



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:40 PM UTC

PDB ID : 7VF0 / pdb_00007vf0
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

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

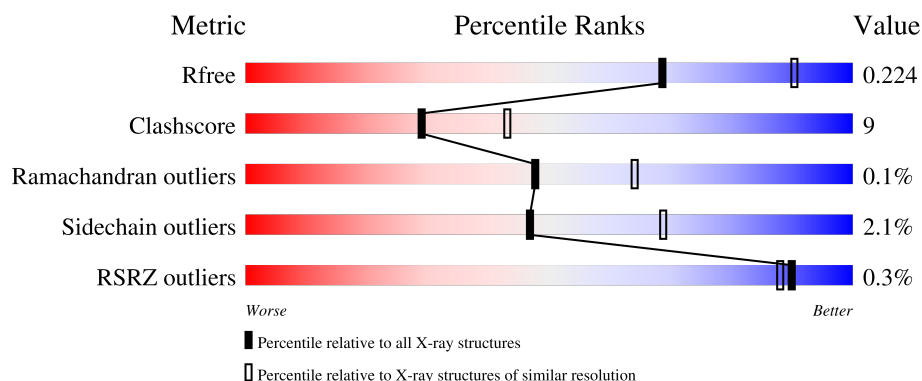
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

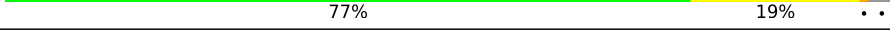
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	 79% 17% .
1	B	404	 80% 16% ..
1	C	404	 78% 19% .
1	D	404	 77% 19% ..

2 Entry composition [i](#)

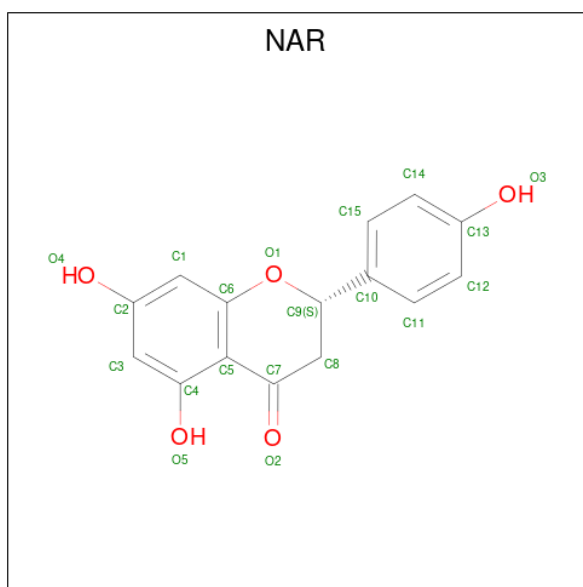
There are 4 unique types of molecules in this entry. The entry contains 12820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	391	Total	C	N	O	S	0	0	0
			3010	1919	511	558	22			
1	B	396	Total	C	N	O	S	0	0	0
			3049	1940	517	570	22			
1	C	396	Total	C	N	O	S	0	0	0
			3049	1940	517	570	22			
1	D	392	Total	C	N	O	S	0	0	0
			3018	1923	513	560	22			

- Molecule 2 is NARINGENIN (CCD ID: NAR) (formula: C₁₅H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



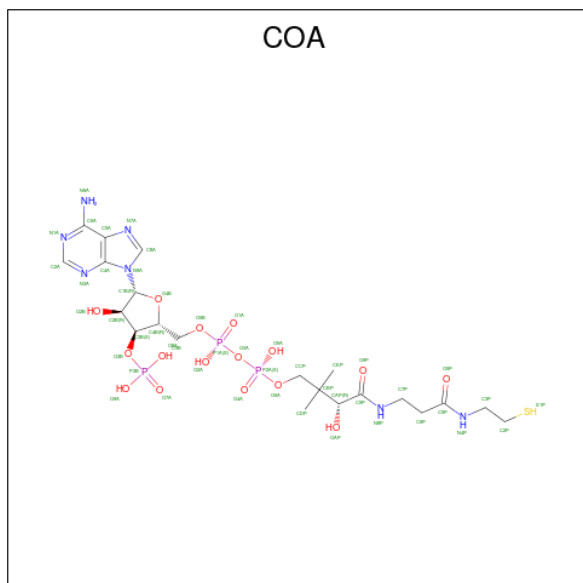
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	15	5		
2	B	1	Total	C	O	0	0
			20	15	5		

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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 (CCD ID: 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		

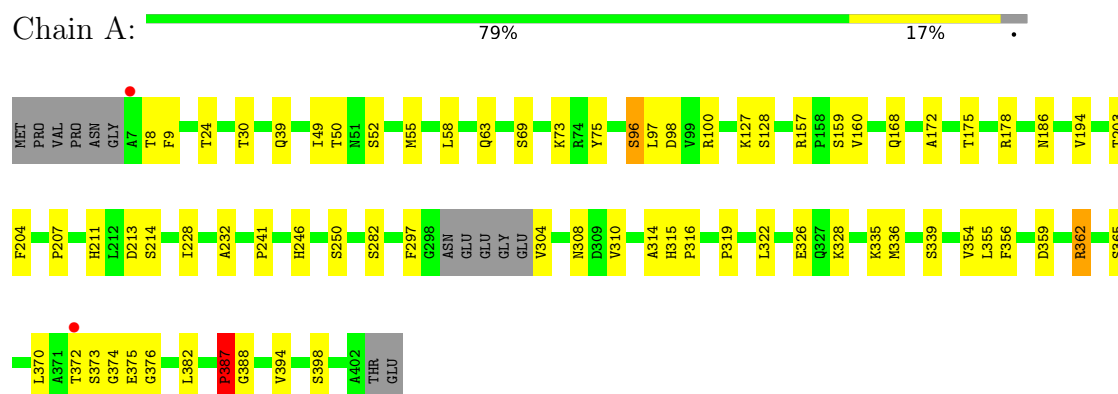
- Molecule 4 is water.

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		

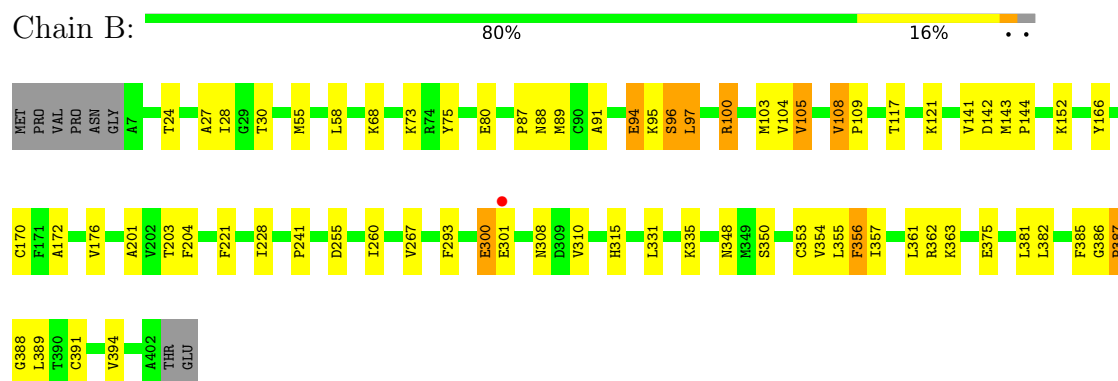
3 Residue-property plots

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

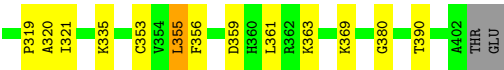


• Molecule 1: chalcone synthase

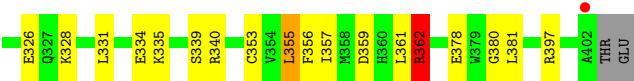
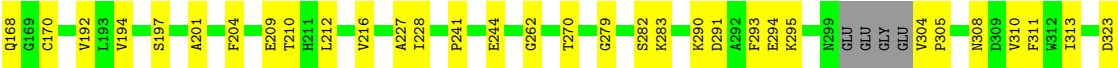
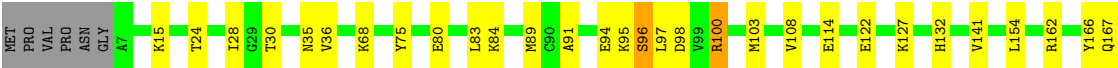


• Molecule 1: chalcone synthase





● Molecule 1: chalcone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.2 (32.48-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.179 , 0.225 0.180 , 0.224	Depositor DCC
R_{free} test set	2004 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12820	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	2/3076 (0.1%)	0.64	4/4168 (0.1%)
1	B	0.79	10/3116 (0.3%)	0.70	7/4223 (0.2%)
1	C	0.75	4/3116 (0.1%)	0.69	2/4223 (0.0%)
1	D	0.67	5/3084 (0.2%)	0.61	1/4179 (0.0%)
All	All	0.71	21/12392 (0.2%)	0.66	14/16793 (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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	353	CYS	C-O	-6.50	1.16	1.24
1	A	362	ARG	C-O	-6.03	1.17	1.24
1	B	356	PHE	C-O	-6.00	1.17	1.24
1	B	100	ARG	C-O	-5.84	1.17	1.24
1	B	95	LYS	C-O	-5.83	1.17	1.23
1	B	361	LEU	C-O	-5.73	1.17	1.24
1	B	353	CYS	C-O	-5.70	1.17	1.24
1	C	355	LEU	C-O	-5.68	1.17	1.24
1	D	361	LEU	C-O	-5.60	1.17	1.24
1	A	354	VAL	C-O	-5.39	1.17	1.24
1	B	354	VAL	C-O	-5.31	1.17	1.24
1	B	385	PHE	C-O	-5.29	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	355	LEU	C-O	-5.18	1.18	1.24
1	C	353	CYS	C-O	-5.16	1.18	1.24
1	D	362	ARG	C-O	-5.13	1.18	1.24
1	B	386	GLY	C-O	-5.07	1.17	1.24
1	C	100	ARG	C-O	-5.05	1.18	1.24
1	D	95	LYS	C-O	-5.05	1.17	1.24
1	B	391	CYS	C-O	-5.04	1.18	1.24
1	C	96	SER	C-O	-5.04	1.17	1.24
1	B	87	PRO	C-O	-5.03	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	SER	CB-CA-C	10.85	132.00	110.42
1	A	96	SER	CB-CA-C	10.08	130.49	110.42
1	D	96	SER	CB-CA-C	8.35	127.04	110.42
1	B	353	CYS	N-CA-C	7.35	118.93	111.07
1	B	387	PRO	N-CA-C	6.90	123.12	113.53
1	B	388	GLY	N-CA-C	6.85	129.41	113.18
1	A	388	GLY	N-CA-C	6.49	128.56	113.18
1	B	96	SER	CB-CA-C	6.41	123.17	110.42
1	C	238	VAL	N-CA-C	-5.98	106.90	111.62
1	A	387	PRO	N-CA-C	5.57	122.80	113.78
1	B	386	GLY	CA-C-N	5.43	125.08	119.05
1	B	386	GLY	C-N-CA	5.43	125.08	119.05
1	A	375	GLU	N-CA-C	5.40	119.03	111.90
1	B	357	ILE	N-CA-C	5.07	116.40	110.62

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	42	0
1	C	3049	0	3052	52	0
1	D	3018	0	3029	56	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	0	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	199	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 9.

