



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:20 PM JST

PDB ID : 6JVC / pdb_00006jvc
Title : Structure of the Cobalt Protoporphyrin IX-Reconstituted CYP102A1 Haem Domain with N-Abietoyl-L-Tryptophan
Authors : Stanfield, J.K.; Matsumoto, A.; Kasai, C.; Sugimoto, H.; Shiro, Y.; Watanabe, Y.; Shoji, O.
Deposited on : 2019-04-16
Resolution : 1.75 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

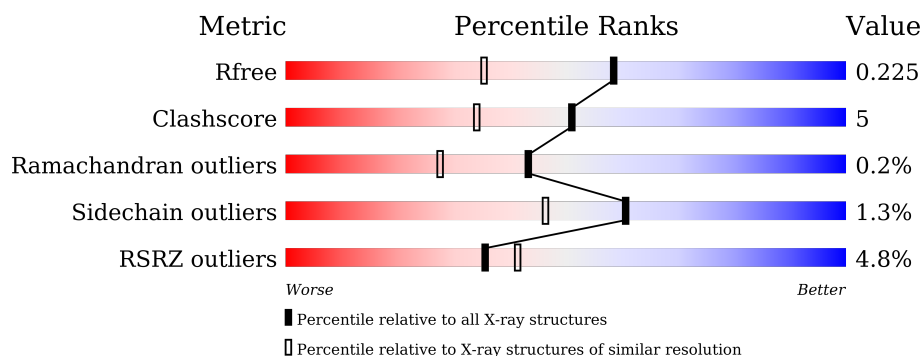
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	456	5% 89% 10%
1	C	456	5% 90% 9%

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

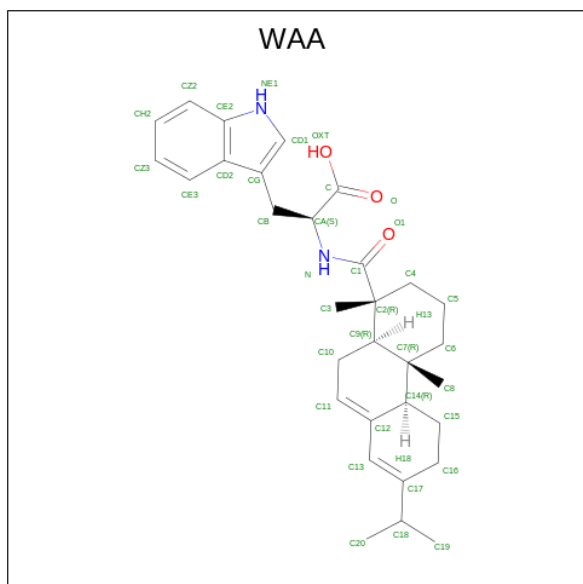
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	505	-	-	X	-
3	GOL	C	509	-	-	X	-
4	COH	A	512[A]	X	-	-	-
4	COH	A	512[B]	X	-	-	-
4	COH	C	514[A]	X	-	-	-
4	COH	C	514[B]	X	-	-	-

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

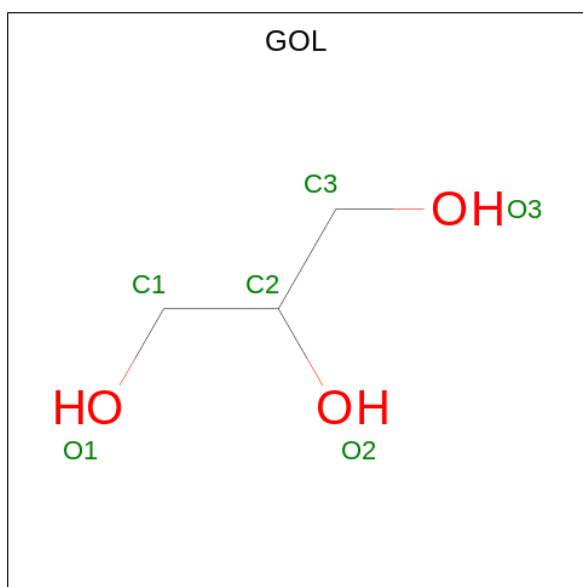
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	17	0
			3795	2416	644	716	19			
1	C	455	Total	C	N	O	S	0	17	0
			3804	2422	649	715	18			

- Molecule 2 is (2S)-2-[[[(1R,4aR,4bR,10aR)-1,4a-dimethyl-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthren-1-yl]carbonylamino]-3-(1H-indol-3-yl)propanoic acid (CCD ID: WAA) (formula: C₃₁H₄₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 36	C 31	N 2	O 3	0	0
2	C	1	Total 36	C 31	N 2	O 3	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



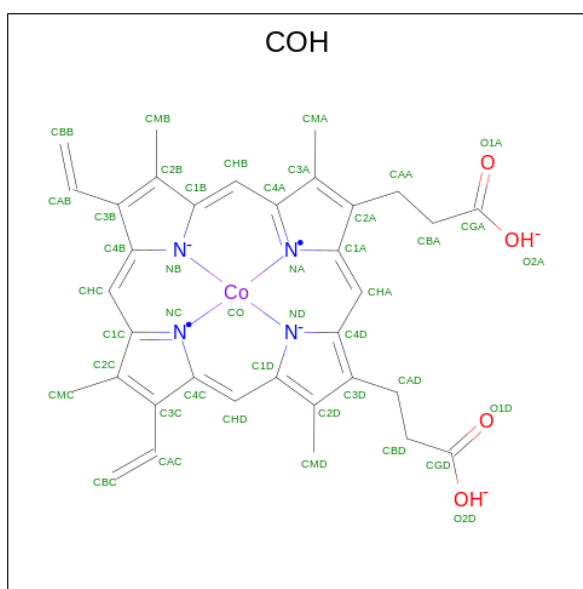
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	1
			12	6	6		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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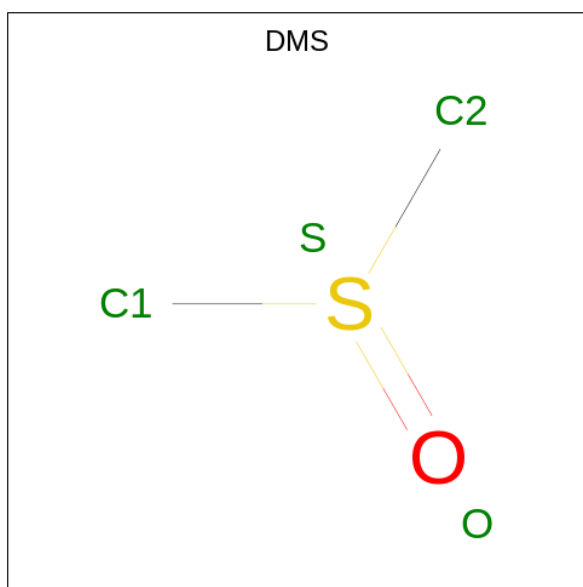
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 12	C 6	O 6	0	1
3	C	1	Total 12	C 6	O 6	0	1

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: $\text{C}_{34}\text{H}_{32}\text{CoN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



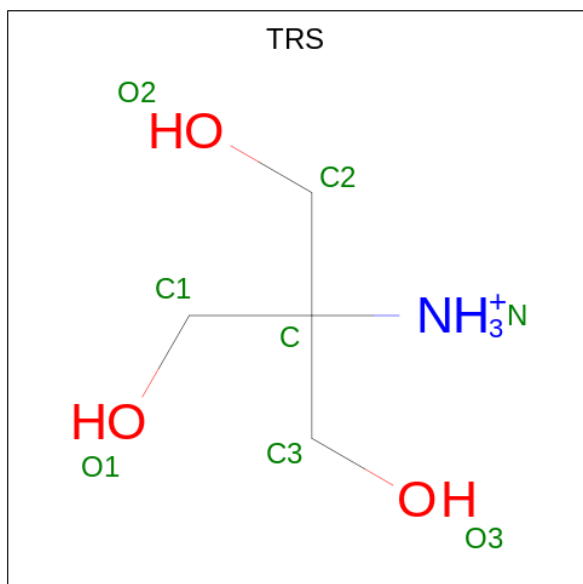
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 86	C 68	Co 2	N 8	O 8	0	1
4	C	1	Total 86	C 68	Co 2	N 8	O 8	0	1

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			8	4	1	3		

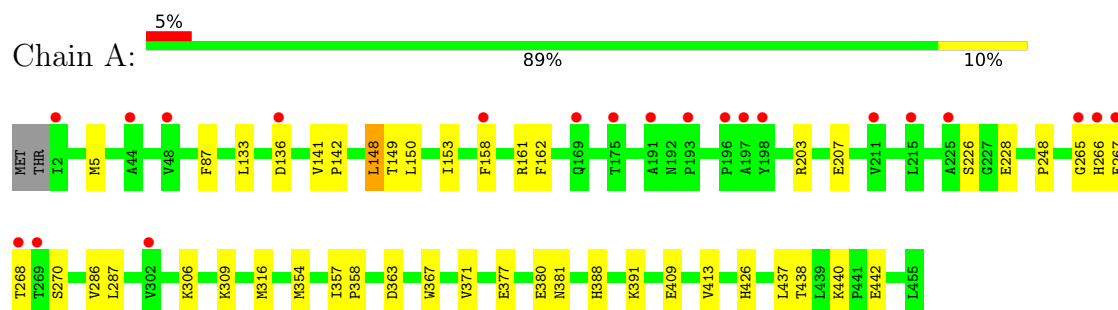
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	301	Total 301	O 301	0	0
7	C	278	Total 278	O 278	0	0

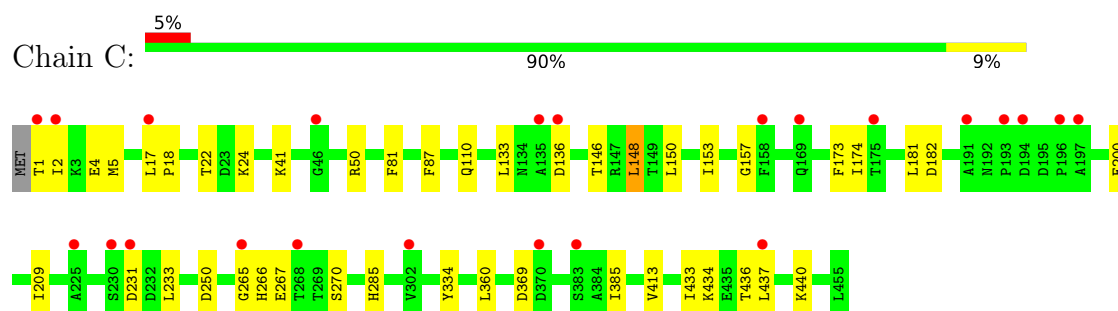
3 Residue-property plots [i](#)

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: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.90Å 148.25Å 63.22Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	47.87 – 1.75 47.87 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.87-1.75) 99.8 (47.87-1.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.220 0.195 , 0.225	Depositor DCC
R_{free} test set	5319 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, TRS, GOL, WAA, COH

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	1.04	2/3881 (0.1%)	1.25	2/5247 (0.0%)
1	C	1.08	2/3890 (0.1%)	1.24	3/5256 (0.1%)
All	All	1.06	4/7771 (0.1%)	1.25	5/10503 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	HIS	CE1-NE2	6.03	1.38	1.32
1	C	360	LEU	C-O	5.77	1.30	1.24
1	A	248	PRO	C-O	-5.39	1.16	1.23
1	C	385	ILE	N-CA	5.28	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASP	CB-CA-C	5.65	119.26	110.67
1	C	136	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	250	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	250	ASP	CB-CA-C	5.15	120.24	110.51
1	A	442	GLU	CB-CG-CD	5.03	121.15	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3795	0	3738	36	0
1	C	3804	0	3763	36	0
2	A	36	0	0	0	0
2	C	36	0	0	1	0
3	A	66	0	88	4	0
3	C	90	0	120	12	0
4	A	86	0	60	5	0
4	C	86	0	60	4	0
5	A	4	0	6	3	0
5	C	4	0	6	1	0
6	C	8	0	12	1	0
7	A	301	0	0	4	0
7	C	278	0	0	2	0
All	All	8594	0	7853	83	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 5.

