



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:26 am BST

PDB ID : 6K9S  
Title : Structure of the Carbonylruthenium Mesoporphyrin IX-Reconstituted CYP102A1 Haem Domain with N-Abietoyl-L-Tryptophan  
Authors : Stanfield, J.K.; Omura, K.; Kasai, C.; Sugimoto, H.; Shiro, Y.; Watanabe, Y.; Shoji, O.  
Deposited on : 2019-06-17  
Resolution : 1.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

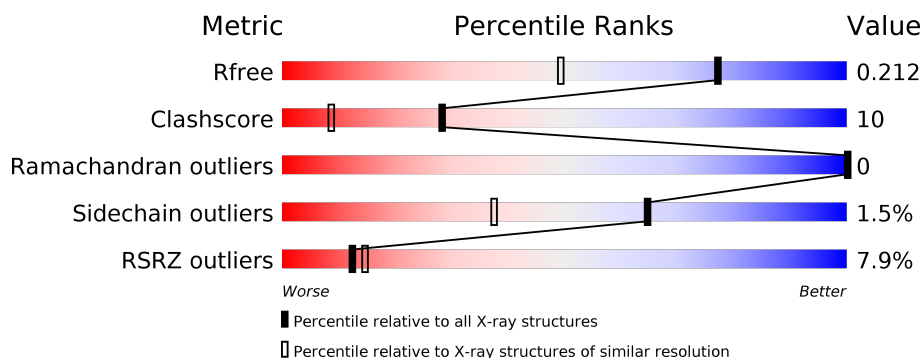
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	456	<div> <div>9%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	B	456	<div> <div>6%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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
4	GOL	B	503	-	-	X	-

## 2 Entry composition [i](#)

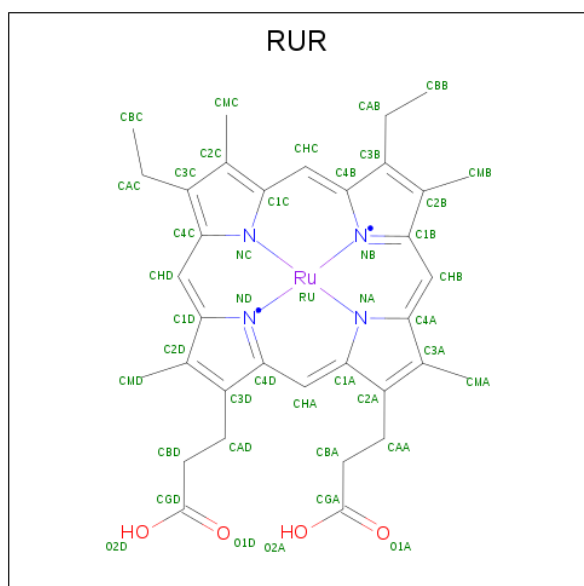
There are 6 unique types of molecules in this entry. The entry contains 8515 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

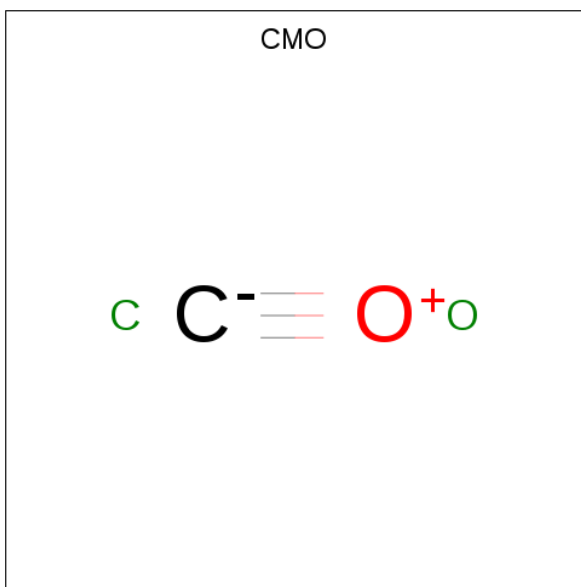
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	26	0
			3856	2456	653	725	22			
1	B	449	Total	C	N	O	S	0	26	0
			3843	2452	655	716	20			

- Molecule 2 is [3,3'-(7,12-diethyl-3,8,13,17-tetramethylporphyrin-2,18-diyl-kappa 4 N 2 1 ,N 22 ,N 23 ,N 24 )dipropanoato(2-)]ruthenium (three-letter code: RUR) (formula: C<sub>34</sub>H<sub>36</sub>N<sub>4</sub>O<sub>4</sub>Ru) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Ru	0	0
			43	34	4	4	1		
2	B	1	Total	C	N	O	Ru	0	0
			43	34	4	4	1		

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		
3	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



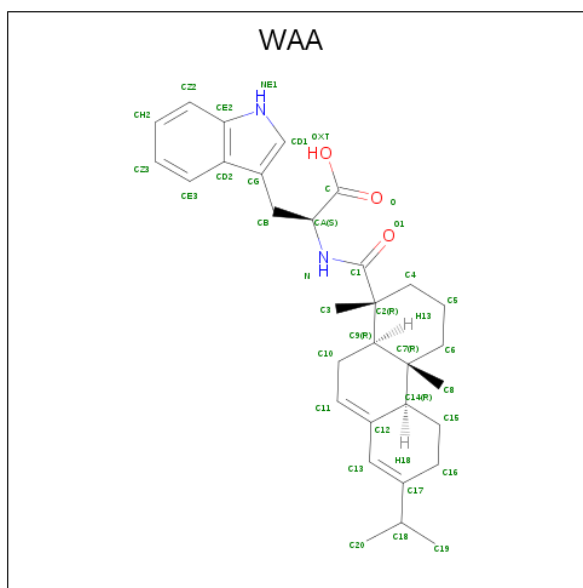
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 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 (three-letter code: WAA) (formula: C<sub>31</sub>H<sub>40</sub>N<sub>2</sub>O<sub>3</sub>).



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

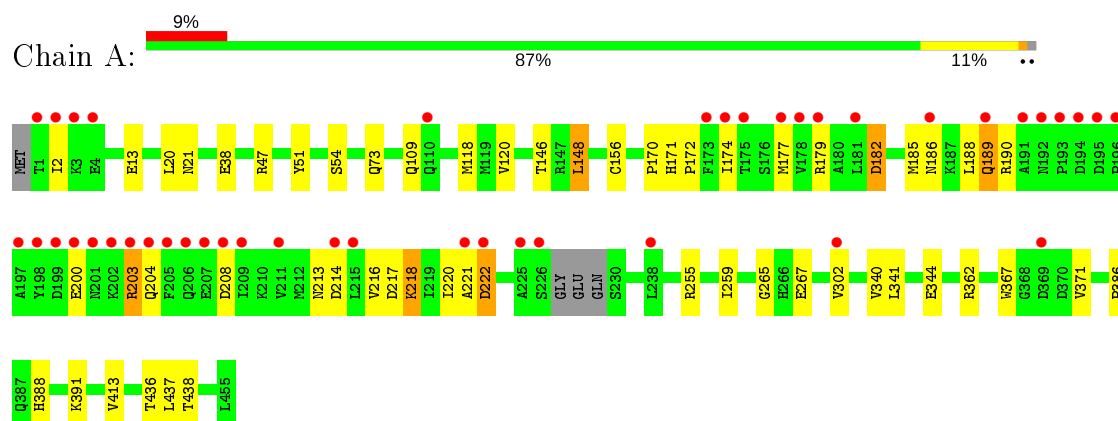
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	255	Total 255	O 255	0	0
6	B	309	Total 309	O 309	0	0