All (199) 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:B:89:MET:HE1	1:B:103:MET:HE1	1.47	0.93
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:C:177:MET:HE1	1:C:228:ILE:HD11	1.62	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PHE:HD1	1:C:65:MET:HE3	1.54	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:C:100:ARG:HA	1:C:103:MET:HE2	1.72	0.71
1:B:89:MET:CE	1:B:103:MET:HE1	2.19	0.70
1:A:186:ASN:O	4:A:604:HOH:O	2.10	0.70
1:B:103:MET:HE3	1:B:201:ALA:HB1	1.73	0.69
1:C:167:GLN:O	4:C:602:HOH:O	2.10	0.69
1:A:314:ALA:HB3	1:A:336:MET:HE1	1.75	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:A:159:SER:O	4:A:607:HOH:O	2.11	0.67
1:C:89:MET:HE1	1:C:103:MET:HE1	1.76	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
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:100:ARG:HA	1:D:103:MET:HE2	1.82	0.61
1:D:291:ASP:OD1	1:D:295:LYS:NZ	2.33	0.61
1:B:55:MET:HE2	1:B:58:LEU:HD23	1.83	0.61
1:B:104:VAL:O	1:B:108:VAL:HG13	2.00	0.60
1:C:65:MET:HE1	1:C:215:LEU:HB3	1.82	0.60
1:C:291:ASP:OD2	1:C:295:LYS:NZ	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:VAL:O	1:A:335:LYS:NZ	2.38	0.56
1:C:103:MET:HE3	1:C:201:ALA:HB1	1.87	0.56
1:D:279:GLY:O	1:D:283:LYS:HG2	2.05	0.56
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:282:SER:OG	1:D:328:LYS:NZ	2.41	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:D:89:MET:HE1	1:D:103:MET:HE1	1.90	0.53
1:D:89:MET:CE	1:D:103:MET:HE1	2.39	0.53
1:A:213:ASP:OD1	1:A:213:ASP:N	2.33	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: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: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
1:B:382:LEU:HB3	1:B:394:VAL:HB	1.93	0.49
1:D:166:TYR:C	1:D:168:GLN:HE21	2.20	0.49
1:A:50:THR:O	4:A:608:HOH:O	2.18	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:C:62:PHE:CD1	1:C:65:MET:HE3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:322:LEU:HB3	1:A:336:MET:HE2	1.97	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:89:MET:CE	1:C:103:MET:HE1	2.44	0.46
1:C:24:THR:HG21	1:C:241:PRO:HB3	1.97	0.46
1:C:44:ASP:OD2	1:C:59:LYS:NZ	2.37	0.46
1:A:373:SER:HG	1:A:398:SER:HB2	1.81	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: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
1:A:297:PHE:HB2	1:A:304:VAL:HG12	2.00	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:C:55:MET:HE2	1:C:209:GLU:HG2	1.98	0.44
1:D:103:MET:HE3	1:D:201:ALA:HB1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:143:MET:HA	1:B:144:PRO:C	2.45	0.42
1:D:378:GLU:O	1:D:397:ARG:HG3	2.19	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: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
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:D:97:LEU:O	1:D:97:LEU:HG	2.19	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:336:MET:HE3	1:A:339:SER:HB2	2.03	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:B:348:ASN:C	1:B:348:ASN:HD22	2.29	0.41
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.82	0.41
1:C:177:MET:HE1	1:C:228:ILE:CD1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:TYR:CE2	1:C:207:PRO:HG3	2.56	0.41
1:C:103:MET:CE	1:C:201:ALA:HB1	2.49	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:D:127:LYS:NZ	1:D:154:LEU:O	2.52	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%)	36	50
1	B	394/404 (98%)	382 (97%)	11 (3%)	1 (0%)	36	50
1	C	394/404 (98%)	384 (98%)	10 (2%)	0	100	100
1	D	388/404 (96%)	375 (97%)	13 (3%)	0	100	100
All	All	1563/1616 (97%)	1513 (97%)	48 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

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

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	327/338 (97%)	324 (99%)	3 (1%)	70	85
1	B	331/338 (98%)	322 (97%)	9 (3%)	39	62
1	C	331/338 (98%)	320 (97%)	11 (3%)	33	55
1	D	328/338 (97%)	324 (99%)	4 (1%)	63	81
All	All	1317/1352 (97%)	1290 (98%)	27 (2%)	47	69

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	250	SER
1	A	387	PRO
1	B	80	GLU
1	B	94	GLU
1	B	97	LEU
1	B	105	VAL
1	B	108	VAL
1	B	203	THR
1	B	300	GLU
1	B	355	LEU
1	B	389	LEU
1	C	60	THR
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	C	369	LYS
1	D	83	LEU

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Mol	Chain	Res	Type
1	D	100	ARG
1	D	355	LEU
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	251	ASN
1	B	32	ASN
1	B	251	ASN
1	B	348	ASN
1	B	360	HIS
1	C	35	ASN
1	C	324	GLN
1	D	125	GLN
1	D	168	GLN
1	D	324	GLN
1	D	341	GLN
1	D	360	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	COA	C	502[A]	-	47,50,50	1.32	7 (14%)	69,75,75	1.81	18 (26%)
3	COA	B	502[B]	-	47,50,50	1.53	9 (19%)	69,75,75	1.85	18 (26%)
2	NAR	D	501	-	22,22,22	1.41	4 (18%)	32,32,32	1.85	10 (31%)
3	COA	B	502[A]	-	47,50,50	1.53	9 (19%)	69,75,75	1.85	18 (26%)
2	NAR	B	501	-	22,22,22	2.01	8 (36%)	32,32,32	1.76	8 (25%)
2	NAR	C	501	-	22,22,22	1.74	9 (40%)	32,32,32	2.09	11 (34%)
3	COA	D	502[B]	-	47,50,50	1.23	6 (12%)	69,75,75	2.04	18 (26%)
2	NAR	A	501	-	22,22,22	1.77	7 (31%)	32,32,32	1.99	9 (28%)
3	COA	D	502[A]	-	47,50,50	1.23	6 (12%)	69,75,75	2.04	18 (26%)
3	COA	C	502[B]	-	47,50,50	1.32	7 (14%)	69,75,75	1.81	18 (26%)

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
3	COA	C	502[A]	-	-	23/48/64/64	0/3/3/3
3	COA	B	502[B]	-	-	13/48/64/64	0/3/3/3
2	NAR	D	501	-	-	0/4/16/16	0/3/3/3
3	COA	B	502[A]	-	-	14/48/64/64	0/3/3/3
2	NAR	B	501	-	-	0/4/16/16	0/3/3/3
2	NAR	C	501	-	-	0/4/16/16	0/3/3/3
3	COA	D	502[B]	-	-	15/48/64/64	0/3/3/3
2	NAR	A	501	-	-	0/4/16/16	0/3/3/3
3	COA	D	502[A]	-	-	16/48/64/64	0/3/3/3
3	COA	C	502[B]	-	-	24/48/64/64	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[A]	COA	C5A-C4A	4.41	1.46	1.39
3	C	502[B]	COA	C5A-C4A	4.41	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	COA	C5A-N7A	-4.37	1.31	1.39
3	B	502[B]	COA	C5A-N7A	-4.37	1.31	1.39
2	A	501	NAR	O1-C6	-4.35	1.32	1.38
3	B	502[A]	COA	C4A-N9A	-3.99	1.29	1.37
3	B	502[B]	COA	C4A-N9A	-3.99	1.29	1.37
2	B	501	NAR	O1-C6	-3.97	1.32	1.38
2	B	501	NAR	C10-C9	-3.57	1.45	1.51
3	D	502[A]	COA	C5A-C4A	3.32	1.45	1.39
3	D	502[B]	COA	C5A-C4A	3.32	1.45	1.39
3	D	502[A]	COA	C5A-N7A	-3.13	1.33	1.39
3	D	502[B]	COA	C5A-N7A	-3.13	1.33	1.39
2	C	501	NAR	C5-C6	2.97	1.45	1.40
2	C	501	NAR	C10-C9	-2.92	1.46	1.51
2	A	501	NAR	C5-C4	2.88	1.46	1.41
3	D	502[A]	COA	C8A-N9A	-2.85	1.32	1.37
3	D	502[B]	COA	C8A-N9A	-2.85	1.32	1.37
3	B	502[A]	COA	C5A-C4A	2.80	1.44	1.39
3	B	502[B]	COA	C5A-C4A	2.80	1.44	1.39
2	B	501	NAR	C5-C4	2.77	1.45	1.41
2	B	501	NAR	O3-C13	-2.77	1.30	1.37
2	C	501	NAR	O1-C6	-2.74	1.34	1.38
2	D	501	NAR	C10-C9	-2.73	1.46	1.51
2	D	501	NAR	C5-C6	2.72	1.45	1.40
2	D	501	NAR	C5-C4	2.66	1.45	1.41
2	B	501	NAR	C5-C6	2.60	1.45	1.40
3	C	502[A]	COA	C5A-C6A	2.59	1.48	1.41
3	C	502[B]	COA	C5A-C6A	2.59	1.48	1.41
3	D	502[A]	COA	C4A-N9A	-2.57	1.32	1.37
3	D	502[B]	COA	C4A-N9A	-2.57	1.32	1.37
2	B	501	NAR	C3-C4	-2.54	1.35	1.38
3	D	502[A]	COA	O5P-C5P	-2.46	1.18	1.23
3	D	502[B]	COA	O5P-C5P	-2.46	1.18	1.23
2	A	501	NAR	C12-C11	-2.46	1.34	1.38
3	B	502[A]	COA	OAP-CAP	2.46	1.46	1.42
3	B	502[B]	COA	OAP-CAP	2.46	1.46	1.42
3	B	502[A]	COA	P2A-O3A	-2.45	1.56	1.59
3	B	502[B]	COA	P2A-O3A	-2.45	1.56	1.59
2	A	501	NAR	C10-C9	-2.44	1.47	1.51
2	C	501	NAR	O4-C2	-2.43	1.31	1.37
2	C	501	NAR	O3-C13	-2.42	1.31	1.37
3	B	502[A]	COA	P3B-O3B	2.40	1.63	1.59
3	B	502[B]	COA	P3B-O3B	2.40	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[A]	COA	C5A-N7A	-2.34	1.34	1.39
3	C	502[B]	COA	C5A-N7A	-2.34	1.34	1.39
3	C	502[A]	COA	P2A-O3A	2.34	1.62	1.59
3	C	502[B]	COA	P2A-O3A	2.34	1.62	1.59
2	C	501	NAR	C5-C4	2.33	1.45	1.41
2	C	501	NAR	C15-C10	-2.33	1.35	1.39
2	C	501	NAR	C12-C11	-2.32	1.35	1.38
3	C	502[A]	COA	C4A-N9A	-2.32	1.32	1.37
3	C	502[B]	COA	C4A-N9A	-2.32	1.32	1.37
2	A	501	NAR	O1-C9	-2.25	1.39	1.44
3	B	502[A]	COA	C8A-N9A	-2.19	1.33	1.37
3	B	502[B]	COA	C8A-N9A	-2.19	1.33	1.37
3	C	502[A]	COA	C8A-N9A	-2.18	1.33	1.37
3	C	502[B]	COA	C8A-N9A	-2.18	1.33	1.37
2	C	501	NAR	O2-C7	-2.15	1.18	1.22
2	D	501	NAR	O1-C9	-2.12	1.39	1.44
3	B	502[A]	COA	O9P-C9P	-2.11	1.19	1.23
3	B	502[B]	COA	O9P-C9P	-2.11	1.19	1.23
2	A	501	NAR	O3-C13	-2.10	1.32	1.37
3	B	502[A]	COA	O5P-C5P	-2.10	1.19	1.23
3	B	502[B]	COA	O5P-C5P	-2.10	1.19	1.23
3	D	502[A]	COA	C5A-C6A	2.06	1.46	1.41
3	D	502[B]	COA	C5A-C6A	2.06	1.46	1.41
2	A	501	NAR	O4-C2	-2.05	1.32	1.37
2	B	501	NAR	O2-C7	-2.03	1.18	1.22
3	C	502[A]	COA	O5P-C5P	-2.01	1.19	1.23
3	C	502[B]	COA	O5P-C5P	-2.01	1.19	1.23
2	B	501	NAR	O4-C2	-2.01	1.32	1.37