All (83) 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:C:285:HIS:ND1	3:C:509:GOL:H12	1.80	0.97
1:C:285:HIS:ND1	3:C:509:GOL:C1	2.39	0.85
3:A:504:GOL:H32	7:A:687:HOH:O	1.81	0.80
1:C:133:LEU:O	6:C:516:TRS:H11	1.89	0.72
1:C:181:LEU:HD22	1:C:437:LEU:HD13	1.73	0.70
1:A:268[A]:THR:HG22	1:A:438[A]:THR:CG2	2.27	0.64
1:A:87:PHE:CD1	5:A:513:DMS:H12	2.34	0.63
1:A:287[B]:LEU:O	1:A:287[B]:LEU:HD23	2.00	0.61
1:A:381[A]:ASN:ND2	7:A:601:HOH:O	2.20	0.61
4:C:514[A]:COH:HBC1	4:C:514[A]:COH:HMC3	1.83	0.61
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.82	0.59
1:C:440:LYS:HD3	7:C:725:HOH:O	2.03	0.58
4:A:512[A]:COH:HBB1	4:A:512[A]:COH:CMB	2.34	0.58
4:C:514[A]:COH:HBC1	4:C:514[A]:COH:CMC	2.34	0.56
1:C:267[B]:GLU:HA	1:C:270[B]:SER:CB	2.35	0.56
1:A:87:PHE:CE1	5:A:513:DMS:H12	2.39	0.56
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.87	0.56
1:C:267[B]:GLU:HA	1:C:270[B]:SER:HB3	1.87	0.56
1:A:316:MET:HE1	1:A:380:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268[A]:THR:HG22	1:A:438[A]:THR:HG22	1.88	0.56
1:C:267[A]:GLU:OE2	3:C:505:GOL:H2	2.06	0.55
1:C:434:LYS:HD3	1:C:440:LYS:NZ	2.22	0.54
1:C:81:PHE:HB3	1:C:209:ILE:HG12	1.88	0.54
1:A:158:PHE:CD1	1:A:158:PHE:N	2.77	0.52
1:A:150:LEU:C	1:A:150:LEU:HD13	2.35	0.52
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.90	0.52
1:A:287[B]:LEU:HD23	1:A:287[B]:LEU:C	2.34	0.52
1:A:161:ARG:NH2	3:A:507:GOL:H12	2.25	0.52
1:C:153:ILE:HG21	1:C:265[A]:GLY:HA3	1.92	0.52
1:A:153:ILE:HG21	1:A:265[A]:GLY:HA3	1.92	0.52
1:C:146:THR:N	1:C:270[B]:SER:OG	2.43	0.52
1:A:268[A]:THR:HG22	1:A:438[A]:THR:HG21	1.93	0.51
1:C:267[A]:GLU:OE1	1:C:437:LEU:HB3	2.12	0.50
4:A:512[A]:COH:HBB1	4:A:512[A]:COH:HMB1	1.94	0.50
1:C:200:GLU:HA	1:C:200:GLU:OE1	2.13	0.49
1:C:334:TYR:CZ	3:C:504:GOL:H11	2.48	0.49
1:A:267[A]:GLU:OE1	1:A:437:LEU:HB3	2.12	0.49
4:A:512[B]:COH:HBC1	4:A:512[B]:COH:HMC1	1.94	0.49
1:A:267[B]:GLU:HA	1:A:270:SER:OG	2.13	0.48
1:A:87:PHE:CE2	5:A:513:DMS:H11	2.48	0.48
1:C:182[B]:ASP:OD1	3:C:505:GOL:O1	2.30	0.48
1:A:226:SER:OG	1:A:228:GLU:HG3	2.14	0.47
1:A:316:MET:CE	1:A:380:GLU:HG3	2.45	0.47
1:C:5:MET:SD	1:C:50:ARG:HG2	2.55	0.47
4:C:514[A]:COH:HMB1	4:C:514[A]:COH:HBB1	1.96	0.47
1:C:150:LEU:HD21	1:C:174:ILE:HG13	1.95	0.47
1:C:150:LEU:HD11	1:C:174:ILE:HD11	1.97	0.47
1:A:286:VAL:HG22	3:A:503:GOL:H32	1.96	0.46
4:A:512[A]:COH:HMC3	4:A:512[A]:COH:HBC1	1.97	0.45
1:A:149:THR:HA	1:A:409:GLU:OE2	2.15	0.45
1:A:5:MET:HE3	1:A:5:MET:HB2	1.82	0.45
1:A:150:LEU:CD1	1:A:162:PHE:CD2	3.01	0.44
1:C:4:GLU:HG3	1:C:5:MET:N	2.33	0.44
1:C:87:PHE:CD1	5:C:515:DMS:H22	2.53	0.44
1:C:285:HIS:ND1	3:C:509:GOL:H11	2.29	0.44
3:C:510:GOL:C1	7:C:754:HOH:O	2.66	0.44
1:A:316:MET:CE	1:A:377:GLU:HA	2.46	0.44
1:A:150:LEU:HD13	1:A:150:LEU:O	2.17	0.44
1:A:203:ARG:NH1	1:A:207:GLU:OE1	2.51	0.44
1:C:267[B]:GLU:OE1	3:C:505:GOL:O3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:LEU:HG	2:C:501:WAA:C19	2.47	0.44
1:C:285:HIS:CE1	3:C:509:GOL:C1	2.99	0.43
1:A:136:ASP:OD1	1:A:136:ASP:N	2.48	0.43
1:C:285:HIS:CE1	3:C:509:GOL:H12	2.51	0.43
1:C:153:ILE:O	1:C:157:GLY:N	2.51	0.43
1:C:436:THR:HG21	3:C:505:GOL:H32	2.00	0.42
4:C:514[A]:COH:HBB1	4:C:514[A]:COH:CMB	2.49	0.42
1:A:287[B]:LEU:C	1:A:287[B]:LEU:CD2	2.91	0.42
1:C:173:PHE:CD1	1:C:173:PHE:C	2.97	0.42
1:C:150:LEU:CD2	1:C:174:ILE:HG13	2.50	0.42
1:A:309:LYS:NZ	7:A:622:HOH:O	2.53	0.42
1:C:157:GLY:HA2	1:C:233:LEU:HD12	2.02	0.41
1:A:440:LYS:HB3	7:A:792:HOH:O	2.19	0.41
1:C:17:LEU:HB3	1:C:18:PRO:HD3	2.02	0.41
1:A:141:VAL:HB	1:A:142:PRO:HD3	2.02	0.41
1:C:267[B]:GLU:HA	1:C:270[B]:SER:HB2	2.02	0.41
4:A:512[A]:COH:HBC1	4:A:512[A]:COH:CMC	2.51	0.41
1:A:357:ILE:N	1:A:358:PRO:CD	2.84	0.41
1:C:24:LYS:HE2	1:C:433:ILE:O	2.20	0.41
1:A:133:LEU:O	3:A:508:GOL:H12	2.21	0.41
1:C:285:HIS:CE1	3:C:509:GOL:H11	2.57	0.40
1:A:354[B]:MET:HE2	1:A:354[B]:MET:HB2	1.97	0.40
1:C:148:LEU:HD21	1:C:413:VAL:HG21	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	469/456 (103%)	452 (96%)	15 (3%)	2 (0%)	30	15
1	C	470/456 (103%)	455 (97%)	13 (3%)	2 (0%)	30	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	939/912 (103%)	907 (97%)	28 (3%)	4 (0%)	43 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266[A]	HIS
1	A	266[B]	HIS
1	C	266[A]	HIS
1	C	266[B]	HIS

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	413/400 (103%)	411 (100%)	2 (0%)	81 75
1	C	414/400 (104%)	406 (98%)	8 (2%)	50 31
All	All	827/800 (103%)	817 (99%)	10 (1%)	61 49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	306	LYS
1	C	1	THR
1	C	2	ILE
1	C	22	THR
1	C	41	LYS
1	C	110	GLN
1	C	148	LEU
1	C	231	ASP
1	C	369	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	C	21	ASN
1	C	70	ASN
1	C	201	ASN
1	C	288	GLN
1	C	359	GLN
1	C	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