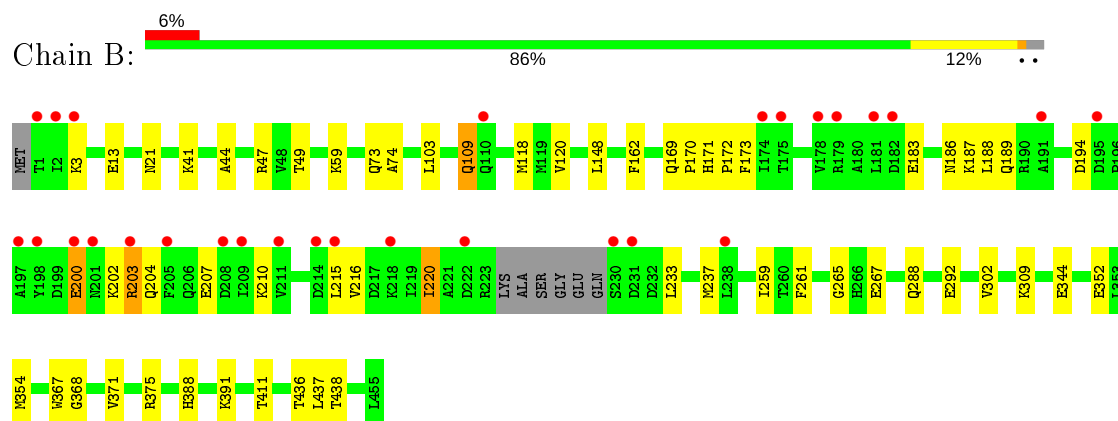
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.12Å 128.56Å 149.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.49 – 1.55 46.45 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.49-1.55) 99.9 (46.45-1.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.167 , 0.205 0.178 , 0.212	Depositor DCC
$R_{free}$ test set	8259 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, GOL, RUR, WAA

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	0.69	0/3940	0.77	0/5319
1	B	0.68	0/3931	0.78	0/5306
All	All	0.68	0/7871	0.77	0/10625

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	3856	0	3811	72	0
1	B	3843	0	3812	81	0
2	A	43	0	34	1	0
2	B	43	0	34	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	42	0	56	1	0
4	B	48	0	64	6	0
5	A	36	0	0	20	0
5	B	36	0	0	18	0
6	A	255	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	309	0	0	6	0
All	All	8515	0	7811	155	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 10.