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502[A]	COA	C5A-C4A-N3A	-6.43	117.86	126.72
3	D	502[B]	COA	C5A-C4A-N3A	-6.43	117.86	126.72
3	B	502[A]	COA	C5A-C4A-N3A	-5.74	118.81	126.72
3	B	502[B]	COA	C5A-C4A-N3A	-5.74	118.81	126.72
3	C	502[A]	COA	C5A-C4A-N3A	-5.61	118.99	126.72
3	C	502[B]	COA	C5A-C4A-N3A	-5.61	118.99	126.72
2	A	501	NAR	O2-C7-C5	-5.00	114.77	122.49
3	D	502[A]	COA	N3A-C4A-N9A	4.95	135.59	127.17
3	D	502[B]	COA	N3A-C4A-N9A	4.95	135.59	127.17
3	B	502[A]	COA	N3A-C4A-N9A	4.63	135.04	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[B]	COA	N3A-C4A-N9A	4.63	135.04	127.17
2	C	501	NAR	C4-C5-C6	4.44	121.65	117.41
2	D	501	NAR	C3-C4-C5	-4.43	115.95	120.92
3	D	502[A]	COA	CDP-CBP-CCP	4.33	115.38	108.22
3	D	502[B]	COA	CDP-CBP-CCP	4.33	115.38	108.22
3	D	502[A]	COA	C2B-C1B-N9A	-4.26	102.73	113.30
3	D	502[B]	COA	C2B-C1B-N9A	-4.26	102.73	113.30
3	D	502[A]	COA	C4A-C5A-N7A	-4.22	105.76	110.58
3	D	502[B]	COA	C4A-C5A-N7A	-4.22	105.76	110.58
3	C	502[A]	COA	N3A-C4A-N9A	4.20	134.30	127.17
3	C	502[B]	COA	N3A-C4A-N9A	4.20	134.30	127.17
2	A	501	NAR	O1-C6-C1	4.18	123.42	116.29
3	C	502[A]	COA	C4A-C5A-N7A	-4.18	105.81	110.58
3	C	502[B]	COA	C4A-C5A-N7A	-4.18	105.81	110.58
3	B	502[A]	COA	O3B-P3B-O7A	-4.08	94.81	109.33
3	B	502[B]	COA	O3B-P3B-O7A	-4.08	94.81	109.33
2	B	501	NAR	O2-C7-C5	-4.06	116.22	122.49
2	D	501	NAR	C4-C5-C6	4.03	121.25	117.41
2	C	501	NAR	C3-C4-C5	-3.96	116.48	120.92
3	D	502[A]	COA	C2A-N3A-C4A	3.91	121.39	111.83
3	D	502[B]	COA	C2A-N3A-C4A	3.91	121.39	111.83
3	B	502[A]	COA	C2A-N3A-C4A	3.86	121.26	111.83
3	B	502[B]	COA	C2A-N3A-C4A	3.86	121.26	111.83
2	A	501	NAR	O1-C6-C5	-3.70	117.93	121.64
3	B	502[A]	COA	N3A-C2A-N1A	-3.63	123.09	128.58
3	B	502[B]	COA	N3A-C2A-N1A	-3.63	123.09	128.58
2	B	501	NAR	C3-C4-C5	-3.63	116.86	120.92
2	C	501	NAR	C6-O1-C9	3.61	121.85	115.54
3	D	502[A]	COA	C4A-N9A-C8A	3.49	109.40	105.74
3	D	502[B]	COA	C4A-N9A-C8A	3.49	109.40	105.74
2	C	501	NAR	O1-C6-C1	3.49	122.25	116.29
2	B	501	NAR	O2-C7-C8	3.41	126.36	120.81
2	A	501	NAR	O2-C7-C8	3.41	126.35	120.81
3	C	502[A]	COA	CEP-CBP-CAP	3.38	114.52	108.77
3	C	502[B]	COA	CEP-CBP-CAP	3.38	114.52	108.77
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	D	502[A]	COA	C5A-N7A-C8A	3.31	108.66	103.45
3	D	502[B]	COA	C5A-N7A-C8A	3.31	108.66	103.45
2	D	501	NAR	O2-C7-C5	-3.31	117.38	122.49
2	D	501	NAR	O1-C6-C1	3.30	121.93	116.29
2	C	501	NAR	C14-C15-C10	-3.30	117.89	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAR	C4-C5-C6	3.27	120.53	117.41
3	C	502[A]	COA	C3P-N4P-C5P	3.27	128.91	122.82
3	C	502[B]	COA	C3P-N4P-C5P	3.27	128.91	122.82
2	C	501	NAR	O2-C7-C5	-3.26	117.44	122.49
3	C	502[A]	COA	C6P-C7P-N8P	-3.24	105.11	112.00
3	C	502[B]	COA	C6P-C7P-N8P	-3.24	105.11	112.00
2	D	501	NAR	O2-C7-C8	3.18	125.99	120.81
2	C	501	NAR	C3-C2-C1	3.17	124.83	120.47
3	C	502[A]	COA	C2A-N3A-C4A	3.13	119.47	111.83
3	C	502[B]	COA	C2A-N3A-C4A	3.13	119.47	111.83
3	C	502[A]	COA	C3B-C2B-C1B	3.05	106.59	99.89
3	C	502[B]	COA	C3B-C2B-C1B	3.05	106.59	99.89
3	D	502[A]	COA	N9A-C8A-N7A	-3.02	109.65	113.94
3	D	502[B]	COA	N9A-C8A-N7A	-3.02	109.65	113.94
3	D	502[A]	COA	O9A-P3B-O8A	2.99	119.01	107.80
3	D	502[B]	COA	O9A-P3B-O8A	2.99	119.01	107.80
2	C	501	NAR	C11-C12-C13	-2.99	116.72	119.88
3	D	502[A]	COA	O3A-P2A-O4A	-2.97	101.76	110.70
3	D	502[B]	COA	O3A-P2A-O4A	-2.97	101.76	110.70
3	D	502[A]	COA	N3A-C2A-N1A	-2.91	124.18	128.58
3	D	502[B]	COA	N3A-C2A-N1A	-2.91	124.18	128.58
2	A	501	NAR	C4-C5-C6	2.86	120.14	117.41
3	C	502[A]	COA	CEP-CBP-CDP	-2.77	103.67	109.20
3	C	502[B]	COA	CEP-CBP-CDP	-2.77	103.67	109.20
3	B	502[A]	COA	O5P-C5P-C6P	-2.71	117.11	122.02
3	B	502[B]	COA	O5P-C5P-C6P	-2.71	117.11	122.02
3	C	502[A]	COA	O5A-P2A-O3A	2.70	114.56	107.27
3	C	502[B]	COA	O5A-P2A-O3A	2.70	114.56	107.27
3	C	502[A]	COA	C5A-N7A-C8A	2.66	107.62	103.45
3	C	502[B]	COA	C5A-N7A-C8A	2.66	107.62	103.45
2	A	501	NAR	C6-O1-C9	2.65	120.17	115.54
2	A	501	NAR	C3-C4-C5	-2.64	117.97	120.92
2	B	501	NAR	C3-C2-C1	2.58	124.01	120.47
3	D	502[A]	COA	C6P-C5P-N4P	2.54	120.96	116.34
3	D	502[B]	COA	C6P-C5P-N4P	2.54	120.96	116.34
3	B	502[A]	COA	O3B-C3B-C2B	2.51	120.67	111.68
3	B	502[B]	COA	O3B-C3B-C2B	2.51	120.67	111.68
2	D	501	NAR	O1-C6-C5	-2.47	119.16	121.64
2	A	501	NAR	O5-C4-C5	-2.47	116.57	121.14
2	C	501	NAR	O1-C6-C5	-2.47	119.16	121.64
3	C	502[A]	COA	C2B-C1B-N9A	-2.44	107.24	113.30
3	C	502[B]	COA	C2B-C1B-N9A	-2.44	107.24	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	COA	P3B-O3B-C3B	-2.42	116.97	123.43
3	B	502[B]	COA	P3B-O3B-C3B	-2.42	116.97	123.43
3	B	502[A]	COA	OAP-CAP-CBP	-2.42	104.58	110.18
3	B	502[B]	COA	OAP-CAP-CBP	-2.42	104.58	110.18
3	B	502[A]	COA	C7P-N8P-C9P	2.40	126.86	122.55
3	B	502[B]	COA	C7P-N8P-C9P	2.40	126.86	122.55
2	C	501	NAR	O5-C4-C3	2.37	125.85	119.45
3	B	502[A]	COA	C6P-C7P-N8P	2.34	116.98	112.00
3	B	502[B]	COA	C6P-C7P-N8P	2.34	116.98	112.00
2	B	501	NAR	O1-C6-C1	2.34	120.29	116.29
3	C	502[A]	COA	C6A-C5A-N7A	2.32	136.56	132.09
3	C	502[B]	COA	C6A-C5A-N7A	2.32	136.56	132.09
3	B	502[A]	COA	CEP-CBP-CCP	2.31	112.04	108.22
3	B	502[B]	COA	CEP-CBP-CCP	2.31	112.04	108.22
3	C	502[A]	COA	C4A-N9A-C8A	2.28	108.13	105.74
3	C	502[B]	COA	C4A-N9A-C8A	2.28	108.13	105.74
3	C	502[A]	COA	C7P-N8P-C9P	-2.27	118.47	122.55
3	C	502[B]	COA	C7P-N8P-C9P	-2.27	118.47	122.55
3	D	502[A]	COA	CEP-CBP-CDP	-2.26	104.70	109.20
3	D	502[B]	COA	CEP-CBP-CDP	-2.26	104.70	109.20
3	D	502[A]	COA	C6A-C5A-N7A	2.25	136.43	132.09
3	D	502[B]	COA	C6A-C5A-N7A	2.25	136.43	132.09
3	B	502[A]	COA	O6A-P2A-O4A	-2.25	100.02	108.94
3	B	502[B]	COA	O6A-P2A-O4A	-2.25	100.02	108.94
2	D	501	NAR	C4-C3-C2	2.24	121.74	119.67
3	B	502[A]	COA	O5A-P2A-O4A	2.24	122.86	112.44
3	B	502[B]	COA	O5A-P2A-O4A	2.24	122.86	112.44
2	D	501	NAR	C3-C2-C1	2.24	123.54	120.47
2	A	501	NAR	O5-C4-C3	2.23	125.46	119.45
3	B	502[A]	COA	O3A-P2A-O4A	-2.21	104.06	110.70
3	B	502[B]	COA	O3A-P2A-O4A	-2.21	104.06	110.70
3	C	502[A]	COA	CDP-CBP-CAP	2.17	112.47	108.77
3	C	502[B]	COA	CDP-CBP-CAP	2.17	112.47	108.77
2	D	501	NAR	O5-C4-C3	2.17	125.32	119.45
2	B	501	NAR	C15-C10-C11	2.14	120.96	118.30
3	D	502[A]	COA	O5P-C5P-C6P	-2.14	118.14	122.02
3	D	502[B]	COA	O5P-C5P-C6P	-2.14	118.14	122.02
3	B	502[A]	COA	C5A-C6A-N6A	-2.10	118.10	123.29
3	B	502[B]	COA	C5A-C6A-N6A	-2.10	118.10	123.29
2	C	501	NAR	C15-C10-C11	2.08	120.89	118.30
3	B	502[A]	COA	CEP-CBP-CAP	2.05	112.27	108.77
3	B	502[B]	COA	CEP-CBP-CAP	2.05	112.27	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAR	C1-C6-C5	-2.04	118.23	121.79
3	C	502[A]	COA	C4B-O4B-C1B	2.04	113.96	109.47
3	C	502[B]	COA	C4B-O4B-C1B	2.04	113.96	109.47
3	C	502[A]	COA	N3A-C2A-N1A	-2.03	125.50	128.58
3	C	502[B]	COA	N3A-C2A-N1A	-2.03	125.50	128.58
3	B	502[A]	COA	O4B-C1B-C2B	-2.03	102.27	106.62
3	B	502[B]	COA	O4B-C1B-C2B	-2.03	102.27	106.62
2	D	501	NAR	C15-C10-C11	2.01	120.80	118.30
3	D	502[A]	COA	O4B-C1B-N9A	2.01	111.95	108.09
3	D	502[B]	COA	O4B-C1B-N9A	2.01	111.95	108.09