35 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	$\# Z > 2$
6	TRS	C	516	-	7,7,7	0.21	0	9,9,9	0.59	0
3	GOL	C	512[B]	-	5,5,5	0.09	0	5,5,5	0.28	0
3	GOL	C	505	-	5,5,5	0.15	0	5,5,5	0.53	0
3	GOL	C	502	-	5,5,5	0.12	0	5,5,5	0.35	0
3	GOL	C	503[B]	-	5,5,5	0.18	0	5,5,5	0.43	0
3	GOL	C	504	-	5,5,5	0.20	0	5,5,5	0.55	0
4	COH	A	512[B]	5	50,50,50	1.87	17 (34%)	68,82,82	3.93	34 (50%)
3	GOL	A	502	-	5,5,5	0.14	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	511	-	5,5,5	0.12	0	5,5,5	0.39	0
4	COH	C	514[B]	5	50,50,50	1.87	12 (24%)	68,82,82	3.95	37 (54%)
3	GOL	C	506	-	5,5,5	0.28	0	5,5,5	0.60	0
5	DMS	A	513	4	3,3,3	0.33	0	3,3,3	0.57	0
3	GOL	A	505	-	5,5,5	0.09	0	5,5,5	0.21	0
3	GOL	C	513[B]	-	5,5,5	0.10	0	5,5,5	0.27	0
3	GOL	A	503	-	5,5,5	0.09	0	5,5,5	0.35	0
3	GOL	A	504	-	5,5,5	0.10	0	5,5,5	0.23	0
3	GOL	A	506	-	5,5,5	0.13	0	5,5,5	0.33	0
3	GOL	A	511[B]	-	5,5,5	0.12	0	5,5,5	0.20	0
2	WAA	A	501	-	40,40,40	1.23	4 (10%)	51,61,61	1.30	6 (11%)
3	GOL	A	508	-	5,5,5	0.09	0	5,5,5	0.22	0
3	GOL	C	510	-	5,5,5	0.11	0	5,5,5	0.32	0
2	WAA	C	501	-	40,40,40	1.20	5 (12%)	51,61,61	1.44	9 (17%)
3	GOL	C	512[A]	-	5,5,5	0.11	0	5,5,5	0.29	0
3	GOL	C	503[A]	-	5,5,5	0.15	0	5,5,5	0.42	0
5	DMS	C	515	4	3,3,3	0.42	0	3,3,3	0.36	0
3	GOL	C	509	-	5,5,5	0.25	0	5,5,5	0.73	0
4	COH	A	512[A]	5	50,50,50	1.82	13 (26%)	68,82,82	3.79	36 (52%)
3	GOL	C	508	-	5,5,5	0.14	0	5,5,5	0.27	0
3	GOL	A	507	-	5,5,5	0.14	0	5,5,5	0.37	0
3	GOL	A	509	-	5,5,5	0.10	0	5,5,5	0.35	0
3	GOL	A	510	-	5,5,5	0.10	0	5,5,5	0.38	0
4	COH	C	514[A]	5	50,50,50	1.86	14 (28%)	68,82,82	3.93	36 (52%)
3	GOL	C	507	-	5,5,5	0.10	0	5,5,5	0.35	0
3	GOL	C	513[A]	-	5,5,5	0.09	0	5,5,5	0.28	0
3	GOL	A	511[A]	-	5,5,5	0.11	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	C	516	-	-	0/9/9/9	-
3	GOL	C	512[B]	-	-	2/4/4/4	-
3	GOL	C	505	-	-	1/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	C	503[B]	-	-	2/4/4/4	-
4	COH	A	512[B]	5	1/1/3/9	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	504	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	C	511	-	-	2/4/4/4	-
4	COH	C	514[B]	5	1/1/3/9	2/14/54/54	-
3	GOL	C	506	-	-	2/4/4/4	-
3	GOL	A	505	-	-	0/4/4/4	-
3	GOL	C	513[B]	-	-	2/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	A	511[B]	-	-	1/4/4/4	-
2	WAA	A	501	-	-	2/22/66/66	0/5/5/5
3	GOL	A	508	-	-	3/4/4/4	-
3	GOL	C	510	-	-	4/4/4/4	-
2	WAA	C	501	-	-	2/22/66/66	0/5/5/5
3	GOL	C	512[A]	-	-	1/4/4/4	-
3	GOL	C	503[A]	-	-	4/4/4/4	-
3	GOL	C	509	-	-	4/4/4/4	-
4	COH	A	512[A]	5	1/1/3/9	2/14/54/54	-
3	GOL	C	508	-	-	0/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	A	509	-	-	3/4/4/4	-
3	GOL	A	510	-	-	1/4/4/4	-
4	COH	C	514[A]	5	1/1/3/9	2/14/54/54	-
3	GOL	C	507	-	-	4/4/4/4	-
3	GOL	C	513[A]	-	-	4/4/4/4	-
3	GOL	A	511[A]	-	-	2/4/4/4	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	514[B]	COH	CHB-C1B	4.72	1.47	1.38
4	C	514[B]	COH	CHC-C4B	4.35	1.46	1.38
4	C	514[A]	COH	CHD-C4C	4.03	1.46	1.38
4	C	514[B]	COH	C3C-C2C	4.02	1.45	1.37
4	C	514[A]	COH	CHC-C4B	4.00	1.46	1.38
4	C	514[A]	COH	CHA-C1A	3.96	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	512[A]	COH	C1D-ND	-3.95	1.32	1.38
4	C	514[A]	COH	C3B-C2B	3.94	1.45	1.37
4	A	512[B]	COH	CHC-C4B	3.86	1.45	1.38
2	A	501	WAA	C13-C17	3.84	1.40	1.34
4	A	512[B]	COH	C4C-NC	-3.58	1.33	1.39
4	A	512[B]	COH	C3C-C2C	3.52	1.44	1.37
4	C	514[B]	COH	C2A-C3A	3.42	1.44	1.36
4	A	512[A]	COH	C3B-C2B	3.42	1.44	1.37
4	A	512[B]	COH	CHB-C1B	3.36	1.44	1.38
4	A	512[B]	COH	C3B-C2B	3.34	1.44	1.37
4	A	512[A]	COH	CHA-C1A	3.33	1.45	1.38
4	A	512[B]	COH	C4A-NA	-3.27	1.32	1.38
4	C	514[B]	COH	C3B-C2B	3.25	1.43	1.37
4	A	512[A]	COH	CHC-C4B	3.23	1.44	1.38
4	A	512[B]	COH	C2A-C3A	3.19	1.43	1.36
4	A	512[A]	COH	C2A-C3A	3.09	1.43	1.36
4	C	514[A]	COH	C2A-C3A	3.04	1.43	1.36
4	C	514[B]	COH	CHA-C4D	3.02	1.46	1.39
4	C	514[A]	COH	C3C-C2C	3.02	1.43	1.37
4	C	514[A]	COH	CHC-C1C	3.02	1.46	1.39
4	A	512[A]	COH	C3C-C2C	3.01	1.43	1.37
4	A	512[A]	COH	CHB-C1B	3.00	1.44	1.38
4	C	514[A]	COH	C1B-C2B	2.96	1.51	1.45
4	C	514[B]	COH	CHC-C1C	2.94	1.45	1.39
4	A	512[A]	COH	C4C-NC	-2.79	1.34	1.39
4	C	514[B]	COH	CHA-C1A	2.78	1.44	1.38
4	C	514[A]	COH	CHB-C4A	2.74	1.45	1.39
4	C	514[B]	COH	C1C-C2C	2.68	1.49	1.44
4	A	512[A]	COH	CHD-C4C	2.64	1.43	1.38
4	A	512[A]	COH	CHB-C4A	2.62	1.45	1.39
4	A	512[A]	COH	C1B-NB	-2.55	1.34	1.38
4	A	512[B]	COH	CHA-C4D	2.54	1.45	1.39
2	A	501	WAA	CD2-CG	-2.50	1.39	1.44
4	A	512[A]	COH	CHC-C1C	2.47	1.44	1.39
2	C	501	WAA	C13-C12	2.45	1.50	1.44
4	A	512[B]	COH	CHA-C1A	2.43	1.43	1.38
2	A	501	WAA	C13-C12	2.43	1.50	1.44
2	C	501	WAA	CD2-CG	-2.43	1.39	1.44
4	C	514[A]	COH	CHB-C1B	2.42	1.43	1.38
4	A	512[B]	COH	CHD-C4C	2.42	1.43	1.38
4	A	512[B]	COH	CHB-C4A	2.40	1.44	1.39
4	A	512[B]	COH	CHC-C1C	2.40	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	512[B]	COH	C4B-NB	-2.40	1.34	1.38
2	C	501	WAA	OXT-C	-2.39	1.22	1.30
4	A	512[A]	COH	C1B-C2B	2.35	1.50	1.45
4	A	512[B]	COH	C1C-C2C	2.32	1.49	1.44
2	A	501	WAA	OXT-C	-2.31	1.23	1.30
4	C	514[B]	COH	CHB-C4A	2.30	1.44	1.39
2	C	501	WAA	CD2-CE2	-2.26	1.38	1.41
4	C	514[A]	COH	C4C-NC	-2.25	1.35	1.39
4	C	514[A]	COH	C4B-NB	-2.21	1.35	1.38
4	A	512[B]	COH	CHD-C1D	2.15	1.44	1.39
4	C	514[A]	COH	CHA-C4D	2.13	1.44	1.39
4	C	514[B]	COH	CHD-C1D	2.07	1.44	1.39
2	C	501	WAA	C13-C17	2.05	1.37	1.34
4	C	514[A]	COH	C3D-C2D	2.04	1.44	1.38
4	A	512[B]	COH	C1B-C2B	2.03	1.49	1.45
4	C	514[B]	COH	C4C-NC	-2.02	1.35	1.39
4	A	512[B]	COH	C1A-NA	-2.02	1.35	1.39