All (155) 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:A:437:LEU:HB3	5:A:509:WAA:C16	1.84	1.07
1:B:233:LEU:HD21	1:B:261[A]:PHE:CD2	1.93	1.02
1:B:437:LEU:HB3	5:B:510:WAA:C15	1.93	0.99
1:A:437:LEU:HB3	5:A:509:WAA:C15	1.93	0.98
1:B:49:THR:HG21	1:B:354[A]:MET:HG2	1.44	0.97
1:B:437:LEU:HB3	5:B:510:WAA:C16	1.95	0.96
1:B:292[B]:GLU:HG2	6:B:749:HOH:O	1.70	0.90
1:B:73:GLN:N	5:B:510:WAA:OXT	2.06	0.88
1:A:185[A]:MET:CE	1:A:437:LEU:H	1.86	0.88
1:A:118[A]:MET:HE2	6:A:615:HOH:O	1.74	0.88
1:A:185[A]:MET:HE3	1:A:437:LEU:H	1.38	0.87
1:A:386:PRO:HB3	4:A:506:GOL:H11	1.56	0.86
1:B:109:GLN:HA	1:B:109:GLN:OE1	1.77	0.84
1:B:375[B]:ARG:HG3	6:B:767:HOH:O	1.81	0.81
1:A:73:GLN:N	5:A:509:WAA:OXT	2.15	0.78
1:B:375[B]:ARG:CG	6:B:767:HOH:O	2.30	0.77
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.18	0.77
1:B:49:THR:CG2	1:B:354[A]:MET:HG2	2.16	0.76
1:A:267:GLU:HG2	1:A:438[B]:THR:HG21	1.69	0.72
1:A:47:ARG:CD	5:A:509:WAA:CZ3	2.67	0.72
1:B:233:LEU:HD21	1:B:261[A]:PHE:CE2	2.24	0.72
1:B:216:VAL:O	1:B:220[B]:ILE:HG23	1.90	0.72
1:B:220[B]:ILE:HD12	1:B:220[B]:ILE:C	2.10	0.71
1:B:237:MET:CE	1:B:261[A]:PHE:CE2	2.74	0.71
1:A:185[A]:MET:HE3	1:A:437:LEU:N	2.07	0.69
1:B:173:PHE:CD1	1:B:215[B]:LEU:HD23	2.27	0.69
1:A:185[A]:MET:CE	6:A:702:HOH:O	2.41	0.68
1:B:411:THR:HG21	4:B:503:GOL:H2	1.75	0.67
1:A:437:LEU:CB	5:A:509:WAA:C15	2.70	0.67
1:A:218:LYS:HE2	1:A:222:ASP:OD1	1.94	0.67
1:B:437:LEU:CB	5:B:510:WAA:C15	2.71	0.67
1:B:215[A]:LEU:O	1:B:215[A]:LEU:HD22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HE2	1:B:344:GLU:CD	2.15	0.66
1:A:182[A]:ASP:O	1:A:186[A]:ASN:ND2	2.29	0.65
1:B:73:GLN:HB2	5:B:510:WAA:CE3	2.25	0.65
1:A:47:ARG:HD3	5:A:509:WAA:CZ3	2.28	0.63
1:B:188:LEU:HB3	5:B:510:WAA:NE1	2.12	0.63
1:B:162:PHE:CE1	1:B:215[B]:LEU:HD21	2.33	0.63
1:A:47:ARG:CZ	5:A:509:WAA:CD2	2.77	0.63
1:B:49:THR:HG21	1:B:354[A]:MET:CG	2.23	0.62
1:B:59[B]:LYS:NZ	6:B:602:HOH:O	2.32	0.62
1:B:237:MET:HE2	1:B:261[A]:PHE:CE2	2.34	0.62
1:A:177:MET:HE1	6:A:739:HOH:O	1.99	0.61
1:B:216:VAL:O	1:B:220[A]:ILE:HG22	2.00	0.61
1:B:288:GLN:O	1:B:292[B]:GLU:HG3	2.01	0.61
1:B:388:HIS:HA	1:B:391[A]:LYS:HD3	1.82	0.61
1:A:186[B]:ASN:HD22	1:A:190:ARG:HH21	1.48	0.60
1:A:185[A]:MET:HE1	1:A:437:LEU:H	1.66	0.60
1:B:162:PHE:HE1	1:B:215[B]:LEU:HD21	1.66	0.60
1:A:73:GLN:HB2	5:A:509:WAA:CE3	2.33	0.59
1:A:185[A]:MET:HE2	6:A:702:HOH:O	2.02	0.59
1:B:109:GLN:CA	1:B:109:GLN:OE1	2.50	0.59
1:A:47:ARG:CZ	5:A:509:WAA:CE3	2.81	0.58
1:A:214:ASP:O	1:A:217:ASP:OD1	2.21	0.57
1:B:103:LEU:HD13	1:B:261[A]:PHE:HZ	1.70	0.57
1:A:185[A]:MET:HE1	6:A:702:HOH:O	2.01	0.57
1:B:267:GLU:HG2	1:B:438[B]:THR:HG21	1.87	0.56
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.87	0.56
1:B:188:LEU:HD13	5:B:510:WAA:C4	2.36	0.56
1:B:13:GLU:CD	1:B:13:GLU:H	2.08	0.56
1:B:267:GLU:CG	1:B:438[B]:THR:HG21	2.36	0.56
1:B:216:VAL:HG21	1:B:259:ILE:HG13	1.87	0.56
1:B:47:ARG:HD3	5:B:510:WAA:CZ3	2.35	0.56
1:A:216:VAL:HG21	1:A:259:ILE:HG13	1.88	0.55
1:A:217:ASP:HB3	1:A:255[A]:ARG:HH12	1.71	0.55
1:B:237:MET:CE	1:B:261[A]:PHE:CD2	2.89	0.55
1:A:118[A]:MET:HE1	6:A:686:HOH:O	2.05	0.55
1:A:2:ILE:HA	1:A:344:GLU:O	2.06	0.55
1:A:213:ASN:OD1	1:A:255[A]:ARG:HD3	2.07	0.54
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.89	0.54
1:B:73:GLN:CB	5:B:510:WAA:CE3	2.85	0.54
1:B:309:LYS:HA	4:B:503:GOL:C3	2.37	0.54
1:A:38:GLU:HB2	1:A:54[B]:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:CD2	1:B:261[A]:PHE:CD2	2.81	0.54
1:A:218:LYS:CE	1:A:222:ASP:OD1	2.55	0.54
4:B:507:GOL:HO1	4:B:507:GOL:HO3	1.56	0.53
1:A:73:GLN:HG2	5:A:509:WAA:CZ3	2.38	0.53
1:A:118[A]:MET:HE3	1:A:156:CYS:HA	1.91	0.53
1:A:47:ARG:NE	5:A:509:WAA:CE3	2.73	0.52
1:A:51:TYR:OH	5:A:509:WAA:O1	2.22	0.52
1:A:220[B]:ILE:HG22	1:A:221:ALA:N	2.25	0.51
1:B:169:GLN:HG3	1:B:170:PRO:HD2	1.92	0.51
1:A:118[A]:MET:CE	6:A:686:HOH:O	2.58	0.51
1:B:237:MET:HE3	1:B:261[A]:PHE:CE2	2.46	0.51
1:A:20:LEU:CD1	5:A:509:WAA:CD1	2.89	0.51
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.92	0.51
1:A:47:ARG:NE	5:A:509:WAA:CZ3	2.75	0.50
1:B:237:MET:HE3	1:B:261[A]:PHE:CD2	2.47	0.50
1:B:74:ALA:N	5:B:510:WAA:O	2.36	0.50
1:A:146:THR:HG21	1:A:174[B]:ILE:HD12	1.94	0.50
1:A:73:GLN:HG2	5:A:509:WAA:CH2	2.42	0.49
1:A:188:LEU:O	5:A:509:WAA:CZ2	2.60	0.49
1:A:186[A]:ASN:O	1:A:189[A]:GLN:HG3	2.12	0.49
1:B:368:GLY:O	1:B:371:VAL:HG13	2.12	0.49
1:B:437:LEU:HD13	5:B:510:WAA:C16	2.42	0.49
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.95	0.49
1:B:220[B]:ILE:HD12	1:B:220[B]:ILE:O	2.12	0.49
1:A:179:ARG:NH1	1:A:204:GLN:OE1	2.45	0.49
1:A:188:LEU:HB3	5:A:509:WAA:NE1	2.28	0.49
1:A:73:GLN:CB	5:A:509:WAA:CE3	2.91	0.49
1:B:309:LYS:HA	4:B:503:GOL:H31	1.95	0.48
1:B:47:ARG:CZ	5:B:510:WAA:CD2	2.91	0.48
1:B:173:PHE:CD1	1:B:215[B]:LEU:CD2	2.96	0.48
1:A:20:LEU:CD1	5:A:509:WAA:NE1	2.77	0.48
1:B:47:ARG:CD	5:B:510:WAA:CZ3	2.91	0.48
1:B:216:VAL:O	1:B:220[A]:ILE:CG2	2.60	0.48
1:B:47:ARG:CD	5:B:510:WAA:CE3	2.92	0.47
1:A:171:HIS:CG	1:A:172:PRO:HD2	2.48	0.47
1:B:41:LYS:HB3	1:B:41:LYS:HE2	1.56	0.47
1:B:49:THR:HG23	1:B:352[B]:GLU:CD	2.35	0.47
1:B:73:GLN:HG2	5:B:510:WAA:CZ3	2.44	0.47
1:A:109:GLN:OE1	6:A:601:HOH:O	2.20	0.47
1:B:200:GLU:HA	1:B:203:ARG:HG2	1.97	0.47
1:B:204:GLN:NE2	1:B:207:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HE2	1:B:344:GLU:CG	2.44	0.46
1:B:216:VAL:HG21	1:B:259:ILE:CG1	2.45	0.46
1:A:203:ARG:CG	1:A:203:ARG:HH11	2.29	0.46
1:B:194:ASP:HA	1:B:202:LYS:NZ	2.30	0.46
1:A:436:THR:OG1	1:A:438[B]:THR:HG23	2.16	0.46
1:A:267:GLU:CG	1:A:438[B]:THR:HG21	2.42	0.46
1:B:47:ARG:NE	5:B:510:WAA:CE3	2.79	0.46
1:A:203:ARG:NH1	1:A:203:ARG:HG2	2.31	0.45
1:A:47:ARG:CD	5:A:509:WAA:CE3	2.94	0.45
1:B:186[B]:ASN:O	1:B:189:GLN:HG2	2.17	0.45
1:A:216:VAL:HG21	1:A:259:ILE:CG1	2.46	0.45
1:A:265:GLY:HA2	2:A:501:RUR:C2C	2.47	0.45
1:A:200:GLU:HA	1:A:200:GLU:OE1	2.17	0.44
1:A:220[B]:ILE:CG2	1:A:221:ALA:N	2.79	0.44
1:B:118[A]:MET:HB2	1:B:118[A]:MET:HE3	1.73	0.44
1:B:309:LYS:HA	4:B:503:GOL:H32	2.00	0.44
1:A:186[B]:ASN:ND2	1:A:190:ARG:HH21	2.14	0.44
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.99	0.44
1:A:367:TRP:HB2	1:A:371:VAL:HG23	1.99	0.43
1:B:265:GLY:HA2	2:B:501:RUR:C2C	2.47	0.43
1:B:3:LYS:CE	1:B:344:GLU:CD	2.84	0.43
1:A:21:ASN:CG	1:A:189[B]:GLN:HE21	2.22	0.43
1:B:437:LEU:HD22	5:B:510:WAA:C15	2.48	0.43
1:B:436:THR:OG1	1:B:438[B]:THR:HG23	2.18	0.43
1:B:233:LEU:HD11	1:B:261[A]:PHE:CE2	2.54	0.43
1:B:194:ASP:HA	1:B:202:LYS:HZ1	1.83	0.43
1:A:13[A]:GLU:CD	1:A:13[A]:GLU:H	2.22	0.43
1:B:44:ALA:HB3	1:B:47:ARG:HG2	2.01	0.43
1:A:340[B]:VAL:CG2	1:A:340[B]:VAL:O	2.67	0.42
1:B:171:HIS:CG	1:B:172:PRO:HD2	2.54	0.42
1:B:220[B]:ILE:CD1	1:B:220[B]:ILE:C	2.80	0.42
4:B:509:GOL:H12	6:B:726:HOH:O	2.19	0.42
1:A:362:ARG:HA	1:A:371:VAL:CG2	2.50	0.42
1:B:21:ASN:CG	1:B:189:GLN:NE2	2.73	0.42
1:A:170:PRO:HB3	1:A:174[B]:ILE:CD1	2.49	0.41
1:A:362:ARG:HA	1:A:371:VAL:HG21	2.02	0.41
1:A:170:PRO:HB3	1:A:174[B]:ILE:HG12	2.03	0.41
1:B:73:GLN:HG2	5:B:510:WAA:CH2	2.50	0.41
1:A:341[B]:LEU:HD23	1:A:341[B]:LEU:HA	1.82	0.40
1:B:183:GLU:OE2	1:B:187:LYS:HE3	2.21	0.40
1:B:118[A]:MET:CE	6:B:634:HOH:O	2.70	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	474/456 (104%)	457 (96%)	17 (4%)	0	100	100
1	B	471/456 (103%)	459 (98%)	12 (2%)	0	100	100
All	All	945/912 (104%)	916 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/400 (106%)	415 (98%)	8 (2%)	57	28
1	B	421/400 (105%)	413 (98%)	8 (2%)	57	28
All	All	844/800 (106%)	828 (98%)	16 (2%)	65	28

