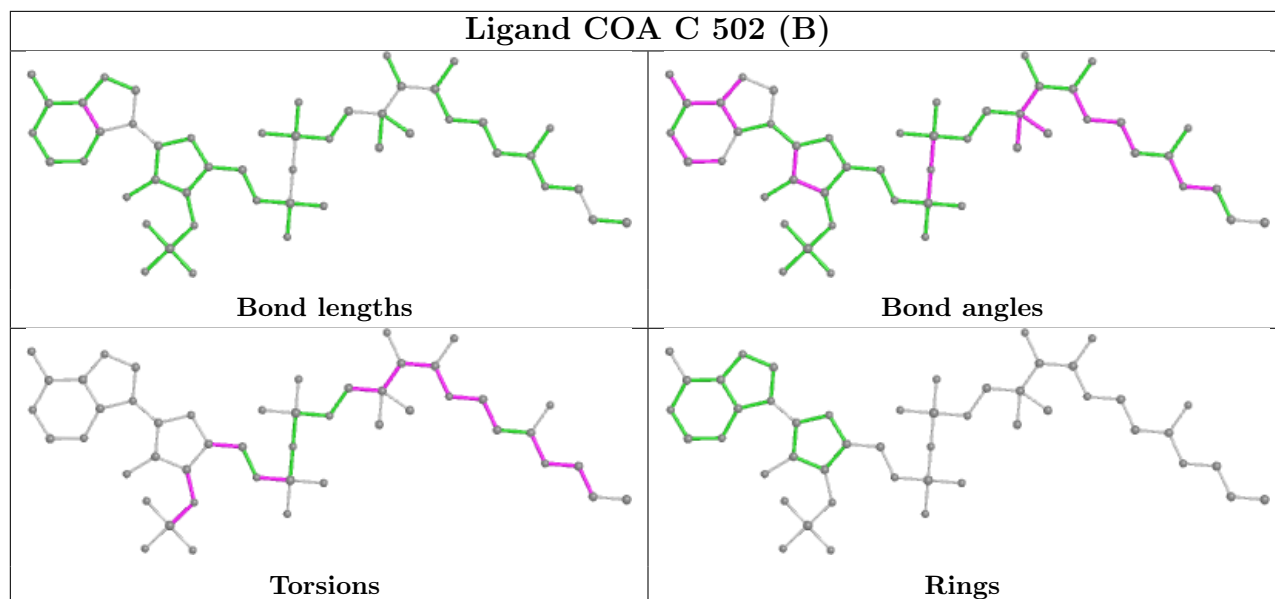
5 monomers are involved in 5 short contacts:

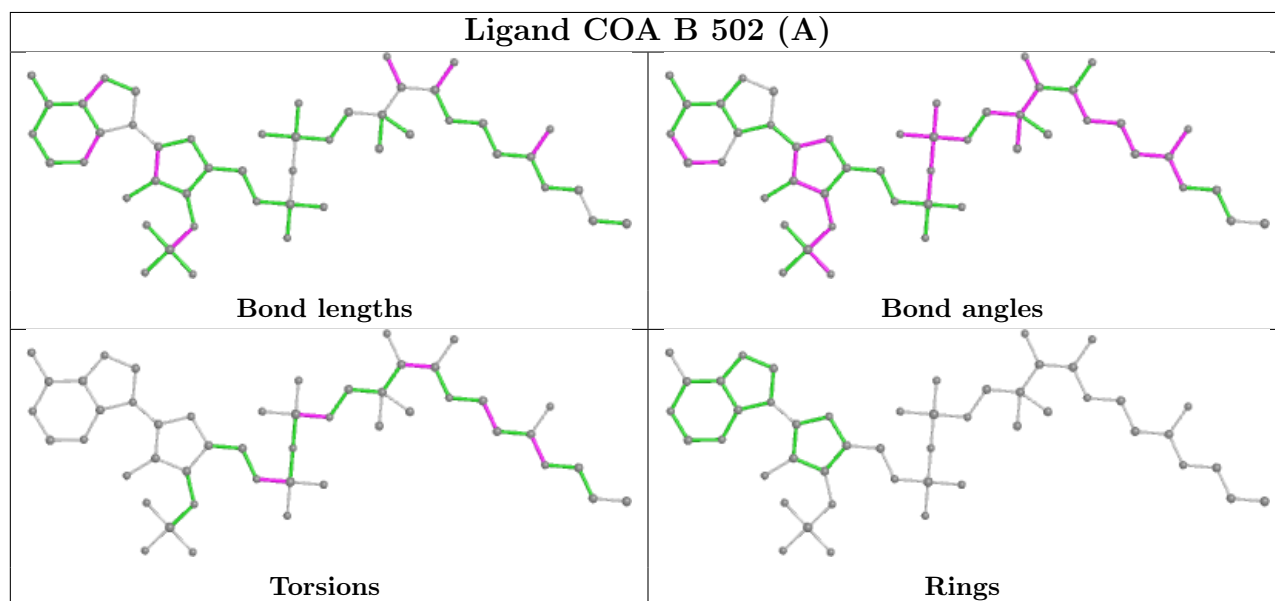
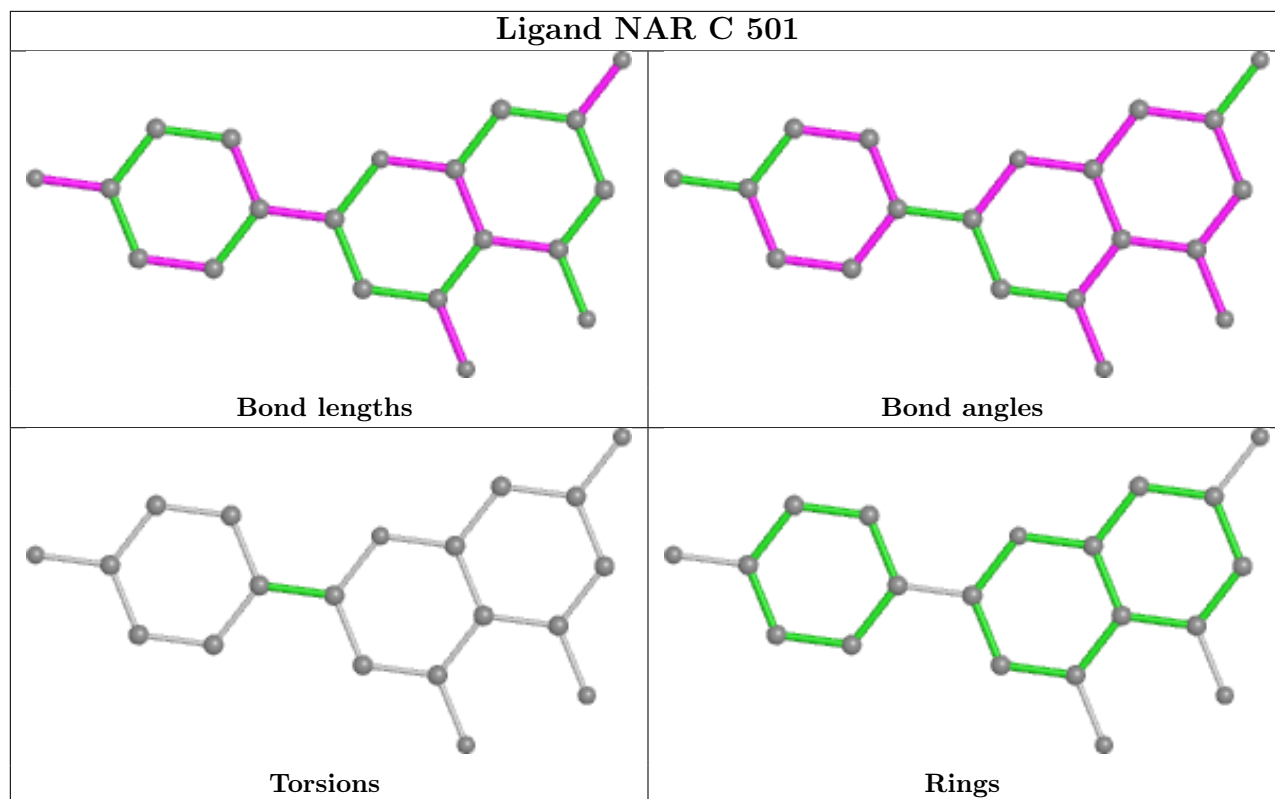
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAR	1	0
2	B	501	NAR	1	0
3	D	502[A]	COA	1	0
3	B	502[B]	COA	1	0
2	C	501	NAR	1	0