There are no chirality outliers.

All (105) 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	C5B-O5B-P1A-O3A
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
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	C5B-O5B-P1A-O3A
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	CDP-CBP-CCP-O6A
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

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Mol	Chain	Res	Type	Atoms
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	CDP-CBP-CCP-O6A
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	C5B-O5B-P1A-O3A
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	C5B-O5B-P1A-O3A
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
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	D	502[A]	COA	C3B-C4B-C5B-O5B
3	D	502[B]	COA	C3B-C4B-C5B-O5B
3	C	502[A]	COA	C9P-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
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	C	502[A]	COA	CEP-CBP-CCP-O6A
3	C	502[A]	COA	C9P-CAP-CBP-CCP
3	C	502[B]	COA	CEP-CBP-CCP-O6A
3	C	502[B]	COA	C9P-CAP-CBP-CCP
3	D	502[A]	COA	CDP-CBP-CCP-O6A
3	D	502[B]	COA	CDP-CBP-CCP-O6A
3	D	502[A]	COA	S1P-C2P-C3P-N4P
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	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	D	502[A]	COA	CEP-CBP-CCP-O6A
3	D	502[B]	COA	CEP-CBP-CCP-O6A
3	D	502[A]	COA	O4B-C4B-C5B-O5B
3	D	502[B]	COA	O4B-C4B-C5B-O5B
3	D	502[A]	COA	N8P-C9P-CAP-OAP
3	D	502[B]	COA	N8P-C9P-CAP-OAP
3	B	502[A]	COA	S1P-C2P-C3P-N4P
3	C	502[A]	COA	CAP-CBP-CCP-O6A
3	C	502[B]	COA	CAP-CBP-CCP-O6A
3	C	502[B]	COA	S1P-C2P-C3P-N4P
3	B	502[A]	COA	P1A-O3A-P2A-O5A
3	B	502[B]	COA	P1A-O3A-P2A-O5A
3	C	502[A]	COA	P2A-O3A-P1A-O2A
3	C	502[B]	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

4 monomers are involved in 4 short contacts:

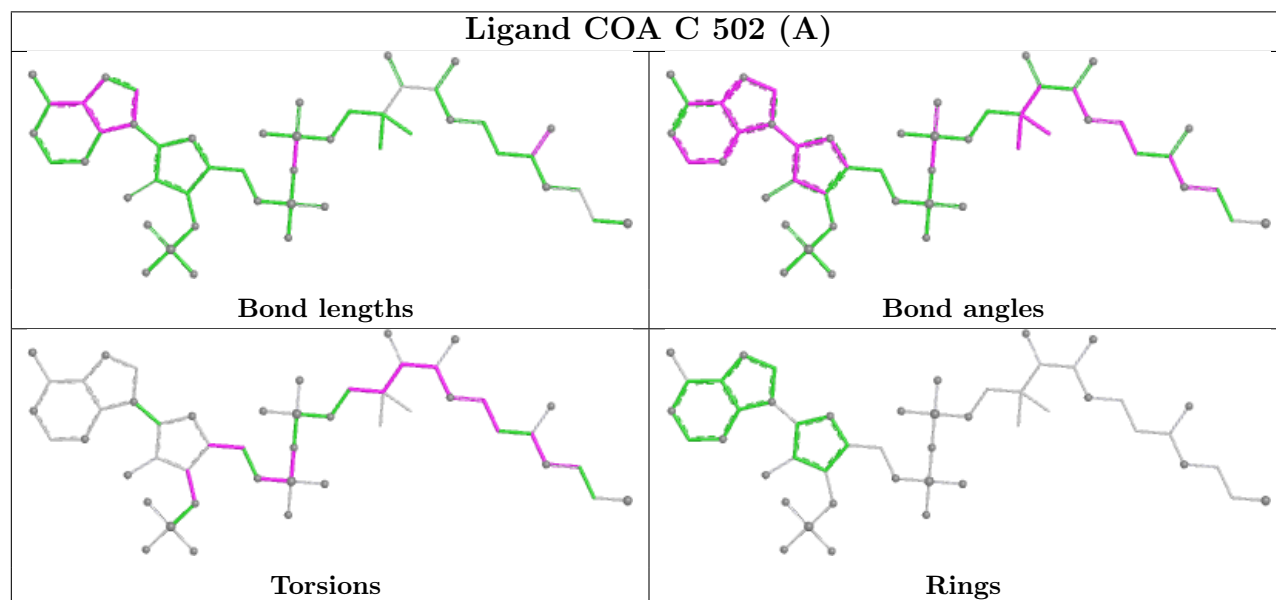
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAR	1	0

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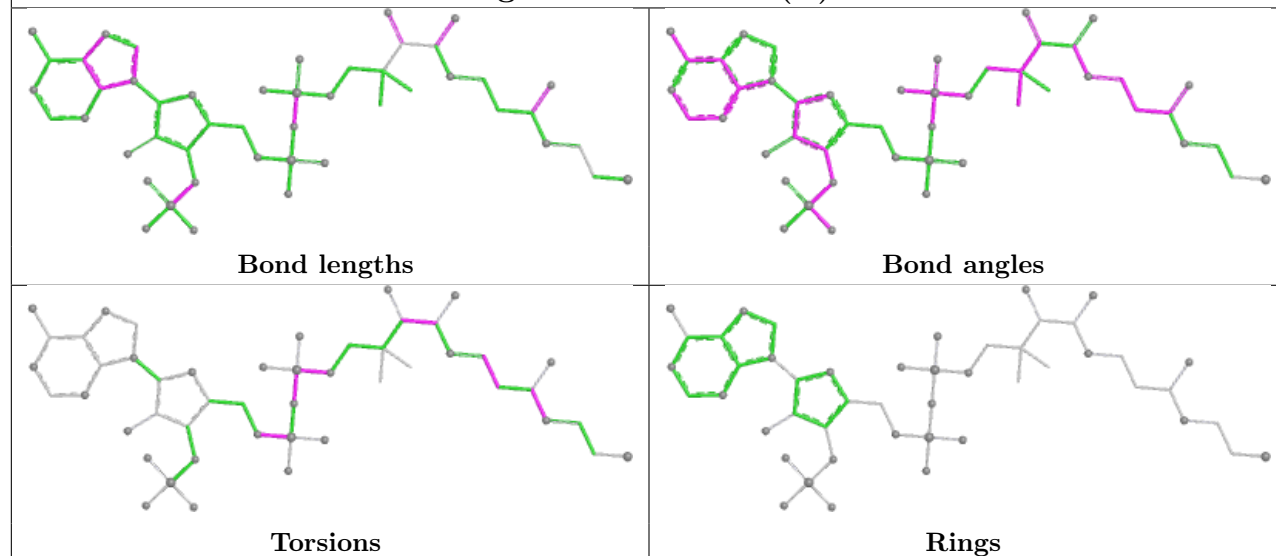
Continued from previous page...