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	182[A]	ASP
1	A	182[B]	ASP
1	A	189[A]	GLN
1	A	189[B]	GLN

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Mol	Chain	Res	Type
1	A	203	ARG
1	A	218	LYS
1	A	222	ASP
1	B	109	GLN
1	B	148	LEU
1	B	200	GLU
1	B	203	ARG
1	B	210[A]	LYS
1	B	210[B]	LYS
1	B	220[A]	ILE
1	B	220[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	503	-	5,5,5	0.14	0	5,5,5	0.29	0
4	GOL	A	503	-	5,5,5	0.14	0	5,5,5	0.34	0
3	CMO	B	502	-	0,1,1	0.00	-	-		
4	GOL	B	507	-	5,5,5	0.13	0	5,5,5	0.25	0
4	GOL	A	507	-	5,5,5	0.14	0	5,5,5	0.33	0
4	GOL	B	508[A]	-	5,5,5	0.12	0	5,5,5	0.34	0
4	GOL	A	508[A]	-	5,5,5	0.12	0	5,5,5	0.33	0
4	GOL	A	508[B]	-	5,5,5	0.12	0	5,5,5	0.32	0
4	GOL	A	504	-	5,5,5	0.10	0	5,5,5	0.25	0
2	RUR	B	501	1	32,50,50	2.04	13 (40%)	18,82,82	1.87	4 (22%)
2	RUR	A	501	1,3	32,50,50	2.08	12 (37%)	18,82,82	2.09	6 (33%)
4	GOL	B	508[B]	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	B	509	-	5,5,5	0.11	0	5,5,5	0.37	0
4	GOL	A	505	-	5,5,5	0.12	0	5,5,5	0.40	0
5	WAA	A	509	-	36,40,40	0.98	2 (5%)	41,61,61	1.52	6 (14%)
4	GOL	A	506	-	5,5,5	0.17	0	5,5,5	0.41	0
4	GOL	B	506	-	5,5,5	0.18	0	5,5,5	0.50	0
5	WAA	B	510	-	36,40,40	0.94	3 (8%)	41,61,61	1.48	6 (14%)
4	GOL	B	504	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	B	505	-	5,5,5	0.12	0	5,5,5	0.31	0
3	CMO	A	502	2	0,1,1	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	A	503	-	-	1/4/4/4	-
4	GOL	B	507	-	-	2/4/4/4	-
4	GOL	A	507	-	-	4/4/4/4	-
4	GOL	B	508[A]	-	-	0/4/4/4	-
4	GOL	A	508[A]	-	-	0/4/4/4	-
4	GOL	A	508[B]	-	-	0/4/4/4	-
4	GOL	A	504	-	-	1/4/4/4	-
2	RUR	B	501	1	-	1/10/54/54	-
2	RUR	A	501	1,3	-	0/10/54/54	-
4	GOL	B	508[B]	-	-	0/4/4/4	-
4	GOL	B	509	-	-	2/4/4/4	-
4	GOL	A	505	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	WAA	A	509	-	-	7/17/66/66	0/5/5/5
4	GOL	A	506	-	-	3/4/4/4	-
4	GOL	B	506	-	-	4/4/4/4	-
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	B	505	-	-	4/4/4/4	-
5	WAA	B	510	-	-	6/17/66/66	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	RUR	C1B-NB	-4.51	1.31	1.36
2	A	501	RUR	C4B-NB	-4.31	1.31	1.37
2	B	501	RUR	C1D-ND	-4.21	1.31	1.37
2	B	501	RUR	C4B-NB	-4.00	1.31	1.37
2	A	501	RUR	C1B-NB	-3.98	1.32	1.36
2	A	501	RUR	C1C-NC	-3.94	1.32	1.36
2	A	501	RUR	C1D-ND	-3.66	1.31	1.37
2	A	501	RUR	C4C-NC	-3.47	1.32	1.36
2	A	501	RUR	C4A-NA	3.11	1.41	1.37
2	B	501	RUR	C2A-C3A	3.00	1.46	1.37
2	B	501	RUR	C3C-C2C	2.97	1.46	1.37
2	A	501	RUR	C1A-C2A	2.78	1.48	1.42
2	A	501	RUR	C3C-C2C	2.77	1.45	1.37
2	B	501	RUR	C4A-NA	2.74	1.40	1.37
2	B	501	RUR	C3B-C2B	2.72	1.45	1.37
2	B	501	RUR	C4C-NC	-2.52	1.33	1.36
2	A	501	RUR	C3B-C2B	2.49	1.45	1.37
2	B	501	RUR	C1C-NC	-2.47	1.33	1.36
2	A	501	RUR	C2A-C3A	2.45	1.44	1.37
5	A	509	WAA	C13-C12	2.40	1.50	1.44
2	A	501	RUR	C3D-C2D	2.36	1.44	1.37
2	B	501	RUR	C1A-C2A	2.30	1.47	1.42
2	B	501	RUR	C3D-C2D	2.26	1.44	1.37
5	B	510	WAA	C15-C14	-2.17	1.49	1.53
5	A	509	WAA	C7-C9	-2.17	1.53	1.56
5	B	510	WAA	CZ3-CE3	2.15	1.41	1.36
2	B	501	RUR	C4B-C3B	2.10	1.47	1.42
2	A	501	RUR	CAD-C3D	-2.09	1.49	1.52
2	B	501	RUR	C1D-C2D	2.03	1.47	1.42
5	B	510	WAA	C13-C12	2.02	1.49	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	RUR	C1C-C2C-C3C	-5.01	103.51	107.00
2	B	501	RUR	C1B-C2B-C3B	-4.70	103.72	107.00
5	A	509	WAA	CB-CA-N	4.65	117.45	109.01
5	B	510	WAA	CB-CA-N	4.62	117.41	109.01
2	A	501	RUR	C1B-C2B-C3B	-4.55	103.83	107.00
5	B	510	WAA	CB-CG-CD1	-3.96	123.08	127.97
5	A	509	WAA	CB-CG-CD1	-3.87	123.19	127.97
2	B	501	RUR	C1C-C2C-C3C	-3.62	104.48	107.00
5	A	509	WAA	C4-C2-C9	3.29	112.10	108.34
5	B	510	WAA	C4-C2-C9	2.98	111.75	108.34
5	B	510	WAA	CB-CG-CD2	2.75	130.53	126.25
5	A	509	WAA	O1-C1-N	-2.52	117.61	122.74
2	A	501	RUR	CBA-CAA-C2A	-2.50	107.86	112.48
5	A	509	WAA	CB-CG-CD2	2.48	130.11	126.25
2	A	501	RUR	CMC-C2C-C3C	2.31	129.29	124.94
2	B	501	RUR	CAD-CBD-CGD	-2.31	108.80	112.67
5	B	510	WAA	C6-C7-C14	2.12	112.37	109.18
2	B	501	RUR	CBA-CAA-C2A	-2.10	108.62	112.48
2	A	501	RUR	C3C-C4C-NC	-2.09	107.78	109.51
5	B	510	WAA	C15-C16-C17	-2.06	108.75	112.33
5	A	509	WAA	C6-C7-C14	2.05	112.27	109.18
2	A	501	RUR	CMA-C3A-C2A	2.01	128.74	124.94