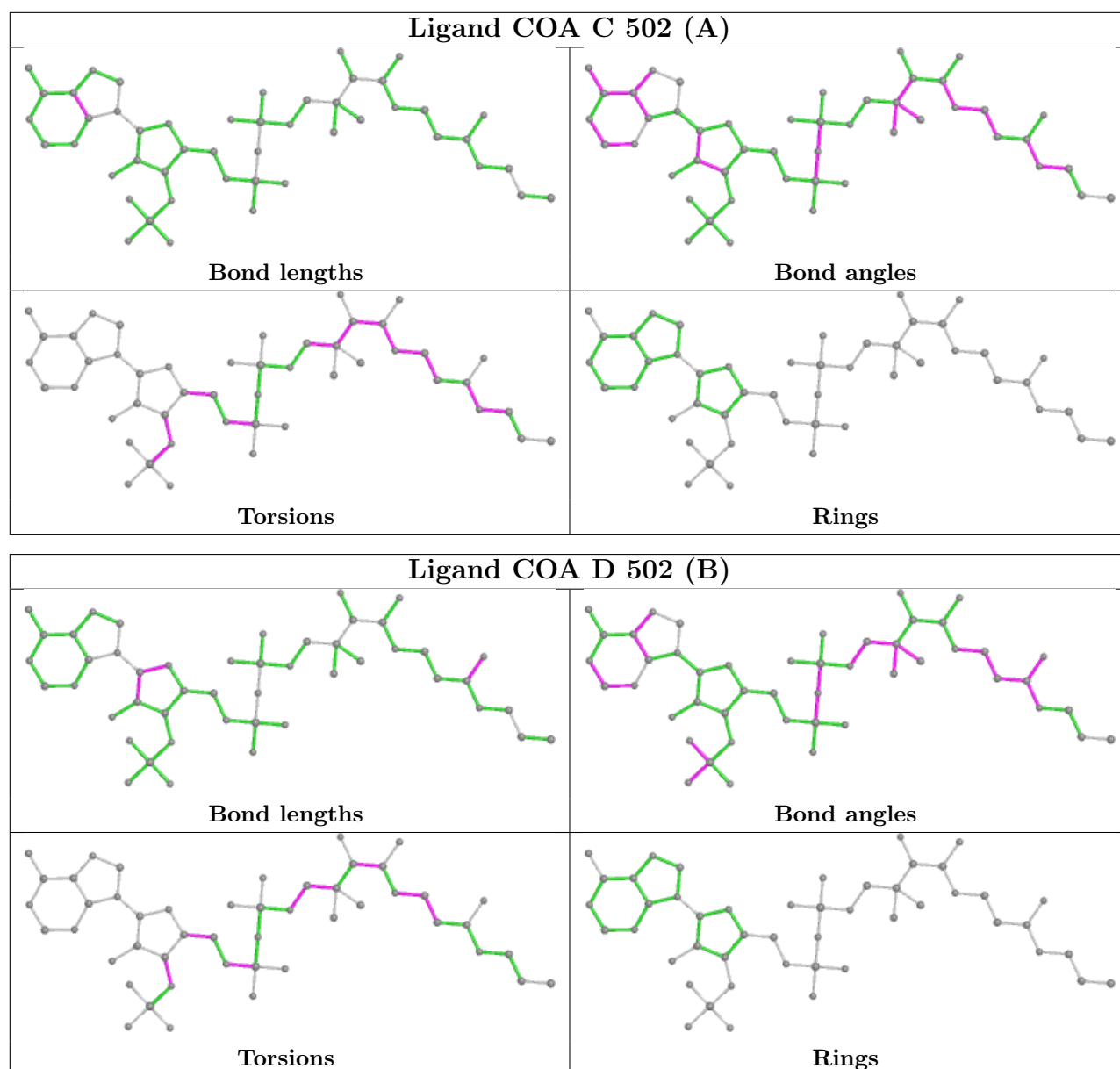
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	391/404 (96%)	0.22	18 (4%) 32 31	15, 23, 34, 44	0
1	B	396/404 (98%)	0.04	16 (4%) 38 37	12, 18, 30, 56	0
1	C	396/404 (98%)	0.13	24 (6%) 21 20	13, 20, 34, 59	0
1	D	392/404 (97%)	0.05	14 (3%) 42 42	14, 20, 33, 42	0
All	All	1575/1616 (97%)	0.11	72 (4%) 32 31	12, 20, 33, 59	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	GLU	5.5
1	C	402	ALA	5.4
1	C	299	ASN	5.3
1	C	301	GLU	5.0
1	B	302	GLY	4.6
1	A	402	ALA	4.5
1	C	302	GLY	4.3
1	C	300	GLU	4.3
1	D	274	MET	3.8
1	C	354	VAL	3.4
1	B	170	CYS	3.4
1	A	238	VAL	3.3
1	A	237	GLU	3.2
1	D	8	THR	3.1
1	C	303	GLU	3.1
1	D	333	THR	3.1
1	C	369	LYS	3.0
1	A	330	GLN	3.0
1	A	354	VAL	3.0
1	D	402	ALA	2.9
1	D	350	SER	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	371	ALA	2.9
1	A	369	LYS	2.8
1	C	170	CYS	2.8
1	C	212	LEU	2.7
1	C	176	VAL	2.7
1	A	170	CYS	2.6
1	C	366	VAL	2.6
1	A	352	ALA	2.6
1	B	172	ALA	2.6
1	B	355	LEU	2.6
1	A	36	VAL	2.6
1	B	176	VAL	2.5
1	C	384	GLY	2.5
1	B	173	GLY	2.5
1	D	170	CYS	2.5
1	B	350	SER	2.5
1	D	304	VAL	2.5
1	C	351	SER	2.5
1	A	13	ALA	2.5
1	B	382	LEU	2.5
1	A	304	VAL	2.5
1	C	316	PRO	2.5
1	A	367	GLU	2.4
1	D	299	ASN	2.4
1	C	352	ALA	2.4
1	A	366	VAL	2.4
1	B	354	VAL	2.4
1	C	173	GLY	2.4
1	A	355	LEU	2.4
1	A	350	SER	2.3
1	B	387	PRO	2.3
1	C	350	SER	2.3
1	D	355	LEU	2.3
1	B	136	CYS	2.2
1	D	401	LEU	2.2
1	B	402	ALA	2.2
1	D	11	PRO	2.2
1	C	330	GLN	2.2
1	D	172	ALA	2.2
1	A	372	THR	2.2
1	C	382	LEU	2.2
1	B	299	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	394	VAL	2.1
1	A	41	THR	2.1
1	C	138	THR	2.1
1	A	351	SER	2.0
1	D	209	GLU	2.0
1	C	64	ARG	2.0
1	C	349	MET	2.0
1	D	298	GLY	2.0
1	B	13	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