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	514[A]	COH	C2B-C1B-NB	10.36	119.72	110.81
4	C	514[A]	COH	C2D-C1D-ND	10.16	119.59	109.69
4	A	512[A]	COH	C2D-C1D-ND	10.15	119.58	109.69
4	A	512[B]	COH	C3C-C2C-C1C	-10.04	99.03	106.49
4	A	512[A]	COH	C2B-C1B-NB	9.88	119.31	110.81
4	C	514[B]	COH	C2B-C1B-NB	9.82	119.26	110.81
4	C	514[A]	COH	C3C-C2C-C1C	-9.70	99.29	106.49
4	A	512[B]	COH	C2B-C1B-NB	9.53	119.01	110.81
4	C	514[B]	COH	C3C-C2C-C1C	-9.39	99.52	106.49
4	C	514[B]	COH	C2D-C1D-ND	9.34	118.79	109.69
4	A	512[B]	COH	C2D-C1D-ND	9.14	118.59	109.69
4	A	512[B]	COH	C3B-C2B-C1B	-8.82	98.65	107.08
4	A	512[A]	COH	C3D-C4D-ND	8.64	118.88	110.68
4	C	514[A]	COH	C3B-C2B-C1B	-8.61	98.86	107.08
4	C	514[B]	COH	C3D-C4D-ND	8.45	118.70	110.68
4	C	514[A]	COH	C3D-C4D-ND	8.44	118.69	110.68
4	A	512[B]	COH	C3C-C4C-NC	8.27	118.23	109.67
4	A	512[B]	COH	C2C-C1C-NC	8.22	120.27	110.83
4	C	514[B]	COH	C2C-C1C-NC	8.21	120.27	110.83
4	C	514[B]	COH	C3B-C2B-C1B	-8.00	99.44	107.08
4	A	512[A]	COH	C3B-C2B-C1B	-7.98	99.45	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	512[A]	COH	C3C-C2C-C1C	-7.66	100.80	106.49
4	C	514[B]	COH	C3C-C4C-NC	7.66	117.60	109.67
4	A	512[B]	COH	C3D-C4D-ND	7.57	117.86	110.68
4	C	514[A]	COH	C2C-C1C-NC	7.24	119.15	110.83
4	A	512[A]	COH	C2C-C1C-NC	6.77	118.61	110.83
4	A	512[A]	COH	C3C-C4C-NC	6.68	116.59	109.67
4	C	514[B]	COH	C3A-C4A-NA	6.57	118.39	110.83
4	C	514[A]	COH	C3C-C4C-NC	6.44	116.34	109.67
4	C	514[B]	COH	C2A-C1A-NA	6.40	118.54	110.58
4	A	512[B]	COH	C4C-NC-C1C	-6.39	98.36	105.05
4	A	512[B]	COH	C3A-C4A-NA	6.39	118.17	110.83
4	A	512[B]	COH	C2A-C1A-NA	6.34	118.47	110.58
4	C	514[B]	COH	C4D-ND-C1D	-6.12	97.78	105.08
4	C	514[B]	COH	C1A-NA-C4A	-6.10	98.66	105.05
4	C	514[B]	COH	C4C-NC-C1C	-6.08	98.68	105.05
4	C	514[A]	COH	C4D-ND-C1D	-5.95	97.99	105.08
4	C	514[A]	COH	C2A-C1A-NA	5.94	117.97	110.58
4	C	514[A]	COH	C4C-NC-C1C	-5.77	99.01	105.05
4	A	512[B]	COH	C4D-ND-C1D	-5.75	98.22	105.08
4	C	514[A]	COH	C3B-C4B-NB	5.69	117.84	109.27
4	A	512[A]	COH	C4D-ND-C1D	-5.66	98.33	105.08
4	A	512[A]	COH	C3A-C4A-NA	5.62	117.29	110.83
4	C	514[A]	COH	C1A-NA-C4A	-5.58	99.21	105.05
4	A	512[A]	COH	C1A-NA-C4A	-5.44	99.35	105.05
4	C	514[A]	COH	C3A-C4A-NA	5.44	117.08	110.83
4	A	512[A]	COH	C2A-C1A-NA	5.43	117.33	110.58
4	A	512[B]	COH	C1A-NA-C4A	-5.39	99.40	105.05
4	A	512[A]	COH	C3B-C4B-NB	5.38	117.37	109.27
4	C	514[A]	COH	C4B-NB-C1B	-5.31	98.75	105.08
4	C	514[A]	COH	CMA-C3A-C4A	5.21	132.98	125.04
4	C	514[B]	COH	C4B-NB-C1B	-5.21	98.87	105.08
4	C	514[A]	COH	CAA-C2A-C1A	5.18	133.72	124.66
4	A	512[A]	COH	C4C-NC-C1C	-5.02	99.80	105.05
4	A	512[A]	COH	C4B-NB-C1B	-4.89	99.25	105.08
4	C	514[B]	COH	C3B-C4B-NB	4.77	116.45	109.27
4	A	512[A]	COH	CAA-C2A-C1A	4.76	132.98	124.66
4	A	512[B]	COH	C3B-C4B-NB	4.70	116.35	109.27
4	C	514[B]	COH	C4A-C3A-C2A	-4.62	102.10	106.96
4	C	514[B]	COH	CHB-C4A-C3A	-4.55	117.88	124.98
4	C	514[A]	COH	CHC-C1C-C2C	-4.53	117.90	124.98
4	A	512[A]	COH	CHC-C1C-C2C	-4.50	117.95	124.98
4	A	512[B]	COH	C1A-C2A-C3A	-4.50	100.34	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	512[B]	COH	C4B-NB-C1B	-4.44	99.78	105.08
4	C	514[A]	COH	C1D-C2D-C3D	-4.42	101.66	106.83
4	C	514[B]	COH	CMD-C2D-C1D	4.37	132.02	125.37
4	C	514[B]	COH	CAD-C3D-C4D	4.27	133.30	124.89
2	A	501	WAA	CZ2-CE2-CD2	-4.19	117.99	122.19
4	A	512[A]	COH	C4D-C3D-C2D	-4.19	100.30	106.89
4	C	514[B]	COH	C4C-C3C-C2C	-4.18	103.80	107.11
4	A	512[B]	COH	CAD-C3D-C4D	4.16	133.09	124.89
4	A	512[B]	COH	CHC-C1C-C2C	-4.12	118.54	124.98
4	A	512[A]	COH	CHB-C4A-C3A	-4.10	118.58	124.98
4	A	512[B]	COH	CHA-C1A-C2A	-3.99	117.83	125.33
4	A	512[A]	COH	CHC-C4B-C3B	-3.99	118.43	125.26
4	C	514[B]	COH	CHA-C1A-C2A	-3.99	117.84	125.33
4	A	512[B]	COH	C4C-C3C-C2C	-3.86	104.05	107.11
4	C	514[A]	COH	CHD-C1D-C2D	-3.81	116.48	127.24
4	C	514[A]	COH	CHA-C1A-C2A	-3.72	118.35	125.33
4	A	512[A]	COH	C4C-C3C-C2C	-3.72	104.16	107.11
4	A	512[A]	COH	CMA-C3A-C4A	3.70	130.67	125.04
4	A	512[B]	COH	CMD-C2D-C1D	3.68	130.98	125.37
2	C	501	WAA	C15-C16-C17	-3.62	106.04	112.33
4	A	512[B]	COH	CAA-C2A-C1A	3.61	130.96	124.66
4	C	514[B]	COH	CAA-C2A-C1A	3.60	130.96	124.66
4	A	512[A]	COH	CMB-C2B-C1B	3.55	130.98	124.71
4	A	512[B]	COH	CMB-C2B-C1B	3.55	130.97	124.71
4	C	514[B]	COH	C1D-C2D-C3D	-3.52	102.71	106.83
4	A	512[B]	COH	CHC-C4B-C3B	-3.50	119.27	125.26
4	C	514[A]	COH	CHB-C1B-C2B	-3.47	118.20	125.48
4	A	512[B]	COH	C1D-C2D-C3D	-3.45	102.80	106.83
2	C	501	WAA	C5-C6-C7	-3.44	108.89	113.17
4	A	512[B]	COH	CHB-C1B-C2B	-3.42	118.31	125.48
4	A	512[A]	COH	CHA-C4D-C3D	-3.40	117.94	125.36
4	C	514[B]	COH	CHC-C4B-C3B	-3.39	119.47	125.26
4	A	512[B]	COH	CHB-C4A-C3A	-3.36	119.72	124.98
4	A	512[A]	COH	C1D-C2D-C3D	-3.35	102.91	106.83
4	A	512[B]	COH	CHD-C1D-C2D	-3.33	117.83	127.24
4	C	514[A]	COH	C1A-C2A-C3A	-3.30	102.09	106.90
4	C	514[B]	COH	CHC-C1C-C2C	-3.30	119.83	124.98
4	C	514[B]	COH	C1A-C2A-C3A	-3.28	102.12	106.90
4	A	512[A]	COH	C4A-C3A-C2A	-3.25	103.54	106.96
4	A	512[B]	COH	CMC-C2C-C1C	3.23	129.96	125.04
4	C	514[B]	COH	CHB-C1B-NB	-3.22	120.51	124.83
4	C	514[B]	COH	CHA-C4D-C3D	-3.22	118.33	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	514[A]	COH	C4A-C3A-C2A	-3.22	103.58	106.96
4	A	512[A]	COH	CHD-C1D-C2D	-3.20	118.19	127.24
4	A	512[A]	COH	C1A-C2A-C3A	-3.18	102.26	106.90
4	A	512[B]	COH	C4A-C3A-C2A	-3.18	103.61	106.96
4	C	514[A]	COH	C4D-C3D-C2D	-3.16	101.92	106.89
4	C	514[B]	COH	C4D-C3D-C2D	-3.16	101.92	106.89
4	A	512[A]	COH	CHB-C1B-NB	-3.15	120.60	124.83
4	C	514[B]	COH	CMB-C2B-C1B	3.15	130.26	124.71
4	C	514[A]	COH	CHA-C4D-C3D	-3.13	118.52	125.36
4	A	512[A]	COH	CHA-C1A-C2A	-3.09	119.53	125.33
4	C	514[A]	COH	CHB-C4A-C3A	-2.99	120.30	124.98
4	C	514[A]	COH	CHC-C4B-C3B	-2.99	120.14	125.26
4	A	512[B]	COH	C4D-C3D-C2D	-2.93	102.28	106.89
4	C	514[A]	COH	CAD-C3D-C4D	2.92	130.63	124.89
2	A	501	WAA	C15-C16-C17	-2.90	107.29	112.33
4	C	514[B]	COH	CHD-C1D-C2D	-2.84	119.21	127.24
4	C	514[A]	COH	CMB-C2B-C1B	2.81	129.67	124.71
4	A	512[A]	COH	CAD-C3D-C4D	2.75	130.29	124.89
4	A	512[B]	COH	CMA-C3A-C4A	2.72	129.17	125.04
4	C	514[B]	COH	CMC-C2C-C1C	2.71	129.16	125.04
4	C	514[B]	COH	CHC-C1C-NC	-2.71	119.84	124.82
4	C	514[A]	COH	CMD-C2D-C3D	2.65	131.34	125.61
2	C	501	WAA	CA-N-C1	2.62	126.51	121.50
2	C	501	WAA	C6-C7-C14	-2.60	105.25	109.18
4	A	512[A]	COH	C4B-C3B-C2B	-2.60	104.61	106.75
4	C	514[A]	COH	CBA-CAA-C2A	-2.59	105.44	112.63
4	A	512[A]	COH	CHB-C1B-C2B	-2.57	120.09	125.48
4	C	514[B]	COH	CBD-CAD-C3D	-2.57	105.50	112.63
4	A	512[B]	COH	CHA-C4D-C3D	-2.54	119.81	125.36
2	A	501	WAA	C10-C9-C7	2.52	114.03	110.51
4	C	514[B]	COH	CHB-C1B-C2B	-2.52	120.19	125.48
4	C	514[B]	COH	CMA-C3A-C4A	2.48	128.81	125.04
2	C	501	WAA	C7-C14-C12	2.47	116.84	112.29
4	C	514[A]	COH	C4B-C3B-C2B	-2.42	104.76	106.75
4	A	512[A]	COH	CHD-C4C-C3C	-2.40	117.39	126.11
4	C	514[A]	COH	CMC-C2C-C1C	2.40	128.69	125.04
4	A	512[B]	COH	CBA-CAA-C2A	-2.39	105.98	112.63
2	A	501	WAA	C6-C7-C9	2.39	110.95	108.02
4	A	512[A]	COH	CBA-CAA-C2A	-2.24	106.42	112.63
2	A	501	WAA	C10-C9-C2	-2.23	110.76	113.21
4	A	512[A]	COH	CMC-C2C-C1C	2.15	128.32	125.04
4	A	512[B]	COH	CBD-CAD-C3D	-2.15	106.67	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	WAA	CB-CA-C	2.13	114.95	110.83
4	C	514[A]	COH	CHC-C4B-NB	-2.10	122.01	124.83
4	C	514[B]	COH	CHD-C4C-C3C	-2.10	118.50	126.11
2	A	501	WAA	C9-C10-C11	-2.07	109.15	113.02
4	C	514[A]	COH	CHB-C1B-NB	-2.07	122.05	124.83
4	A	512[A]	COH	CBD-CAD-C3D	-2.07	106.88	112.63
2	C	501	WAA	C5-C4-C2	-2.05	109.85	113.17
4	C	514[A]	COH	C4D-CHA-C1A	-2.05	121.49	126.34
2	C	501	WAA	CE3-CD2-CG	-2.04	130.85	133.83
4	C	514[B]	COH	C4D-CHA-C1A	-2.03	121.53	126.34
2	C	501	WAA	OXT-C-O	-2.02	119.51	124.09