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	C1-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
4	A	507	GOL	O1-C1-C2-C3
4	B	509	GOL	C1-C2-C3-O3
5	A	509	WAA	C13-C17-C18-C20
5	A	509	WAA	C16-C17-C18-C20
4	A	506	GOL	C1-C2-C3-O3
4	B	506	GOL	O1-C1-C2-O2
4	B	506	GOL	O1-C1-C2-C3
4	B	506	GOL	C1-C2-C3-O3
5	B	510	WAA	C13-C17-C18-C20
5	B	510	WAA	C16-C17-C18-C20
4	A	507	GOL	O1-C1-C2-O2
4	A	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	507	GOL	O1-C1-C2-C3
4	A	507	GOL	C1-C2-C3-O3
4	B	505	GOL	O1-C1-C2-C3
4	B	505	GOL	C1-C2-C3-O3
4	A	505	GOL	O1-C1-C2-C3
4	A	506	GOL	O2-C2-C3-O3
4	B	506	GOL	O2-C2-C3-O3
4	B	505	GOL	O1-C1-C2-O2
4	A	507	GOL	O2-C2-C3-O3
4	A	504	GOL	O1-C1-C2-O2
4	B	505	GOL	O2-C2-C3-O3
5	A	509	WAA	C13-C17-C18-C19
5	A	509	WAA	C16-C17-C18-C19
5	B	510	WAA	C13-C17-C18-C19
5	B	510	WAA	C16-C17-C18-C19
4	B	509	GOL	O2-C2-C3-O3
4	A	505	GOL	O1-C1-C2-O2
4	B	507	GOL	O1-C1-C2-O2
2	B	501	RUR	C2C-C3C-CAC-CBC
4	A	505	GOL	O2-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
5	A	509	WAA	O1-C1-C2-C3
5	A	509	WAA	O1-C1-C2-C9
5	A	509	WAA	N-C1-C2-C3
5	B	510	WAA	O1-C1-C2-C3
5	B	510	WAA	O1-C1-C2-C9





There are no ring outliers.