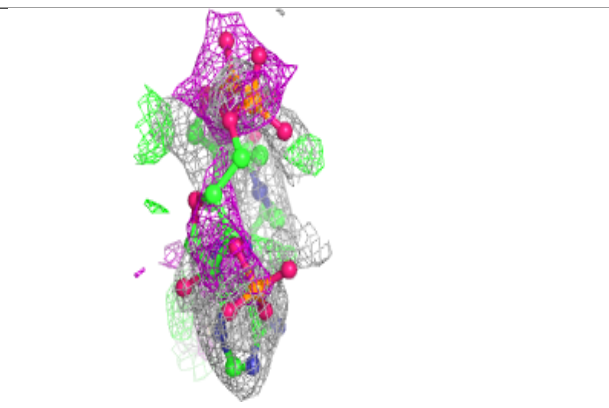
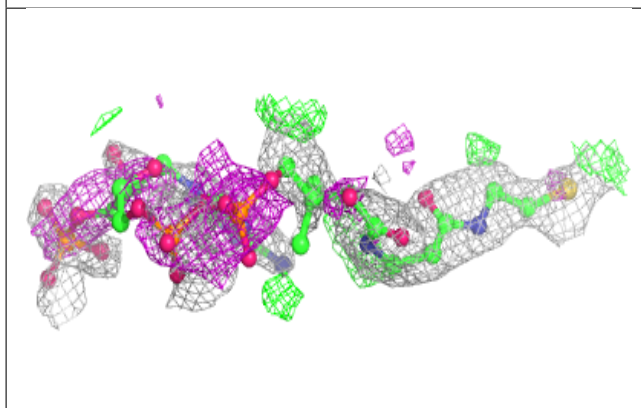
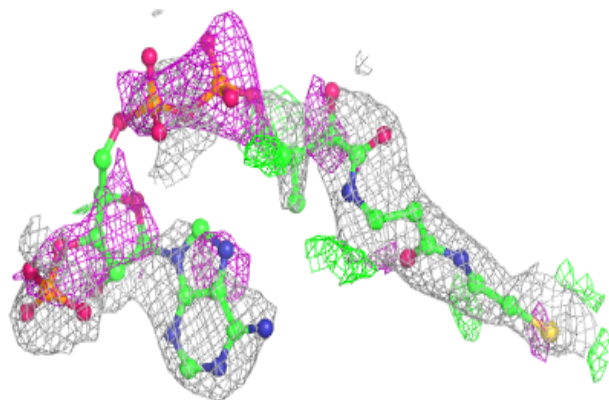
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COA	D	502[A]	48/48	0.54	0.45	23,55,85,104	1
3	COA	D	502[B]	48/48	0.54	0.45	22,55,85,104	1
3	COA	C	502[A]	48/48	0.62	0.45	21,58,78,93	1
3	COA	C	502[B]	48/48	0.62	0.45	21,58,78,93	1
3	COA	B	502[A]	48/48	0.74	0.34	16,46,69,86	1
3	COA	B	502[B]	48/48	0.74	0.34	17,46,69,86	1
2	NAR	D	501	20/20	0.90	0.17	14,26,32,37	0
2	NAR	B	501	20/20	0.91	0.17	12,21,30,32	0
2	NAR	C	501	20/20	0.93	0.14	16,22,26,28	0
2	NAR	A	501	20/20	0.94	0.14	17,23,27,29	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.