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	512[A]	COH	NB
4	A	512[B]	COH	NB
4	C	514[A]	COH	NB
4	C	514[B]	COH	NB

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O2-C2-C3-O3
3	A	506	GOL	C1-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	A	507	GOL	O1-C1-C2-C3
3	A	508	GOL	C1-C2-C3-O3
3	A	509	GOL	C1-C2-C3-O3
3	C	503[A]	GOL	O1-C1-C2-C3
3	C	506	GOL	C1-C2-C3-O3
3	C	507	GOL	O1-C1-C2-O2
3	C	507	GOL	O1-C1-C2-C3
3	C	507	GOL	C1-C2-C3-O3
3	C	507	GOL	O2-C2-C3-O3
3	C	509	GOL	O1-C1-C2-C3
3	C	509	GOL	C1-C2-C3-O3
3	C	510	GOL	C1-C2-C3-O3
3	A	509	GOL	O2-C2-C3-O3
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	511[A]	GOL	O1-C1-C2-C3
3	A	511[B]	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	C	503[A]	GOL	C1-C2-C3-O3
3	C	503[B]	GOL	O1-C1-C2-C3
3	C	504	GOL	O1-C1-C2-C3
3	C	510	GOL	O1-C1-C2-C3
3	C	511	GOL	O1-C1-C2-C3
3	C	512[B]	GOL	O1-C1-C2-C3
3	C	513[A]	GOL	O1-C1-C2-C3
3	C	513[A]	GOL	C1-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	A	508	GOL	O2-C2-C3-O3
3	C	502	GOL	O2-C2-C3-O3
3	C	503[A]	GOL	O1-C1-C2-O2
3	C	509	GOL	O2-C2-C3-O3
3	C	512[B]	GOL	O1-C1-C2-O2
3	A	507	GOL	O1-C1-C2-O2
3	C	503[B]	GOL	O1-C1-C2-O2
3	C	506	GOL	O2-C2-C3-O3
3	C	509	GOL	O1-C1-C2-O2
3	C	510	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	C	511	GOL	O1-C1-C2-O2
3	C	513[A]	GOL	O1-C1-C2-O2
3	A	511[A]	GOL	O1-C1-C2-O2
3	C	503[A]	GOL	O2-C2-C3-O3
3	C	512[A]	GOL	O2-C2-C3-O3
3	C	513[B]	GOL	O1-C1-C2-O2
3	C	505	GOL	C1-C2-C3-O3
2	A	501	WAA	N-C1-C2-C3
2	C	501	WAA	O1-C1-C2-C3
3	A	509	GOL	O1-C1-C2-C3
3	A	510	GOL	O2-C2-C3-O3
4	A	512[A]	COH	CAA-CBA-CGA-O1A
4	A	512[A]	COH	CAA-CBA-CGA-O2A
4	A	512[B]	COH	CAD-CBD-CGD-O2D
4	C	514[A]	COH	CAA-CBA-CGA-O2A
3	A	508	GOL	O1-C1-C2-C3
4	C	514[B]	COH	CAD-CBD-CGD-O2D
3	C	513[A]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	514[A]	COH	CAA-CBA-CGA-O1A
4	A	512[B]	COH	CAD-CBD-CGD-O1D
4	C	514[B]	COH	CAD-CBD-CGD-O1D
3	C	504	GOL	O1-C1-C2-O2
3	C	510	GOL	O1-C1-C2-O2
3	C	513[B]	GOL	O1-C1-C2-C3
2	A	501	WAA	O1-C1-C2-C3
2	C	501	WAA	N-C1-C2-C3

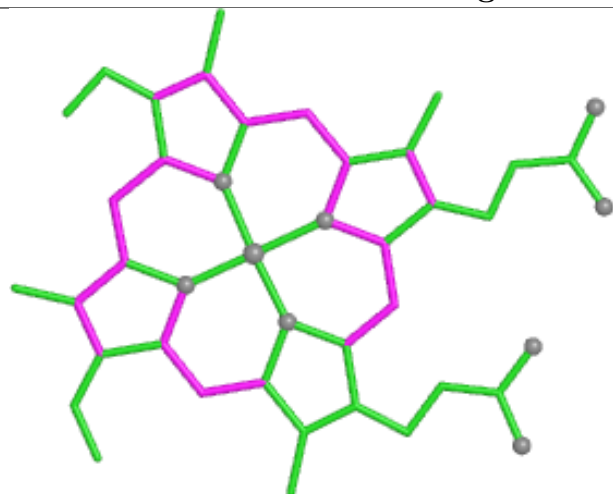
There are no ring outliers.

15 monomers are involved in 31 short contacts:

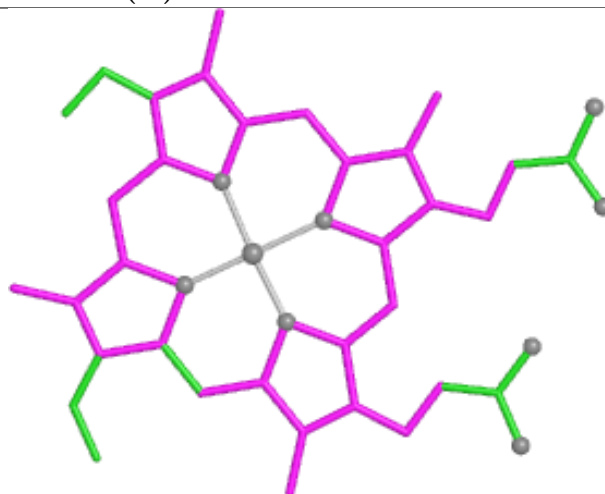
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	516	TRS	1	0
3	C	505	GOL	4	0
3	C	504	GOL	1	0
4	A	512[B]	COH	1	0
5	A	513	DMS	3	0
3	A	503	GOL	1	0
3	A	504	GOL	1	0
3	A	508	GOL	1	0
3	C	510	GOL	1	0
2	C	501	WAA	1	0
5	C	515	DMS	1	0
3	C	509	GOL	6	0
4	A	512[A]	COH	4	0
3	A	507	GOL	1	0
4	C	514[A]	COH	4	0

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.

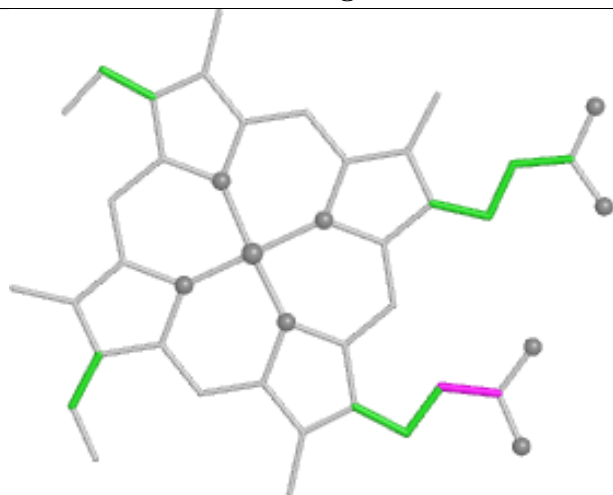
Ligand COH A 512 (B)



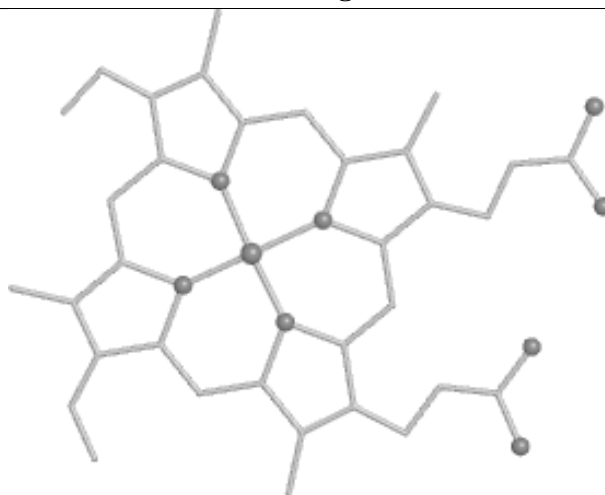
Bond lengths



Bond angles

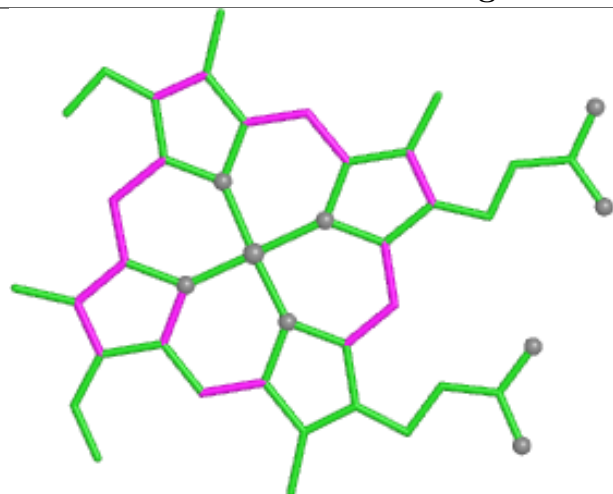


Torsions

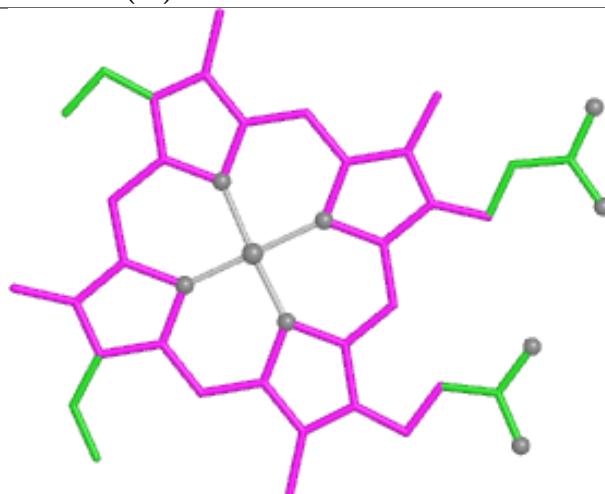


Rings

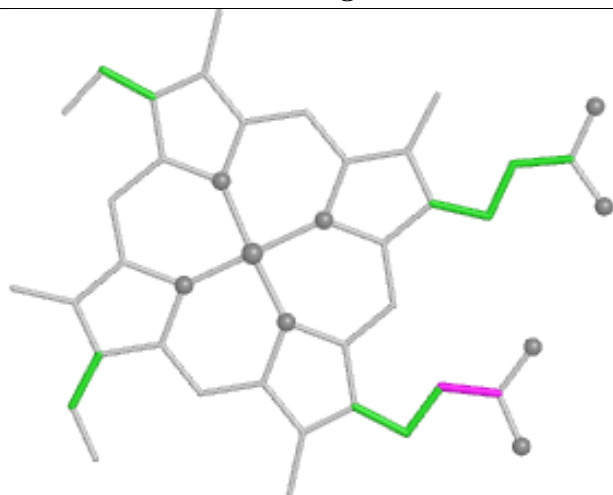
Ligand COH C 514 (B)