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

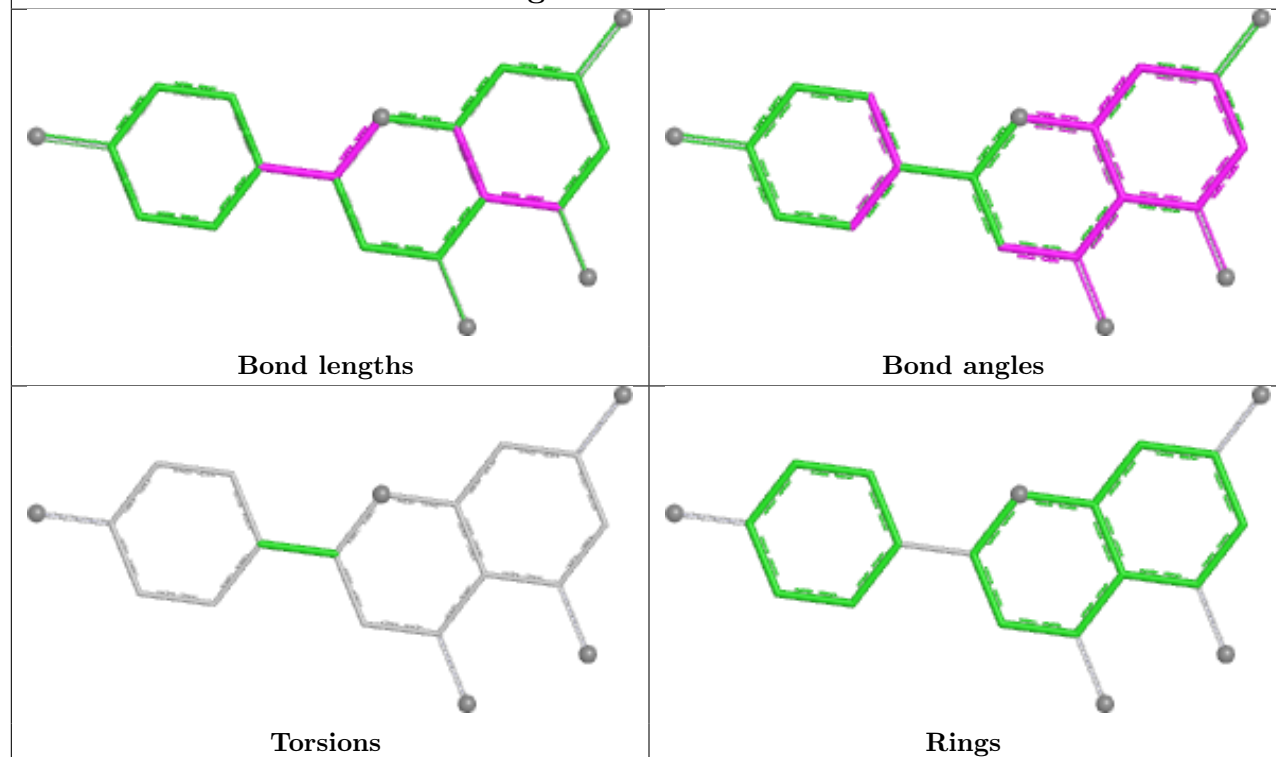
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

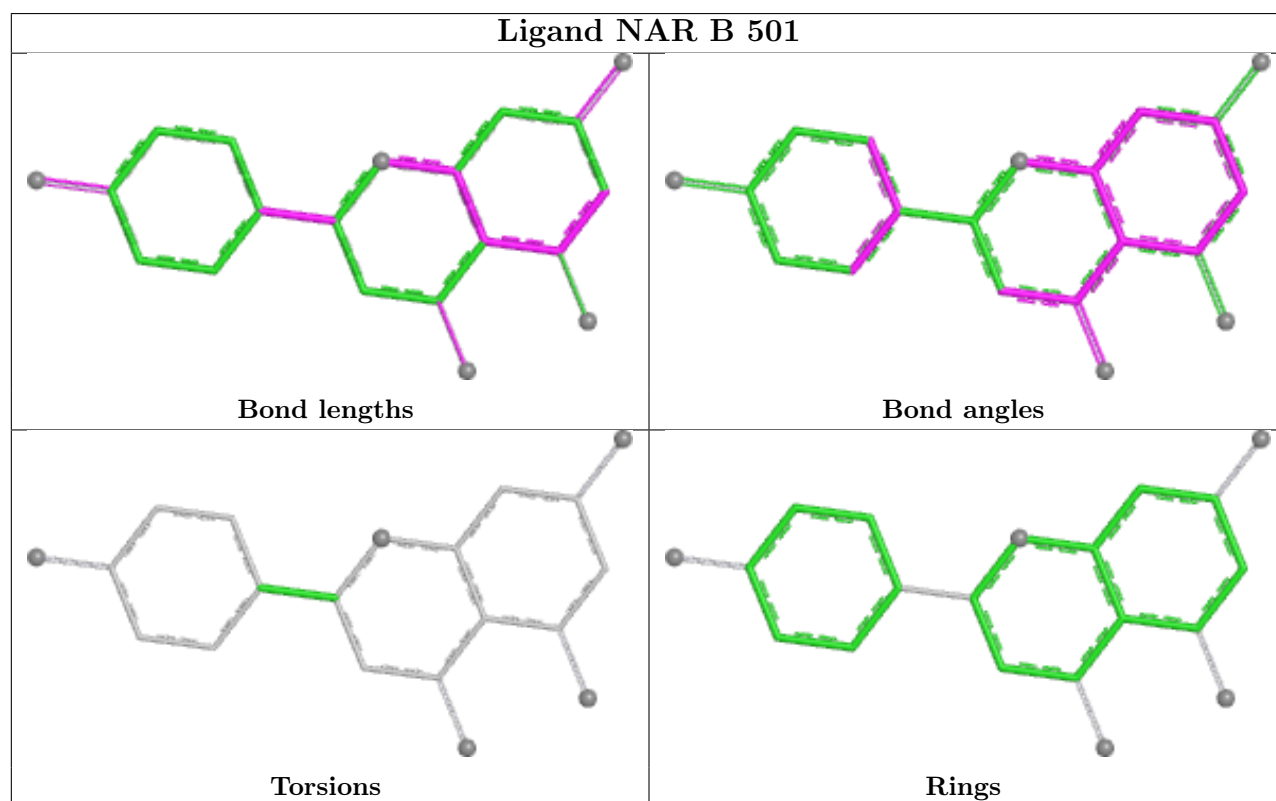
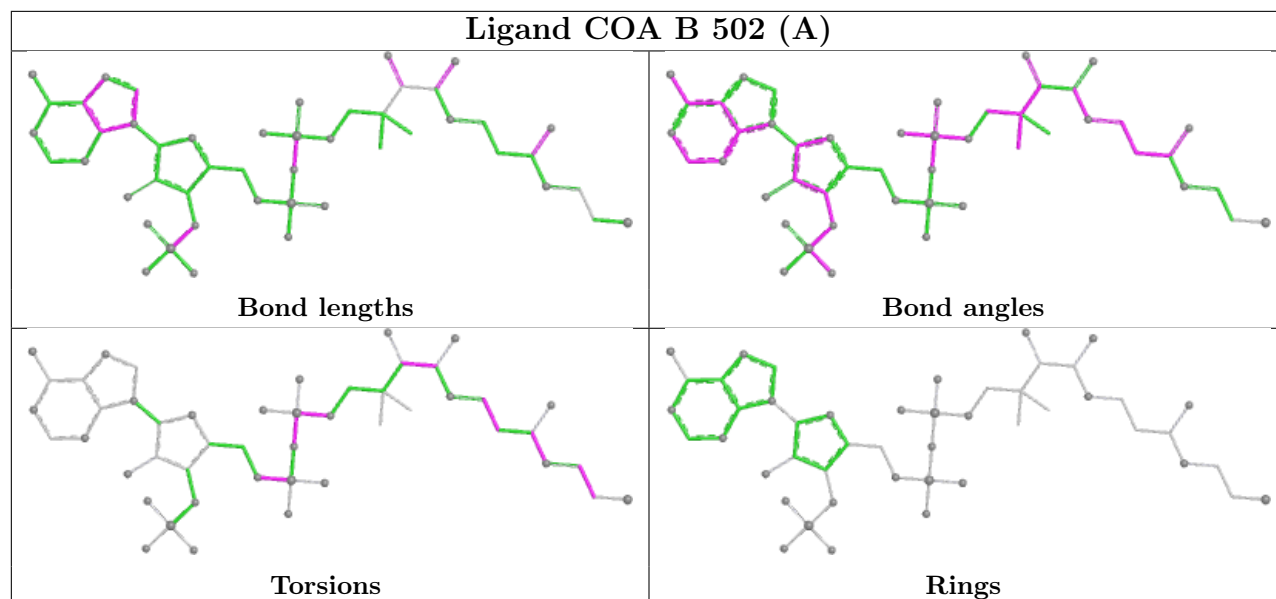