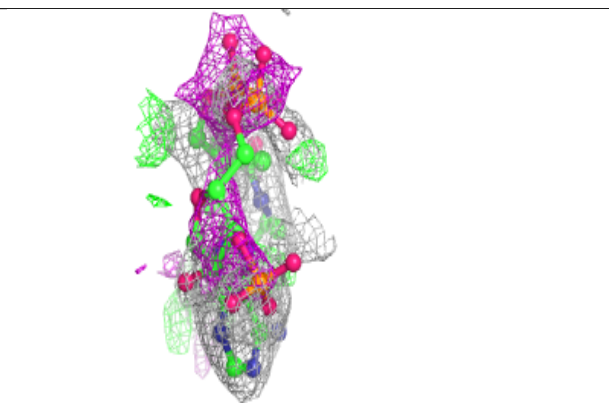
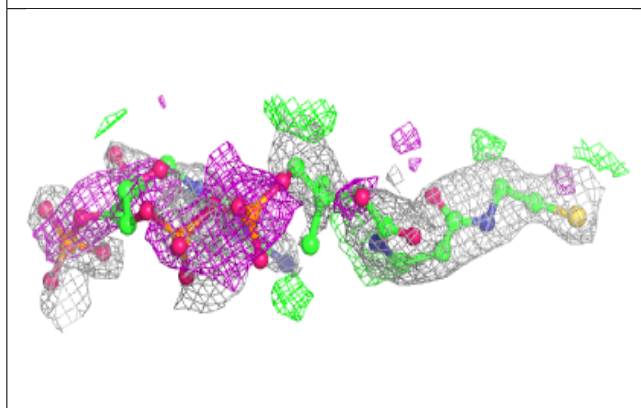
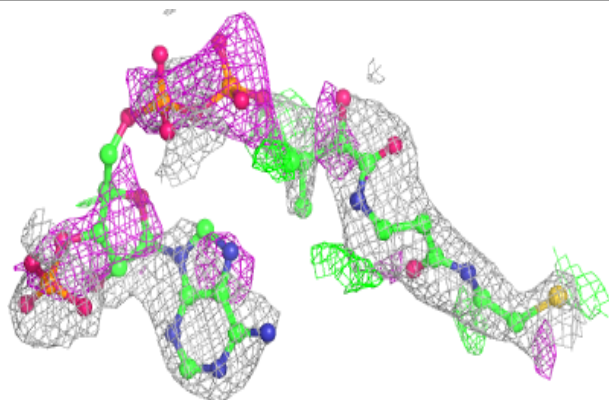
**Electron density around COA D 502 (A):**