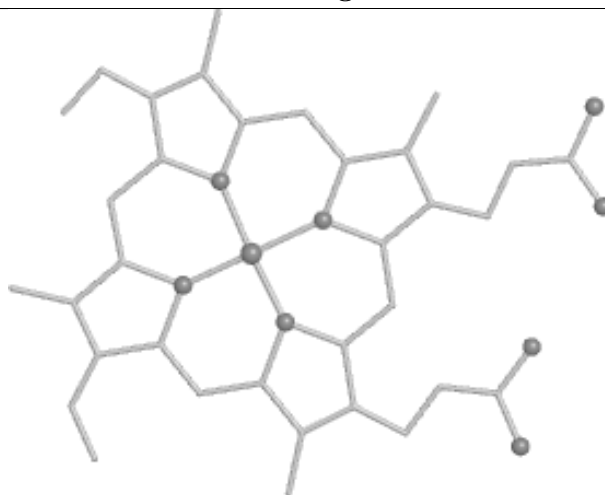
Bond lengths



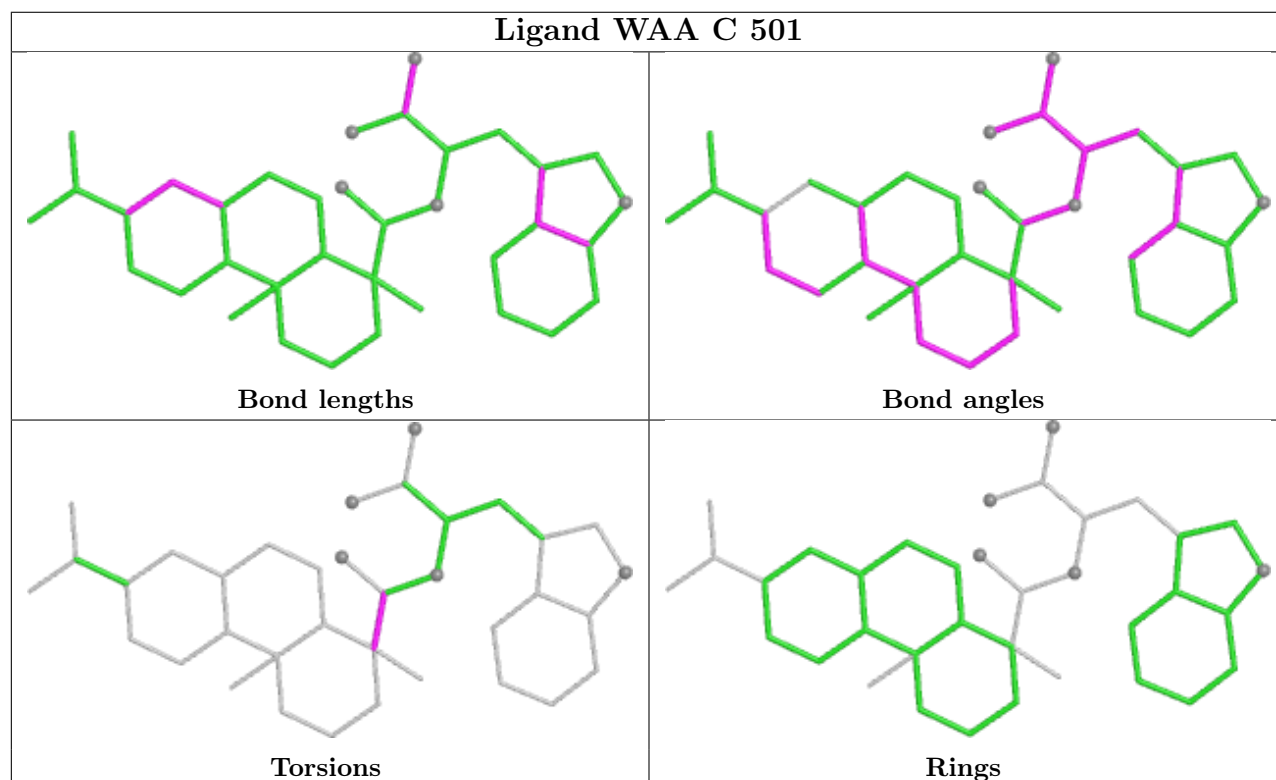
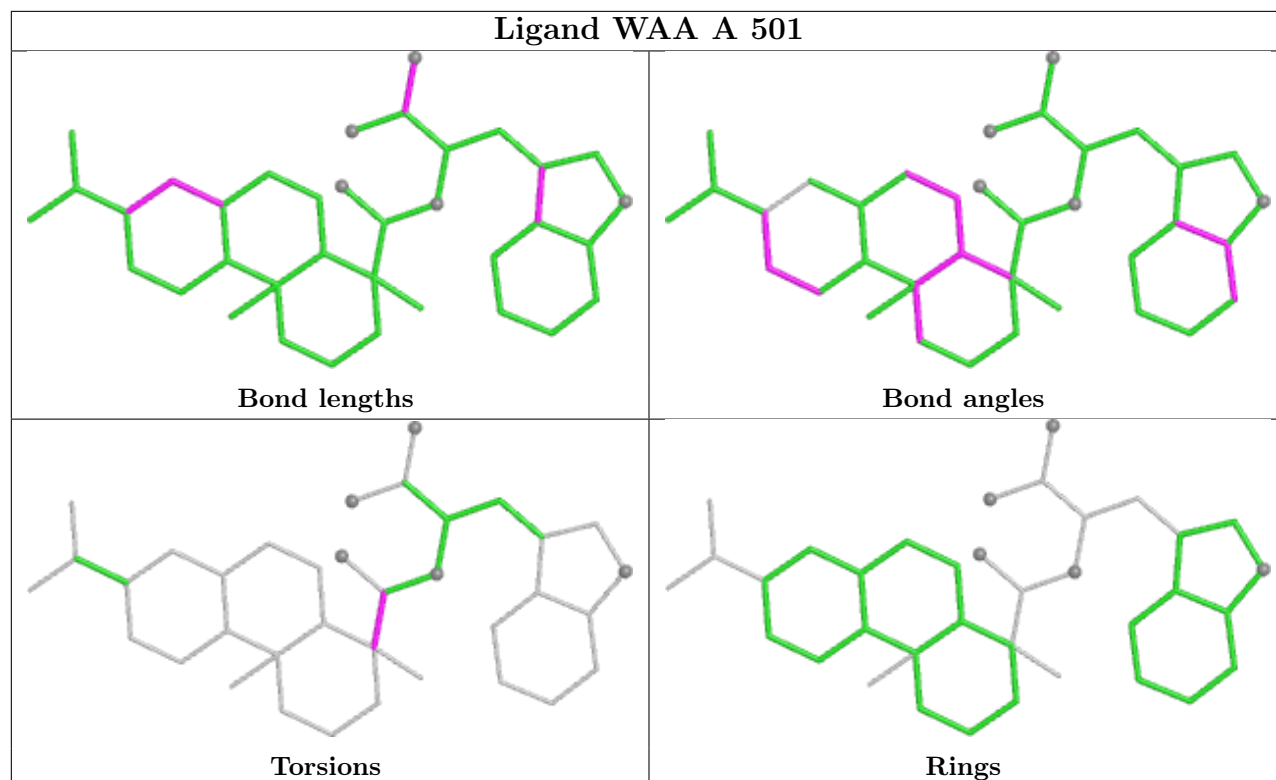
Bond angles