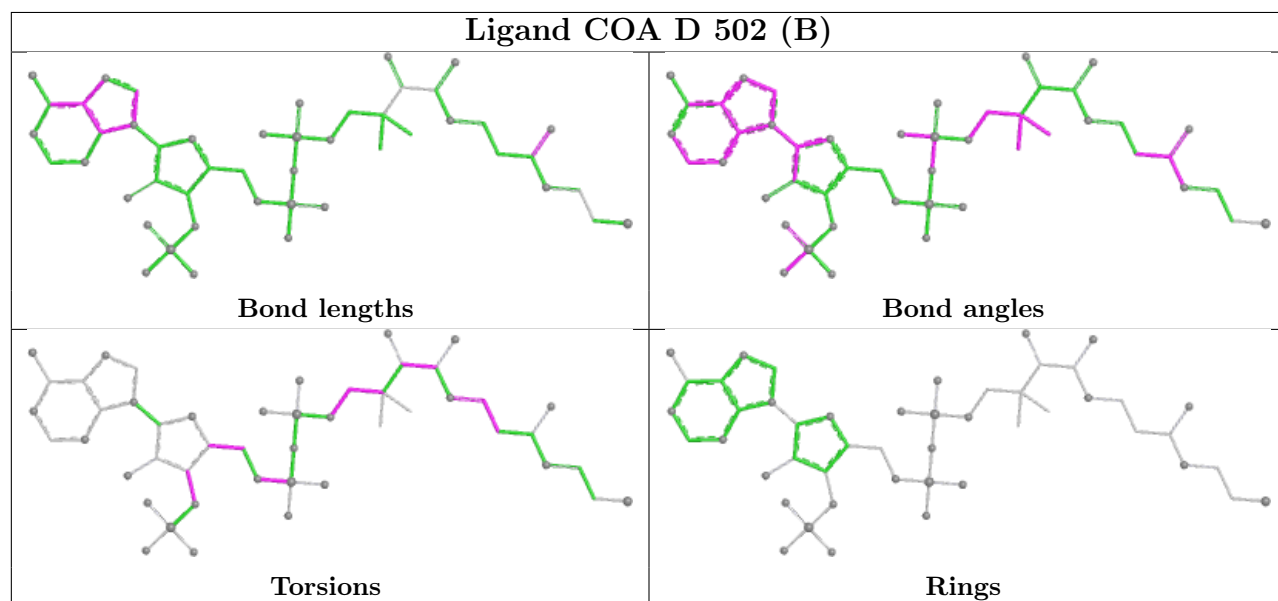
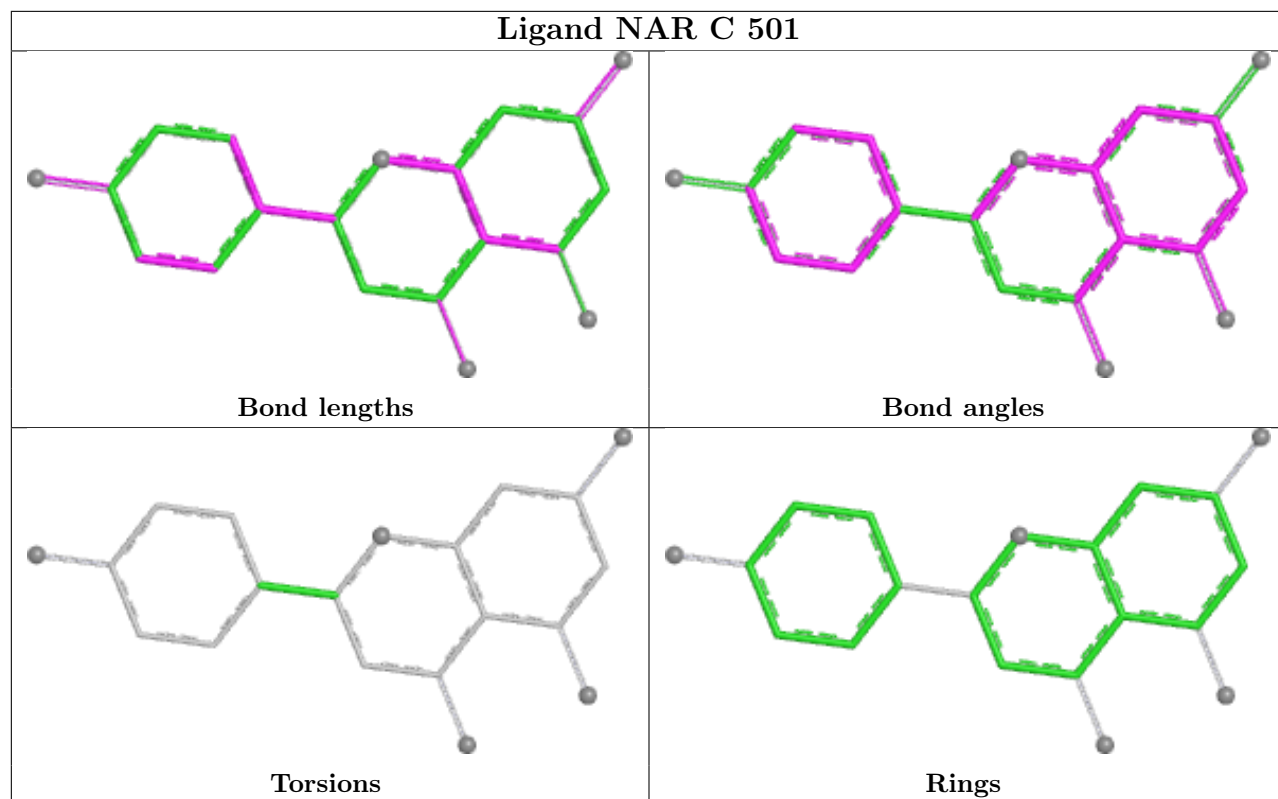
Ligand COA B 502 (B)

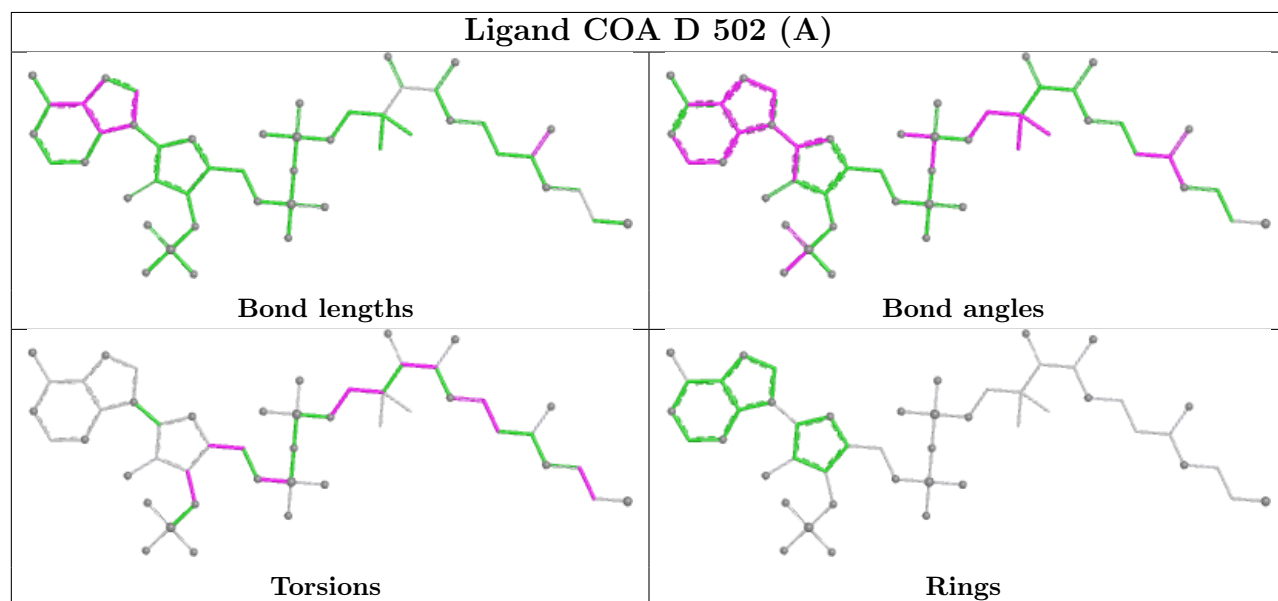
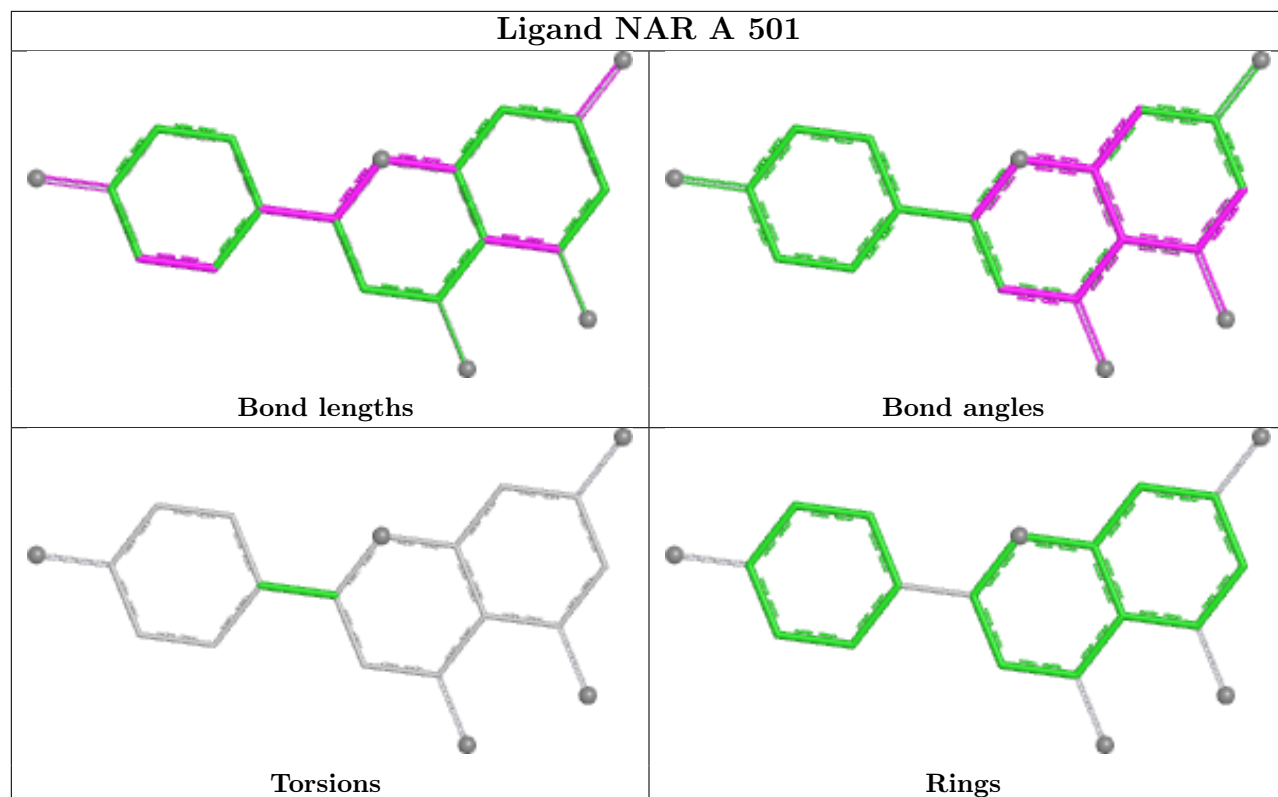