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



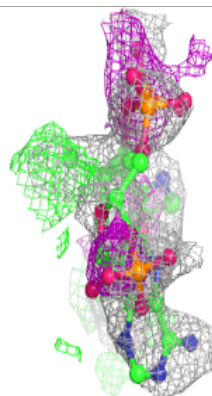
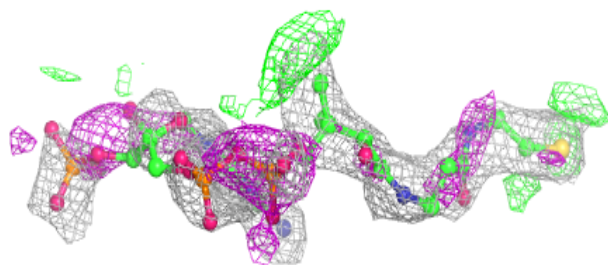
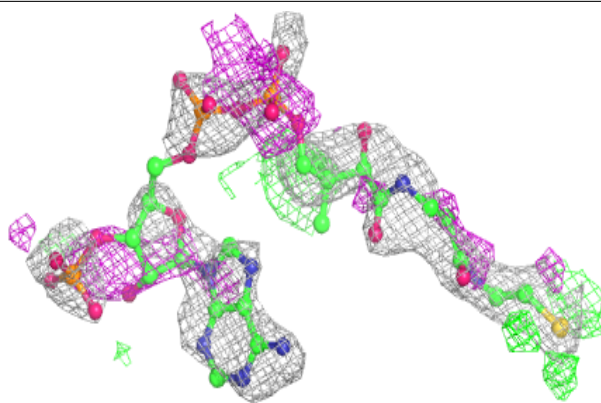
**Electron density around COA D 502 (B):**

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

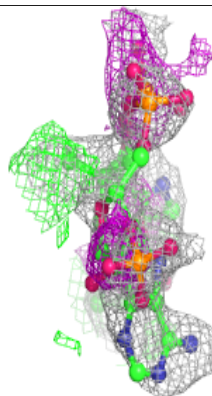
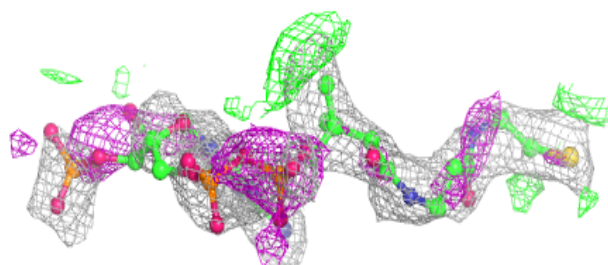
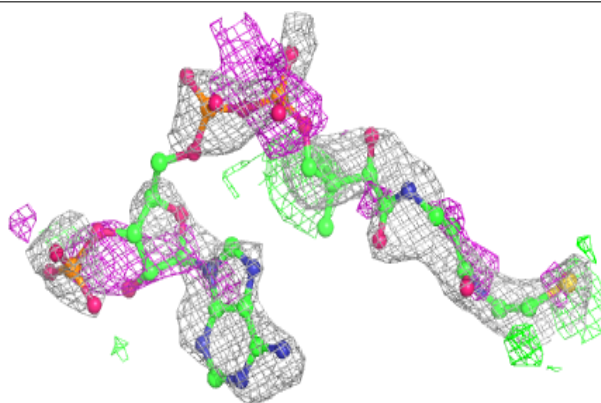