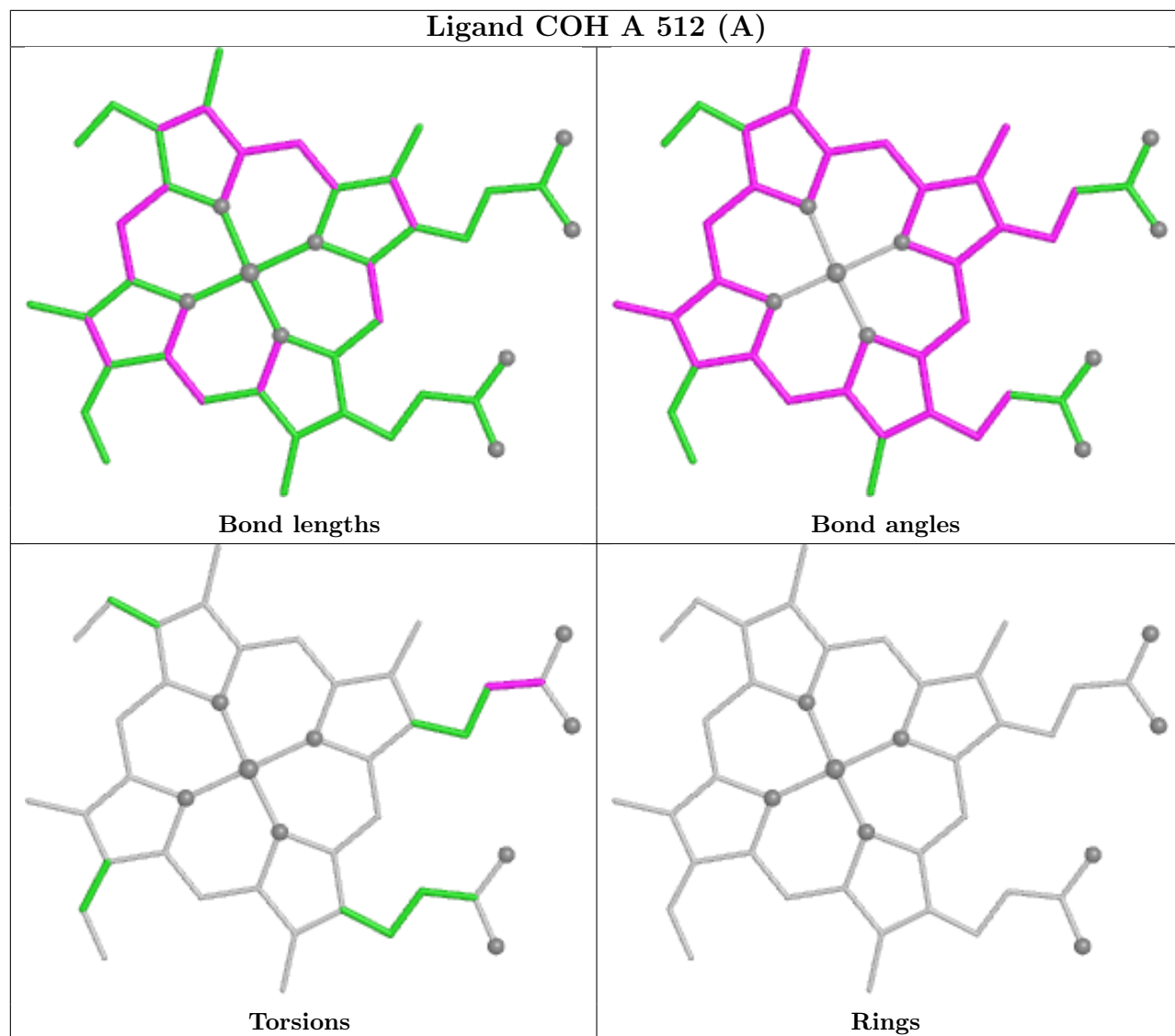
Torsions

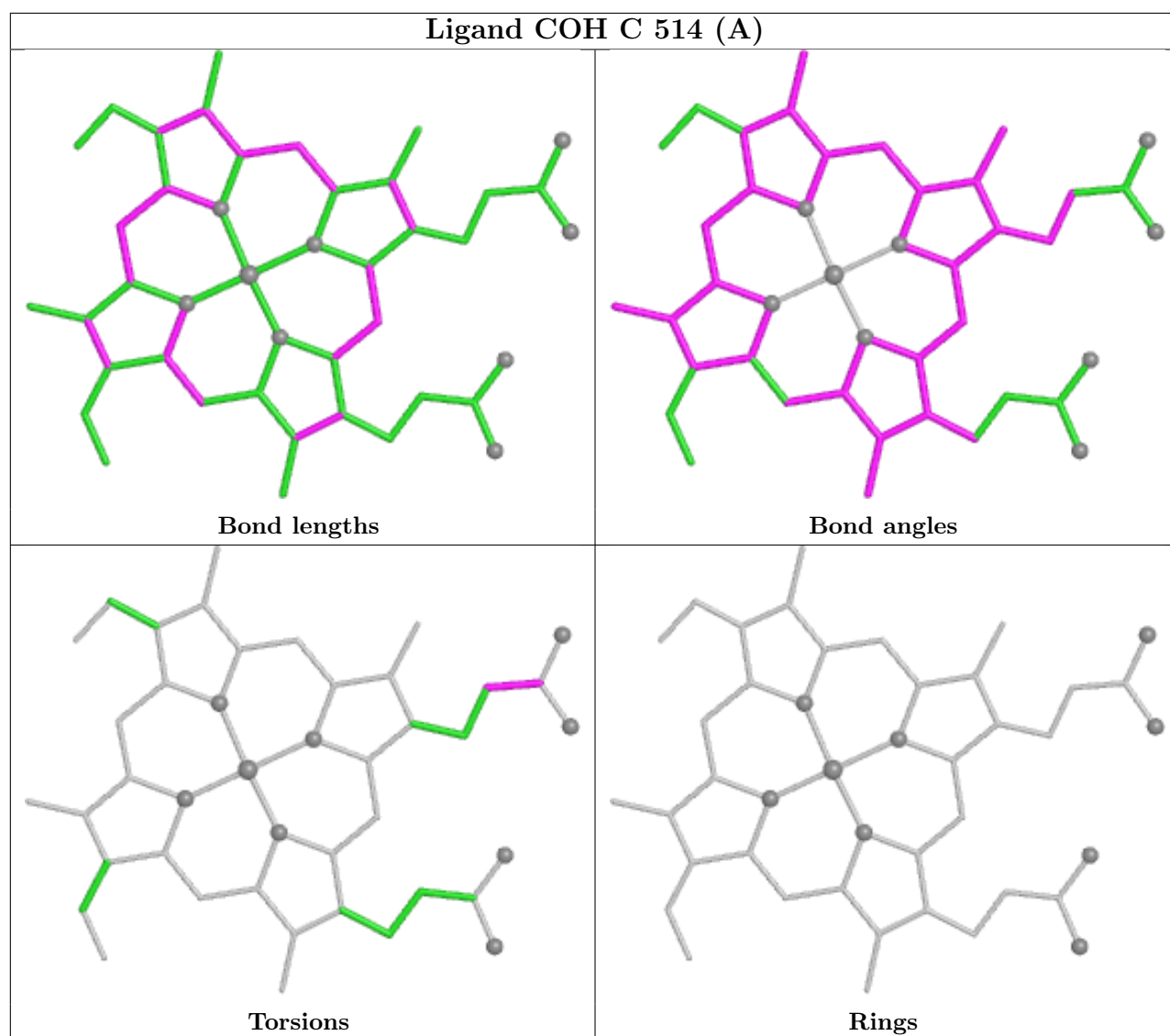


Rings



Ligand COH A 512 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	454/456 (99%)	0.31	21 (4%)	37 43	11, 25, 49, 67	17 (3%)
1	C	455/456 (99%)	0.42	23 (5%)	33 39	9, 26, 50, 77	17 (3%)
All	All	909/912 (99%)	0.37	44 (4%)	35 41	9, 26, 49, 77	34 (3%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	ALA	4.8
1	A	2	ILE	4.2
1	A	191	ALA	4.1
1	C	2	ILE	3.8
1	C	158	PHE	3.7
1	A	196	PRO	3.6
1	A	158	PHE	3.4
1	A	136	ASP	3.3
1	A	198	TYR	3.1
1	C	225	ALA	3.0
1	C	136	ASP	3.0
1	C	265[A]	GLY	3.0
1	A	265[A]	GLY	2.8
1	A	268[A]	THR	2.7
1	C	1	THR	2.7
1	A	267[A]	GLU	2.7
1	A	169	GLN	2.7
1	A	193	PRO	2.7
1	C	197	ALA	2.6
1	A	197	ALA	2.6
1	A	225	ALA	2.6
1	C	231	ASP	2.5
1	C	370	ASP	2.5
1	C	17	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	135	ALA	2.4
1	C	169	GLN	2.4
1	A	175[A]	THR	2.3
1	A	48	VAL	2.3
1	C	196	PRO	2.3
1	A	302	VAL	2.3
1	A	44	ALA	2.2
1	C	230	SER	2.2
1	A	215	LEU	2.2
1	C	437	LEU	2.2
1	C	383	SER	2.2
1	C	194	ASP	2.1
1	C	175	THR	2.1
1	C	46	GLY	2.1
1	A	269[A]	THR	2.1
1	A	211	VAL	2.0
1	C	302	VAL	2.0
1	C	268[A]	THR	2.0
1	C	193	PRO	2.0
1	A	266[A]	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	506	6/6	0.69	0.23	40,59,64,76	0
3	GOL	A	505	6/6	0.75	0.19	56,61,66,66	0
3	GOL	C	504	6/6	0.76	0.18	39,51,54,55	0

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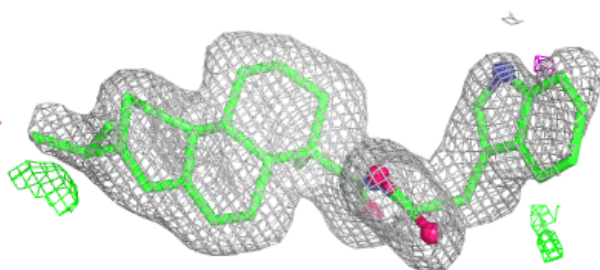
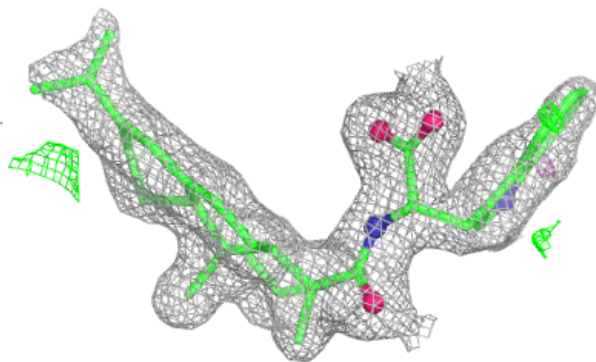
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	503[B]	6/6	0.78	0.21	41,45,47,47	6
3	GOL	C	503[A]	6/6	0.78	0.21	56,61,65,67	6
3	GOL	C	508	6/6	0.78	0.18	54,56,56,58	0
3	GOL	C	505	6/6	0.80	0.18	42,55,63,65	0
3	GOL	C	512[A]	6/6	0.80	0.13	34,41,43,46	6
3	GOL	C	512[B]	6/6	0.80	0.13	59,67,71,72	6
6	TRS	C	516	8/8	0.80	0.18	52,56,60,62	0
3	GOL	C	510	6/6	0.81	0.18	56,59,60,61	0
3	GOL	A	510	6/6	0.82	0.16	53,55,56,58	0
3	GOL	C	513[A]	6/6	0.82	0.19	55,56,58,62	6
3	GOL	C	513[B]	6/6	0.82	0.19	49,50,52,56	6
3	GOL	A	508	6/6	0.82	0.17	50,55,61,66	0
3	GOL	A	504	6/6	0.83	0.16	35,50,56,57	0
3	GOL	C	502	6/6	0.83	0.18	50,53,56,57	0
3	GOL	C	511	6/6	0.83	0.16	39,51,54,57	0
3	GOL	C	507	6/6	0.83	0.13	50,58,60,60	0
3	GOL	A	511[A]	6/6	0.84	0.17	49,54,57,58	6
3	GOL	A	511[B]	6/6	0.84	0.17	37,39,39,40	6
3	GOL	A	509	6/6	0.84	0.16	46,51,53,53	0
3	GOL	A	502	6/6	0.84	0.13	34,45,46,50	0
5	DMS	C	515	4/4	0.85	0.20	33,55,58,63	0
3	GOL	C	506	6/6	0.87	0.14	30,43,44,50	0
5	DMS	A	513	4/4	0.88	0.17	36,51,53,61	0
3	GOL	A	503	6/6	0.88	0.16	38,56,57,65	0
3	GOL	C	509	6/6	0.88	0.13	34,47,49,51	0
3	GOL	A	507	6/6	0.89	0.15	32,51,58,63	0
2	WAA	C	501	36/36	0.92	0.11	25,31,56,58	0
2	WAA	A	501	36/36	0.92	0.10	23,29,42,44	0
4	COH	C	514[B]	43/43	0.97	0.07	16,17,20,21	43
4	COH	C	514[A]	43/43	0.97	0.07	16,18,19,20	43
4	COH	A	512[B]	43/43	0.98	0.06	17,19,20,21	43
4	COH	A	512[A]	43/43	0.98	0.06	17,18,20,20	43