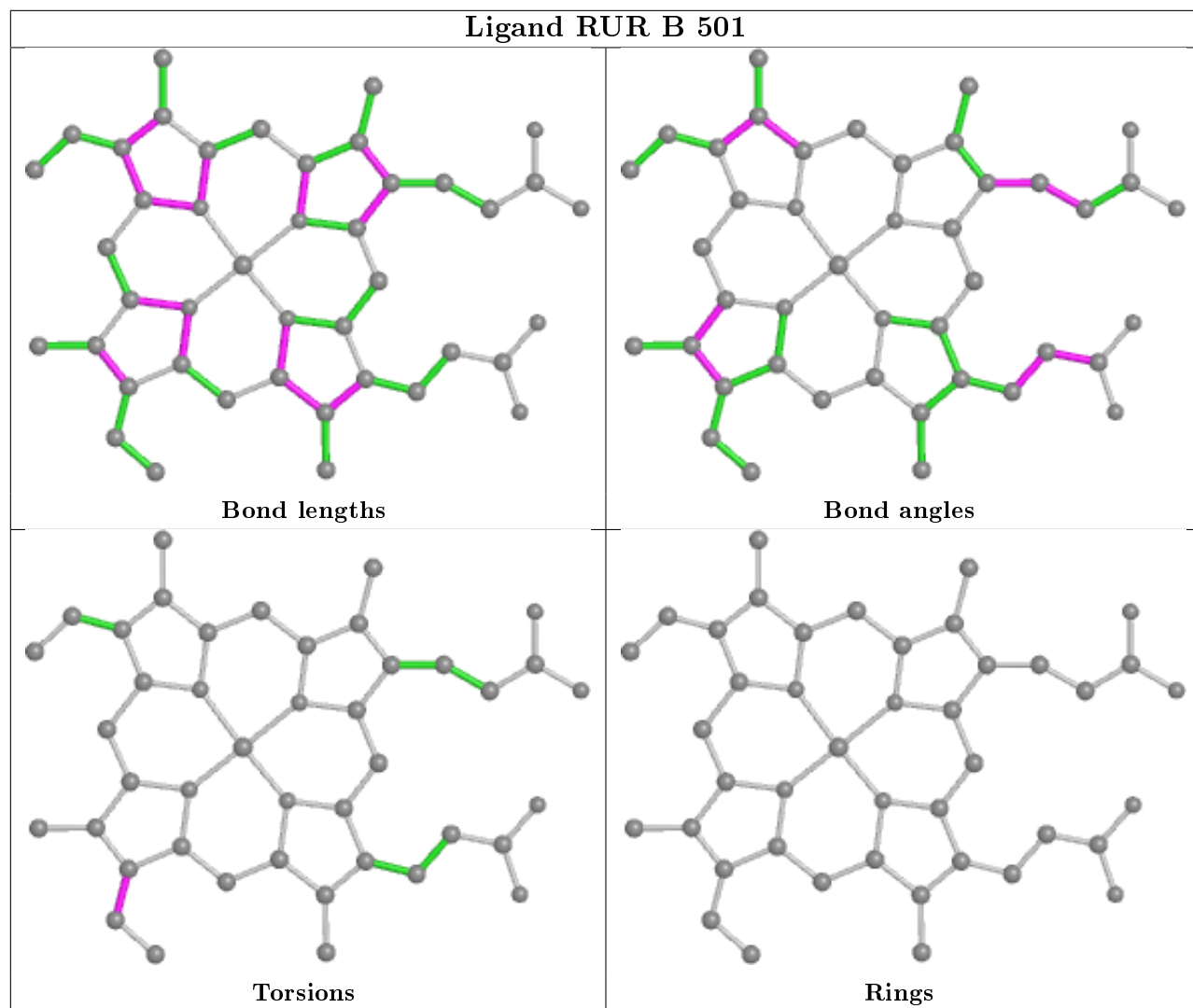
8 monomers are involved in 47 short contacts:

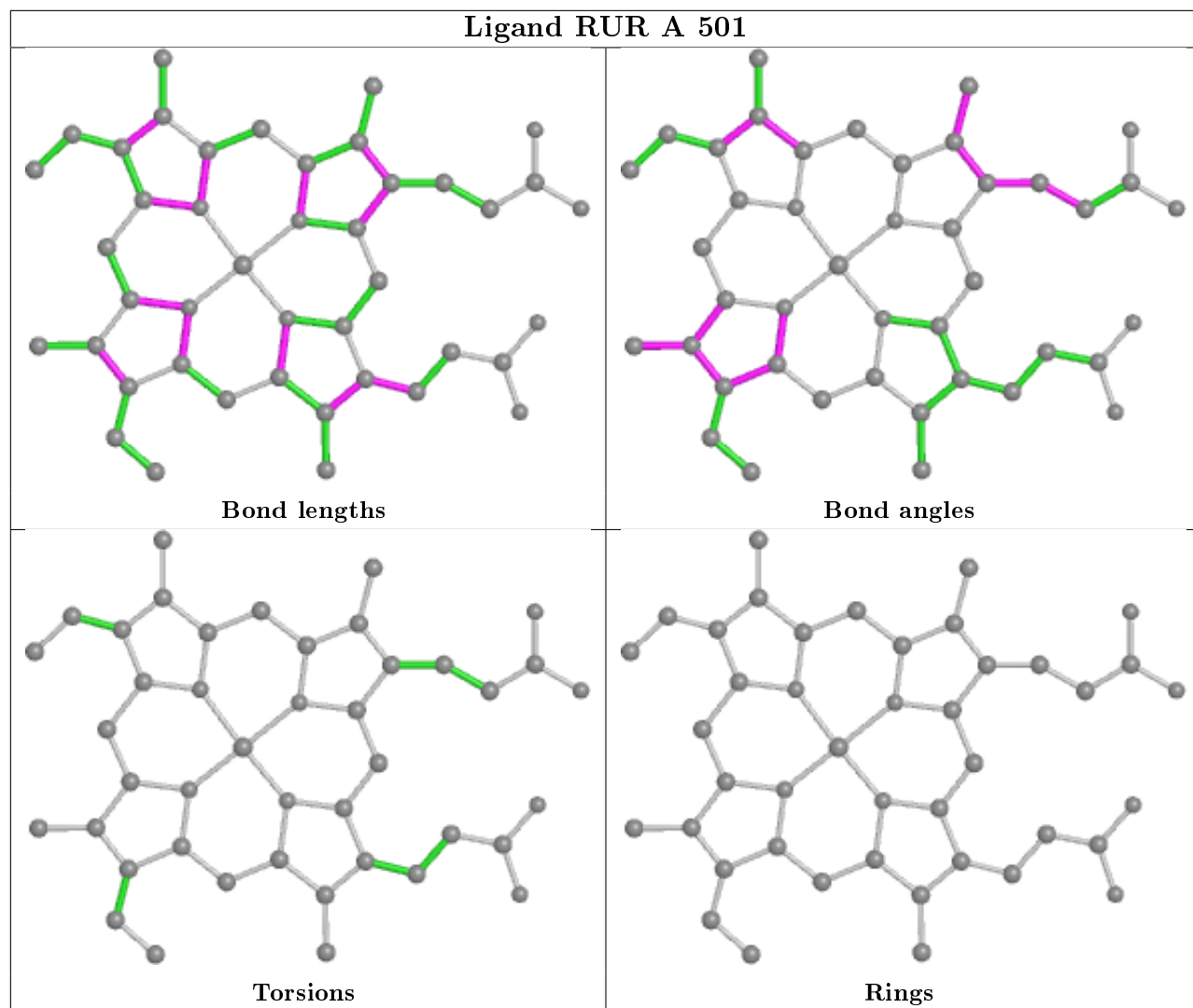
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	GOL	4	0
4	B	507	GOL	1	0
2	B	501	RUR	1	0
2	A	501	RUR	1	0
4	B	509	GOL	1	0
5	A	509	WAA	20	0
4	A	506	GOL	1	0
5	B	510	WAA	18	0