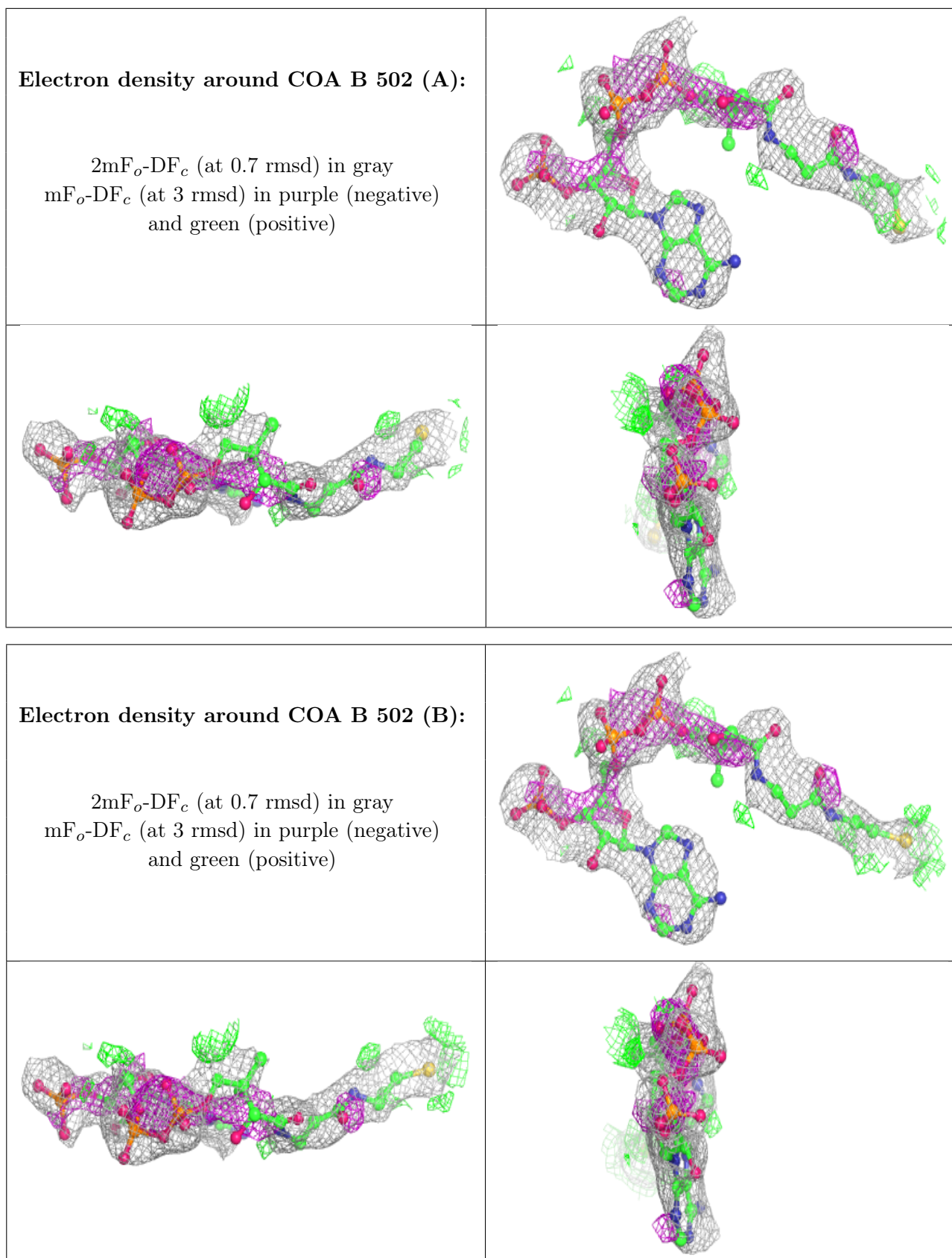
**Electron density around COA C 502 (A):**

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

**Electron density around COA C 502 (B):**

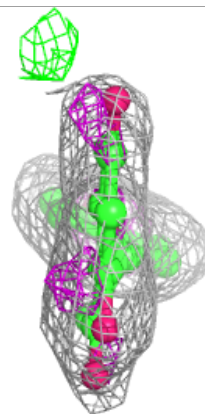
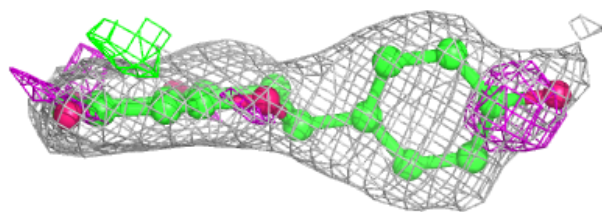
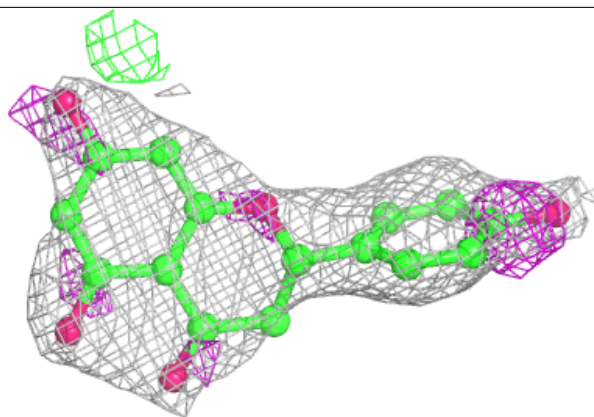
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