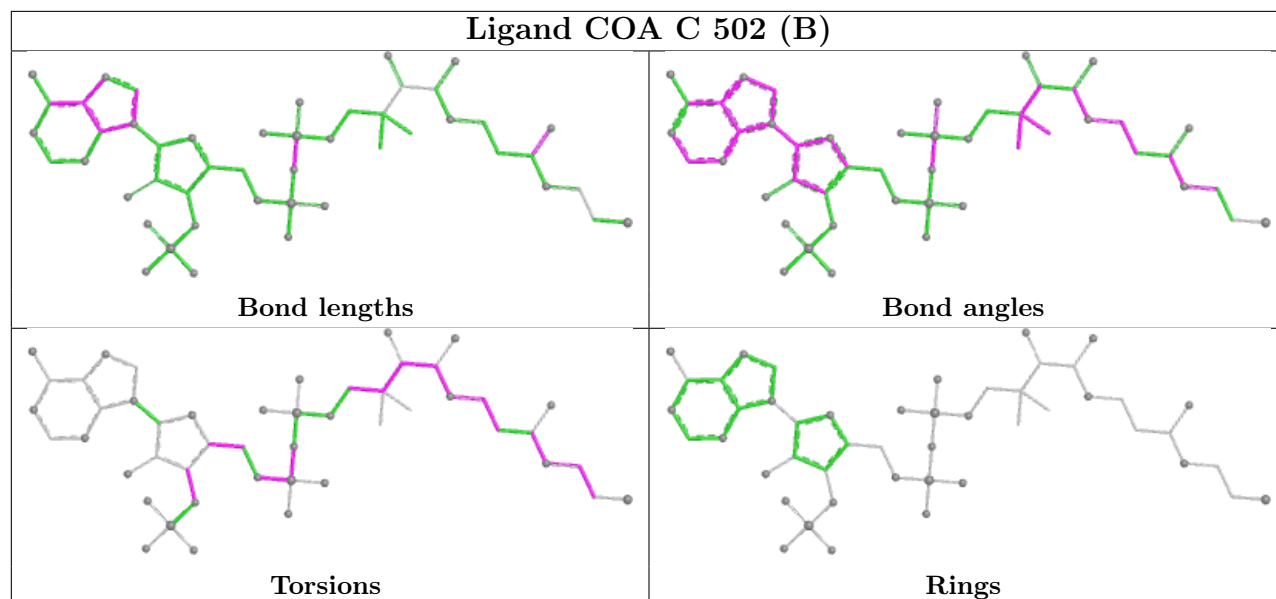
Ligand NAR D 501











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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/404 (96%)	-0.44	2 (0%) 87 85	15, 23, 34, 44	0
1	B	396/404 (98%)	-0.61	1 (0%) 90 88	12, 18, 30, 56	0
1	C	396/404 (98%)	-0.54	0 100 100	13, 20, 34, 59	0
1	D	392/404 (97%)	-0.51	1 (0%) 90 88	14, 20, 33, 42	0
All	All	1575/1616 (97%)	-0.53	4 (0%) 90 88	12, 20, 33, 59	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	402	ALA	2.7
1	B	301	GLU	2.4
1	A	372	THR	2.3
1	A	7	ALA	2.1

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](#)

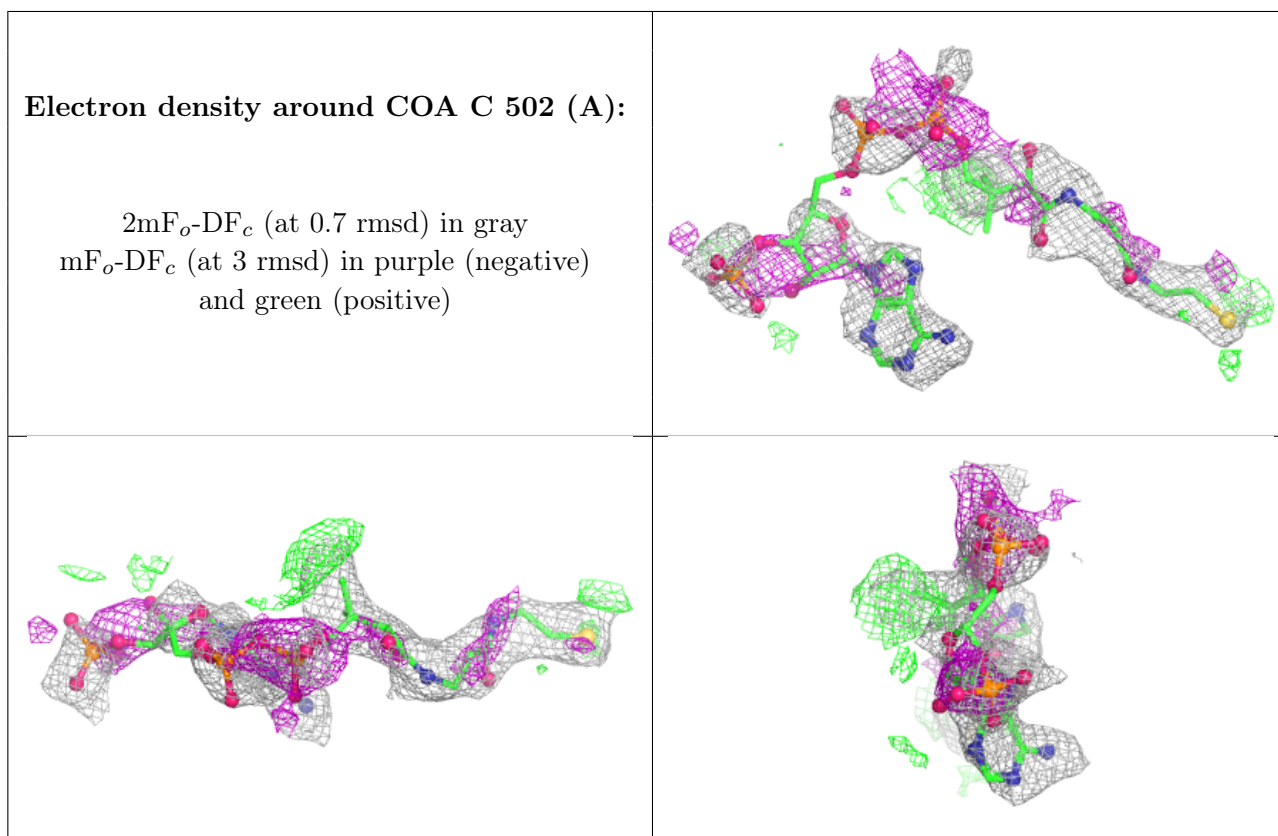
There are no oligosaccharides in this entry.

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.

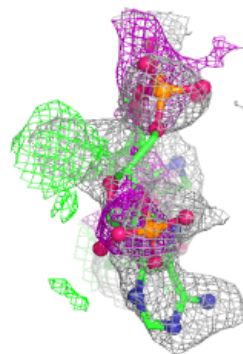
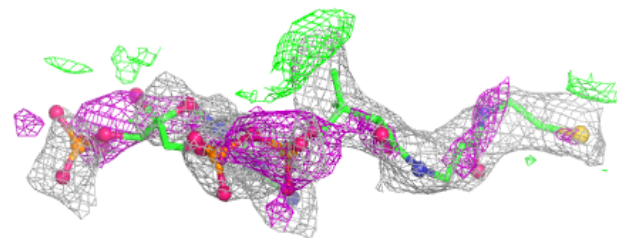
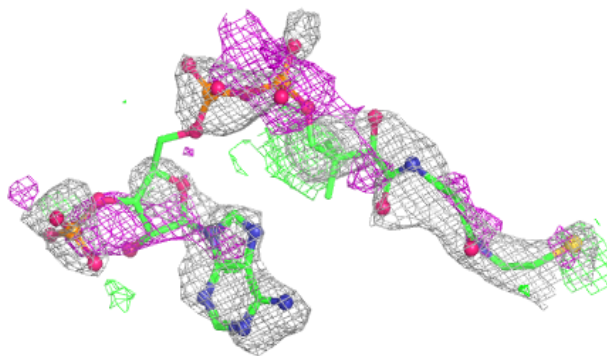
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	COA	C	502[A]	48/48	0.54	0.15	21,58,78,93	1
3	COA	C	502[B]	48/48	0.54	0.15	21,58,78,93	1
3	COA	D	502[A]	48/48	0.59	0.16	23,55,85,104	1
3	COA	D	502[B]	48/48	0.59	0.16	22,55,85,104	1
3	COA	B	502[A]	48/48	0.70	0.12	16,46,69,86	1
3	COA	B	502[B]	48/48	0.70	0.12	17,46,69,86	1
2	NAR	D	501	20/20	0.86	0.09	14,26,32,37	0
2	NAR	B	501	20/20	0.88	0.09	12,21,30,32	0
2	NAR	A	501	20/20	0.89	0.08	17,23,27,29	0
2	NAR	C	501	20/20	0.91	0.07	16,22,26,28	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.