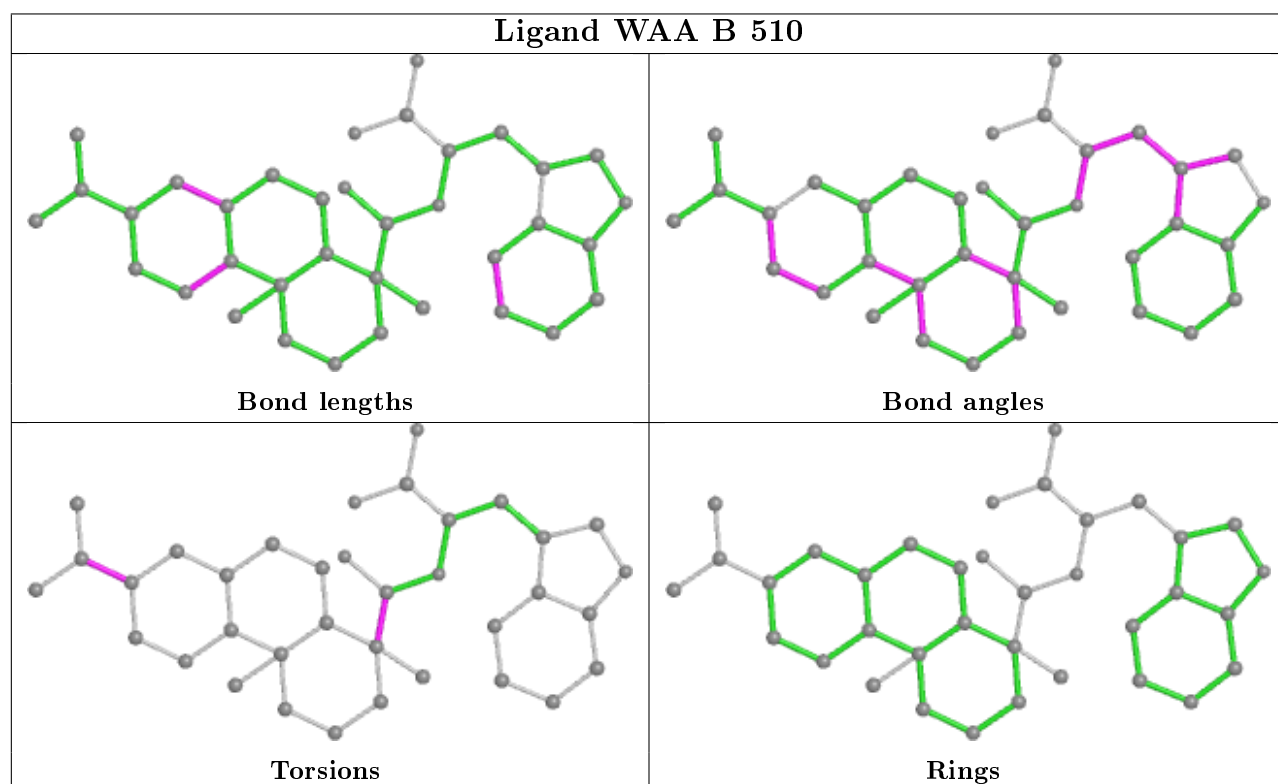
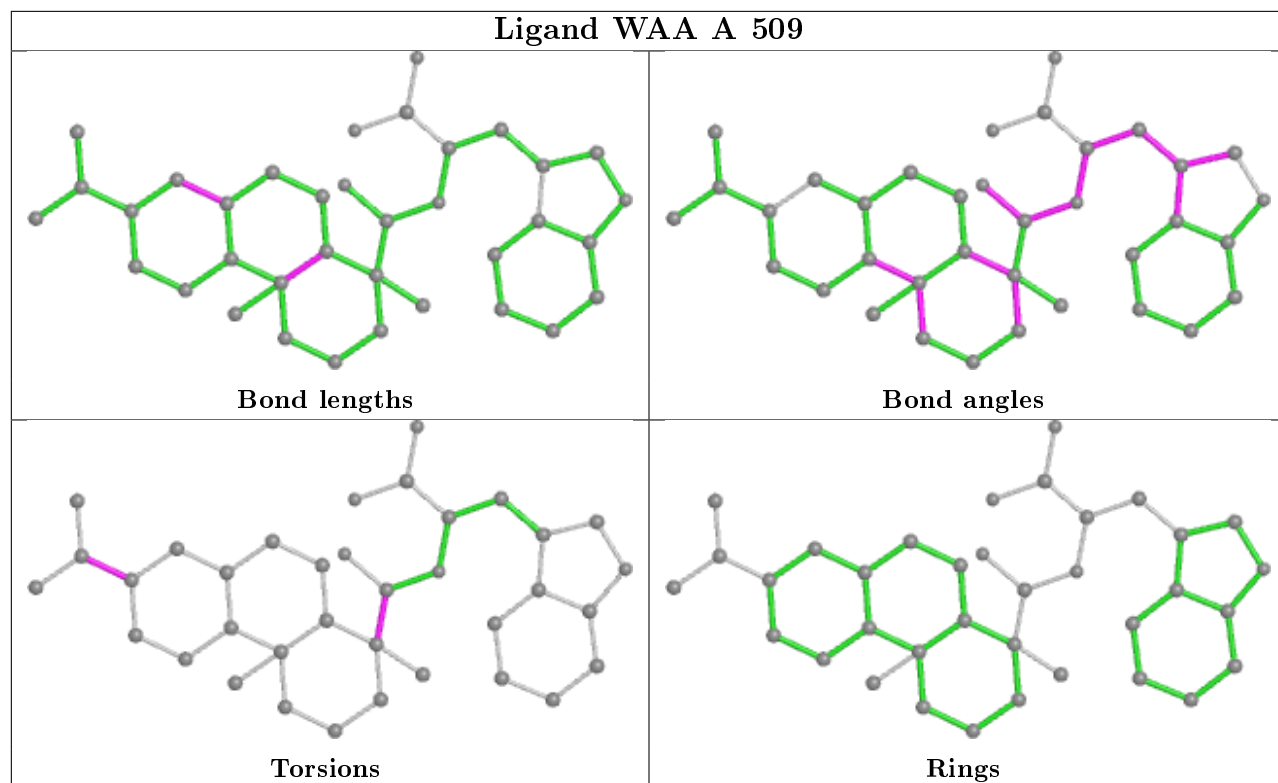
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 CMO B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings









Ligand CMO A 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	452/456 (99%)	0.23	43 (9%) 8 9	18, 29, 56, 84	0
1	B	449/456 (98%)	0.14	28 (6%) 20 24	18, 27, 49, 84	0
All	All	901/912 (98%)	0.18	71 (7%) 12 15	18, 28, 54, 84	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	11.6
1	B	1	THR	9.1
1	A	197	ALA	8.9
1	A	1	THR	8.2
1	B	2	ILE	7.7
1	B	215[A]	LEU	6.7
1	B	197	ALA	6.5
1	A	205	PHE	6.0
1	B	205	PHE	5.1
1	A	174[A]	ILE	4.9
1	A	191	ALA	4.8
1	A	198	TYR	4.8
1	A	215	LEU	4.6
1	A	211	VAL	4.6
1	A	192	ASN	4.3
1	B	222	ASP	4.2
1	B	211	VAL	3.9
1	A	178	VAL	3.8
1	A	195	ASP	3.8
1	B	198	TYR	3.7
1	B	214	ASP	3.7
1	B	181	LEU	3.6
1	B	231	ASP	3.6
1	B	200	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	175	THR	3.6
1	A	196	PRO	3.5
1	B	175	THR	3.5
1	A	200	GLU	3.4
1	A	226	SER	3.4
1	B	3	LYS	3.3
1	A	201	ASN	3.2
1	B	178	VAL	3.1
1	A	179	ARG	3.1
1	B	238	LEU	3.1
1	A	194	ASP	3.1
1	A	221	ALA	3.1
1	A	173	PHE	3.0
1	A	209	ILE	3.0
1	B	110	GLN	3.0
1	A	189[A]	GLN	2.9
1	A	225	ALA	2.9
1	A	208	ASP	2.9
1	A	199	ASP	2.9
1	A	3	LYS	2.8
1	A	204	GLN	2.8
1	A	214	ASP	2.8
1	B	218	LYS	2.8
1	A	203	ARG	2.8
1	A	222	ASP	2.8
1	A	206	GLN	2.7
1	A	181	LEU	2.6
1	A	238	LEU	2.6
1	B	209	ILE	2.6
1	A	4	GLU	2.5
1	A	193	PRO	2.4
1	B	195	ASP	2.4
1	B	174	ILE	2.4
1	B	201	ASN	2.4
1	A	369	ASP	2.4
1	B	179	ARG	2.4
1	B	208	ASP	2.3
1	B	191	ALA	2.3
1	A	302	VAL	2.3
1	B	203	ARG	2.2
1	A	207	GLU	2.2
1	A	177	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	186[A]	ASN	2.1
1	A	202[A]	LYS	2.1
1	B	182	ASP	2.0
1	B	230	SER	2.0
1	A	110	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