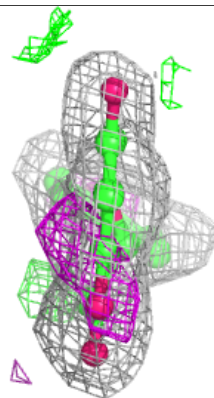
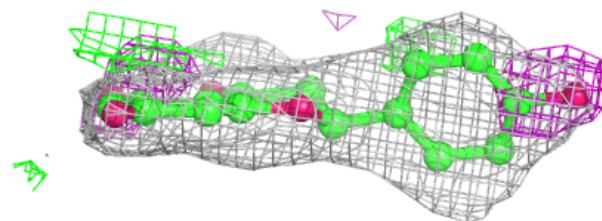
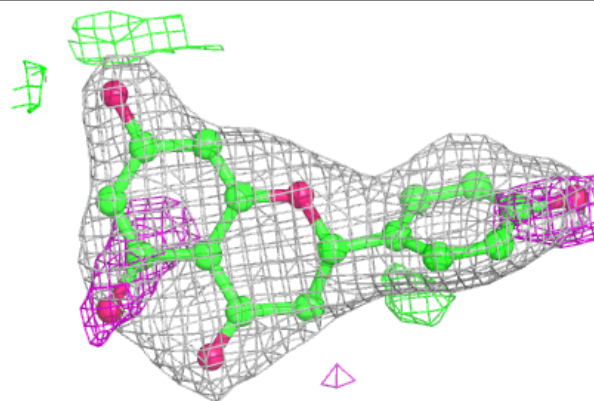


**Electron density around NAR D 501:**

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

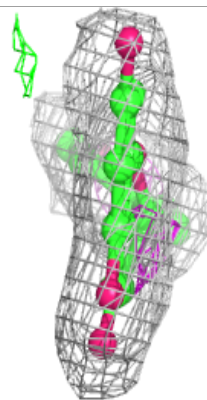
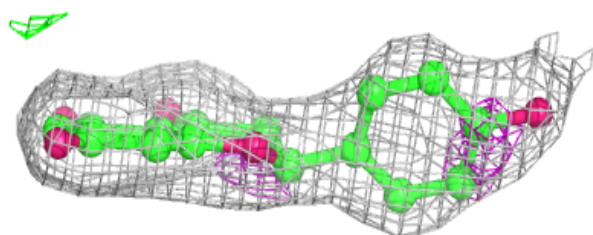
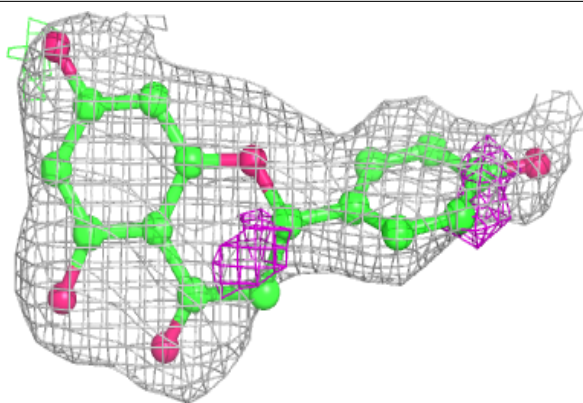
**Electron density around NAR B 501:**

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

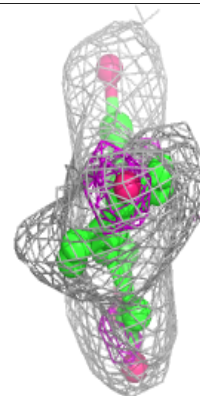
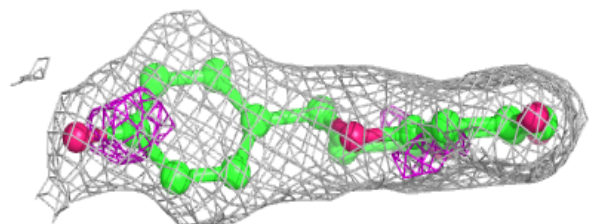
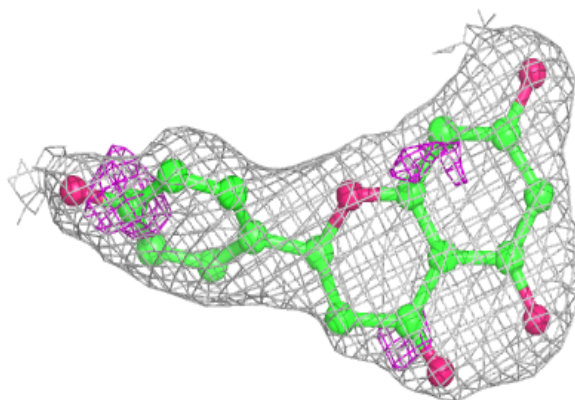


**Electron density around NAR C 501:**

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

**Electron density around NAR A 501:**

$2mF_o-DF_c$  (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.