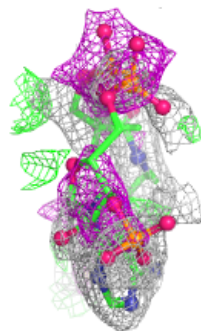
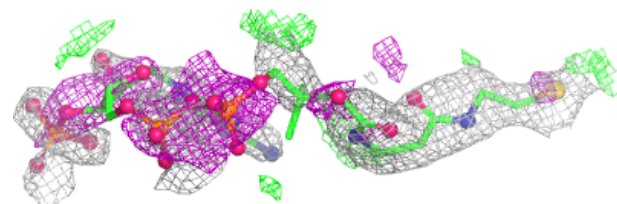
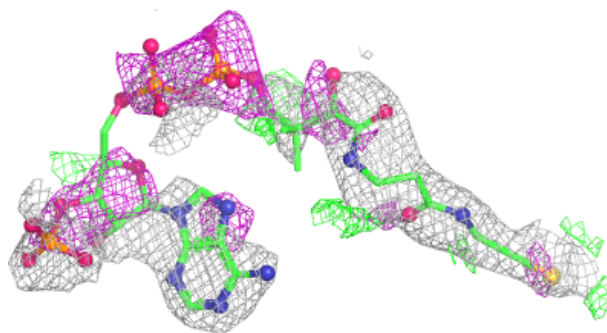


Electron density around COA C 502 (B):

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

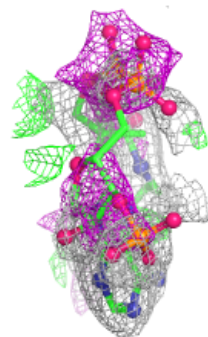
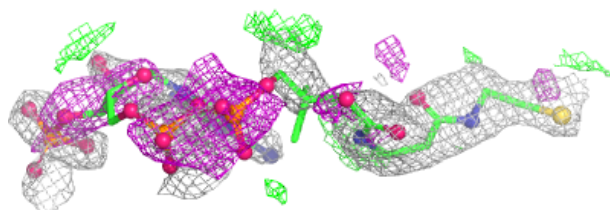
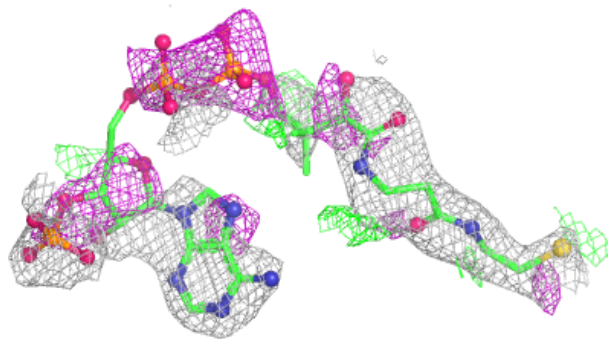
**Electron density around COA D 502 (A):**

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

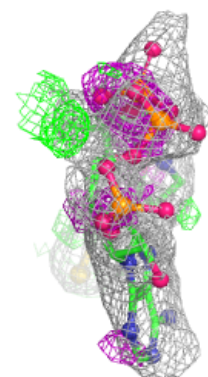
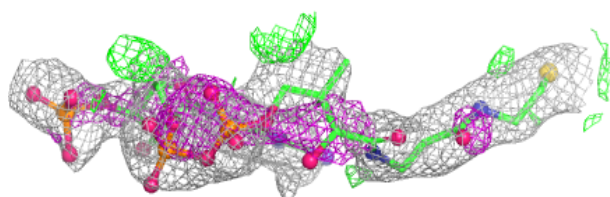
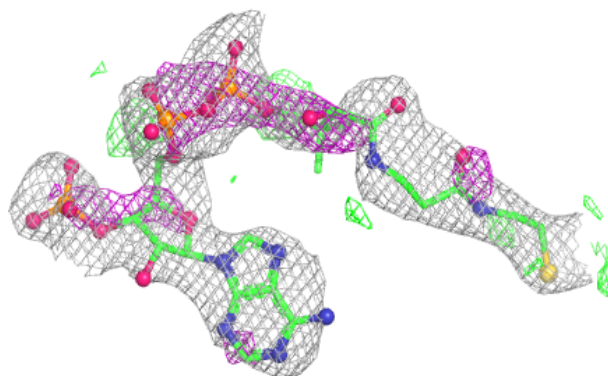


Electron density around COA D 502 (B):

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

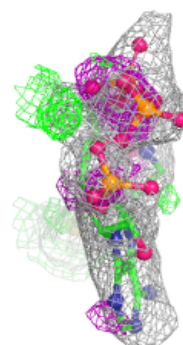
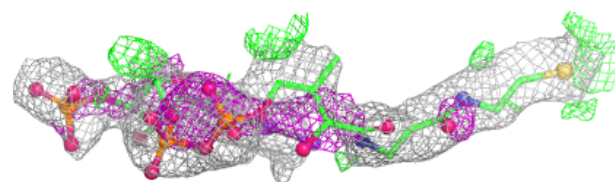
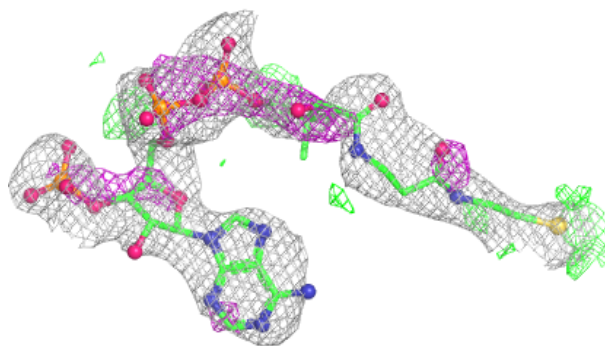
**Electron density around COA B 502 (A):**

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

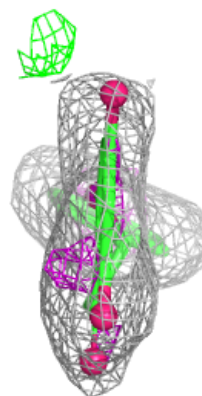
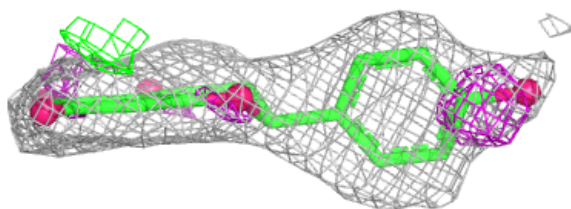
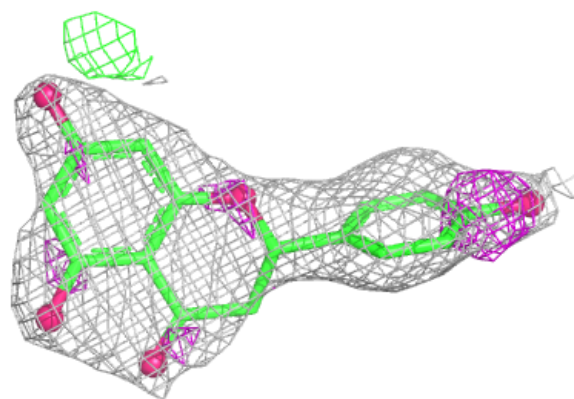


Electron density around COA B 502 (B):

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

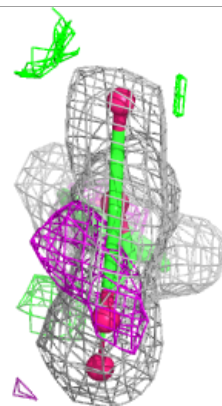
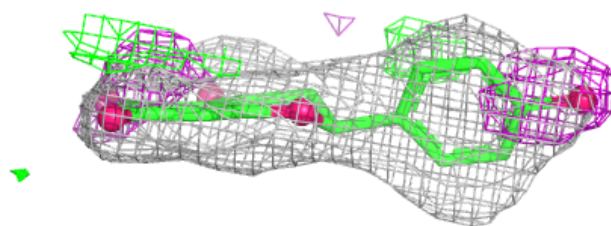
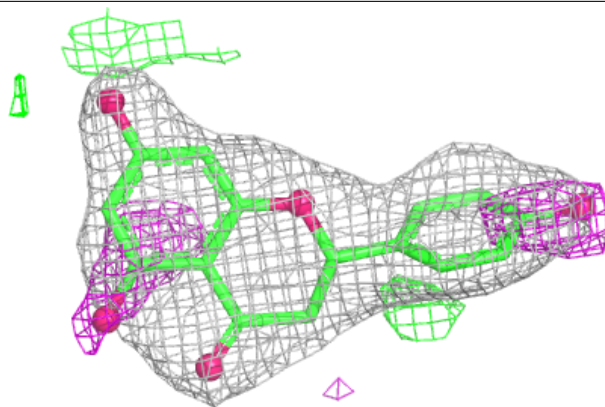
**Electron density around NAR D 501:**

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

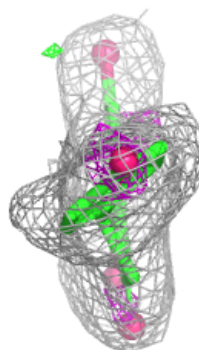
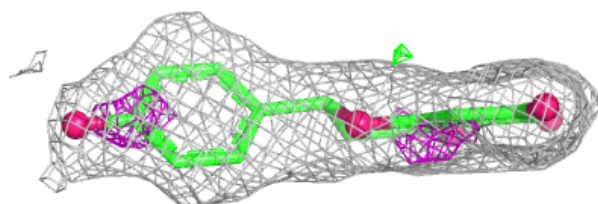
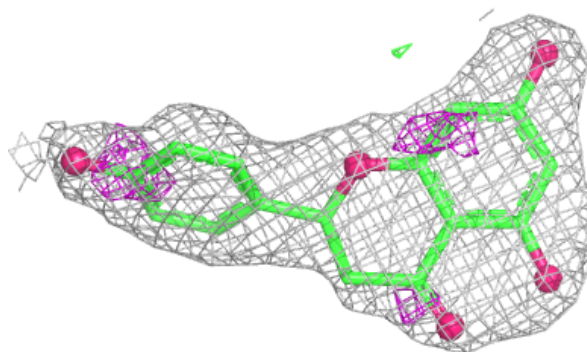


Electron density around NAR B 501:

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

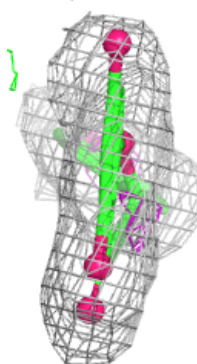
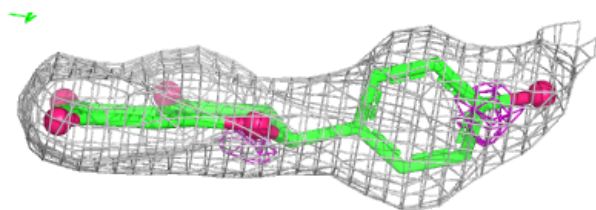
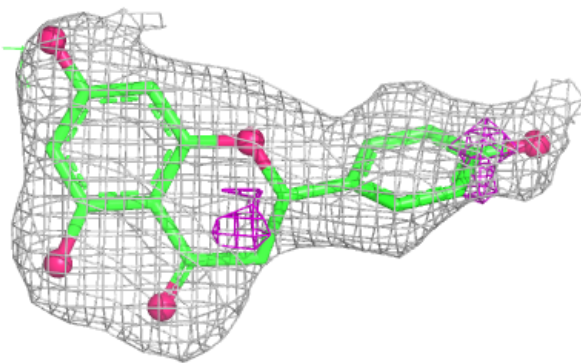
**Electron density around NAR A 501:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.