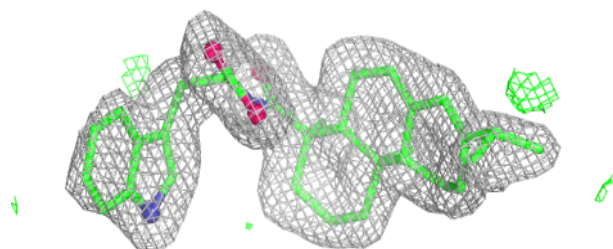
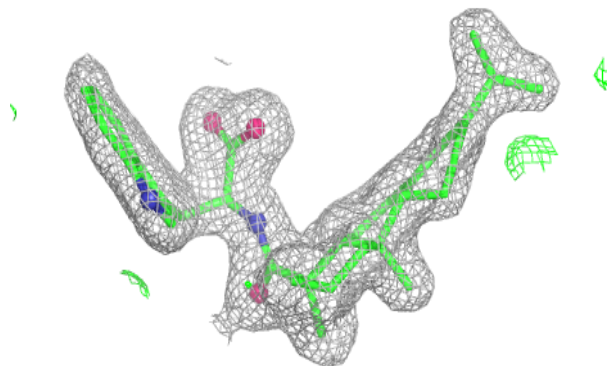
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WAA 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)

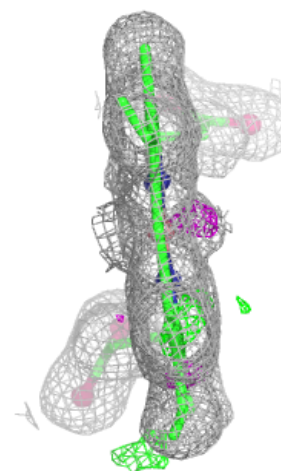
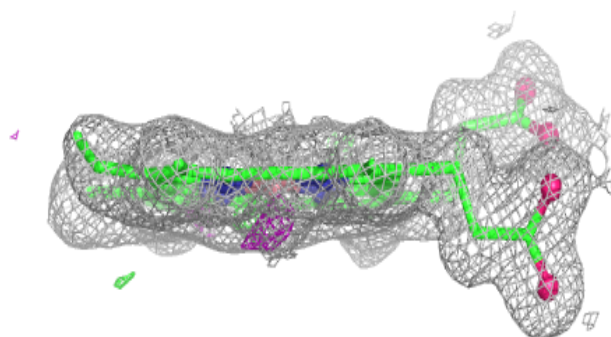
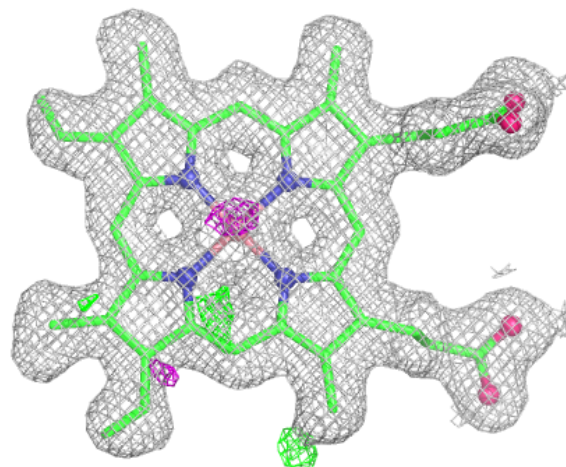
**Electron density around WAA A 501:**

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



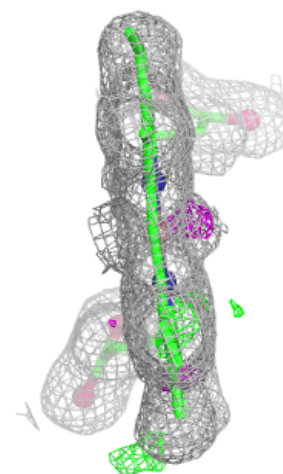
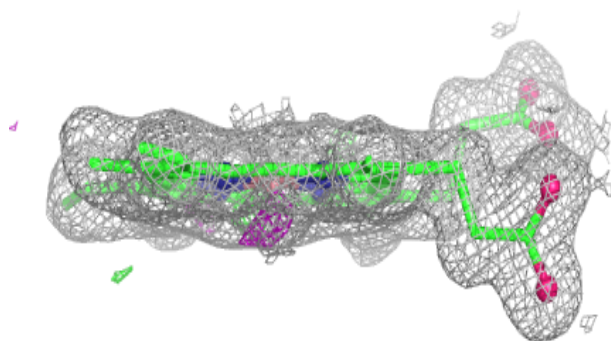
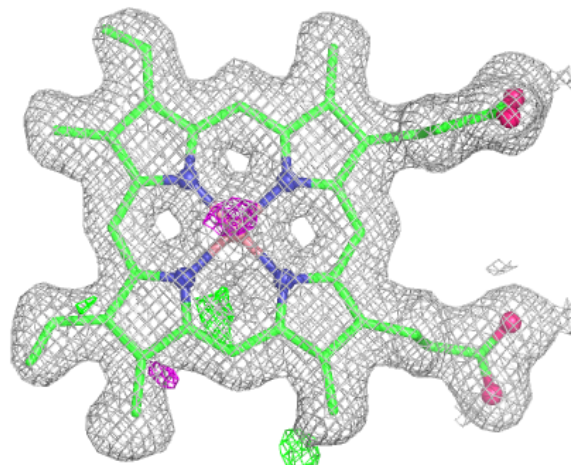
Electron density around COH C 514 (B):

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



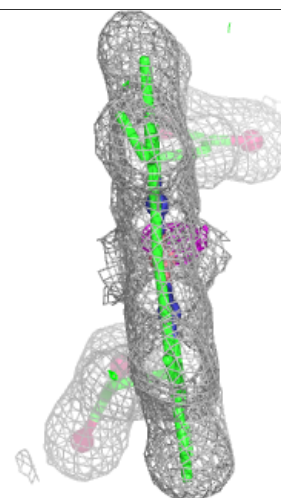
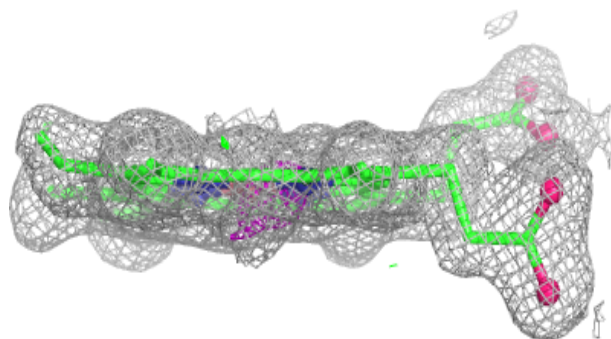
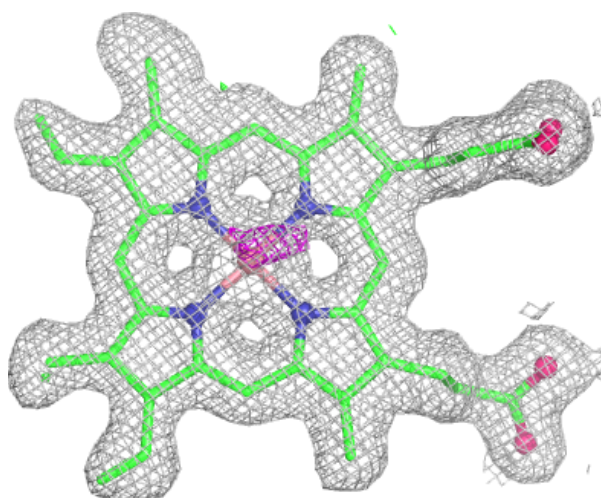
Electron density around COH C 514 (A):

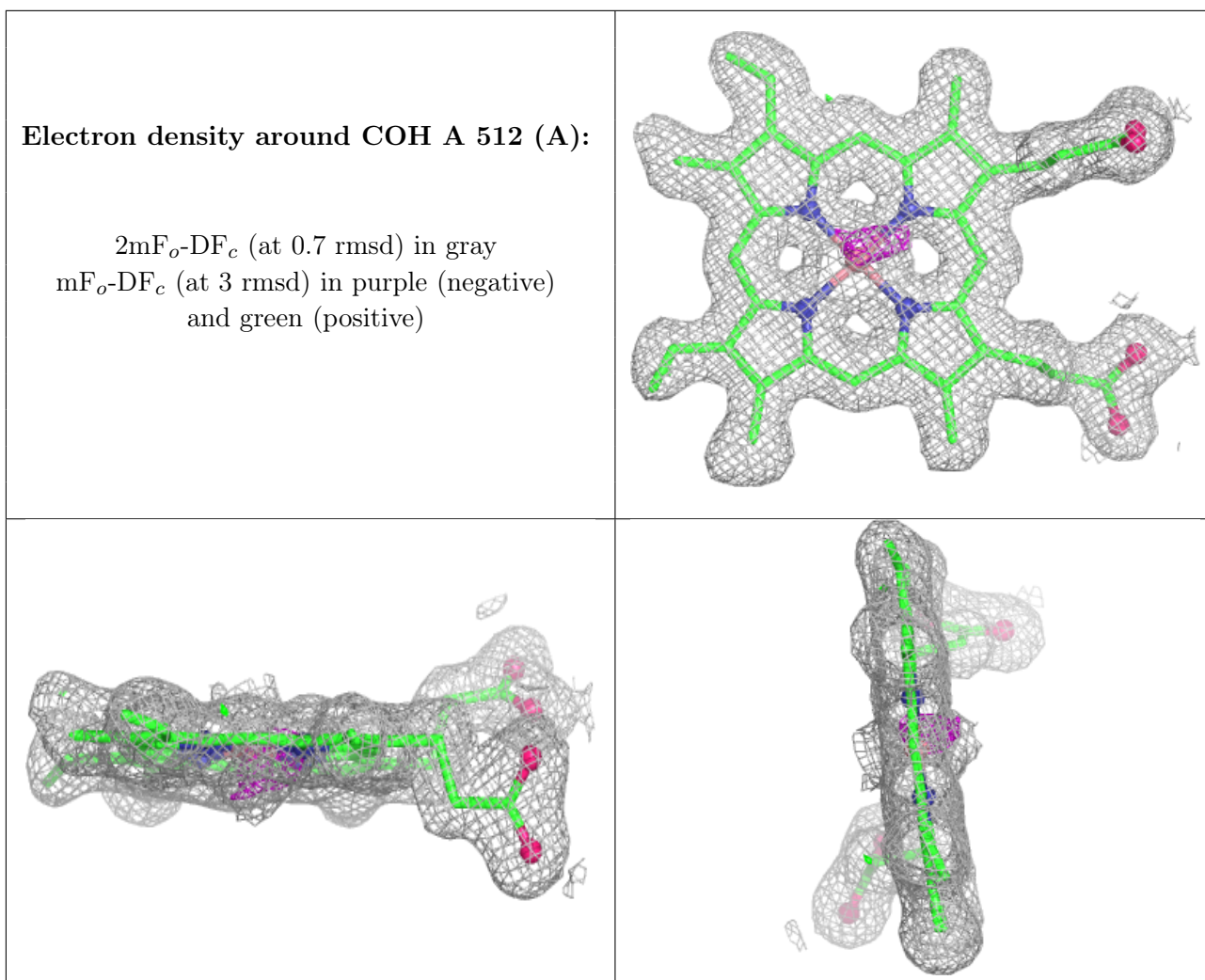
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COH A 512 (B):

$2mF_o-DF_c$ (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.