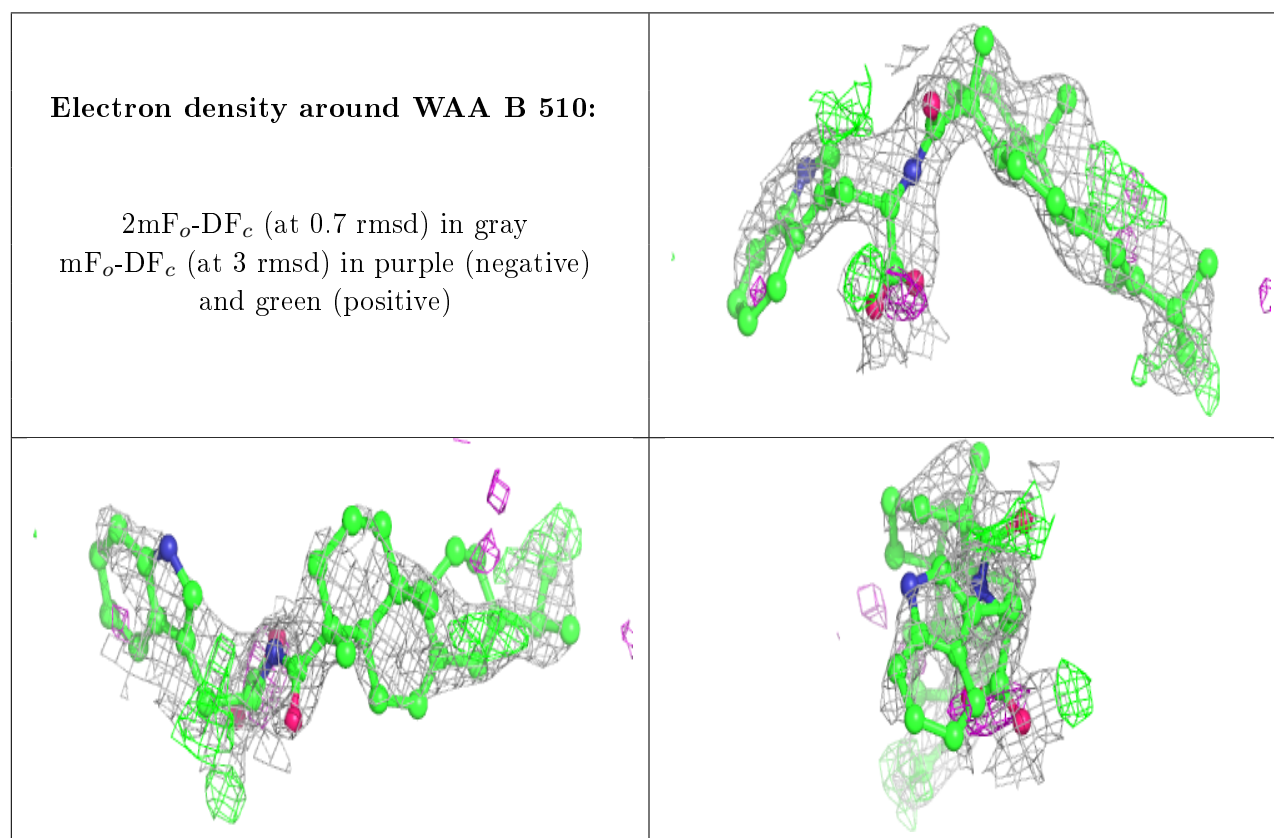
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	508[A]	6/6	0.55	0.23	35,47,51,53	6
4	GOL	B	508[B]	6/6	0.55	0.23	43,51,55,62	6
4	GOL	A	508[A]	6/6	0.71	0.21	45,57,63,63	6
4	GOL	A	508[B]	6/6	0.71	0.21	53,63,65,66	6
5	WAA	B	510	36/36	0.73	0.24	32,44,52,54	36
5	WAA	A	509	36/36	0.78	0.23	39,46,56,63	36
4	GOL	B	507	6/6	0.83	0.15	47,49,51,53	0
4	GOL	A	507	6/6	0.85	0.20	51,57,69,78	0
4	GOL	A	504	6/6	0.86	0.10	53,61,69,69	0
4	GOL	A	503	6/6	0.87	0.11	32,44,53,54	0
4	GOL	B	506	6/6	0.88	0.20	39,45,48,58	0
4	GOL	B	503	6/6	0.90	0.17	34,45,53,55	0
4	GOL	B	505	6/6	0.90	0.25	37,46,52,55	0
4	GOL	A	505	6/6	0.91	0.13	27,49,61,67	0
4	GOL	B	509	6/6	0.91	0.15	48,57,64,74	0
4	GOL	A	506	6/6	0.92	0.28	26,47,56,57	0
4	GOL	B	504	6/6	0.92	0.14	51,62,66,77	0
3	CMO	B	502	2/2	0.98	0.07	25,25,25,25	0

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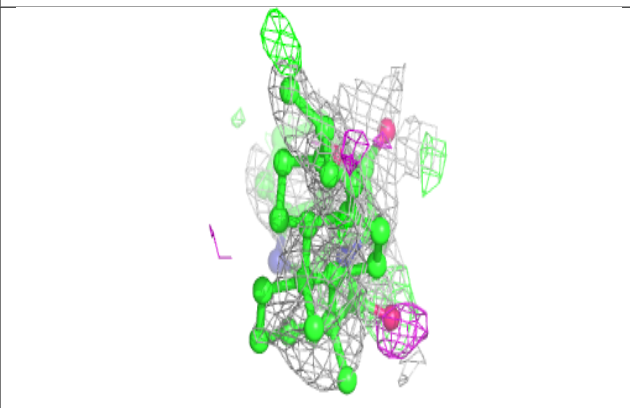
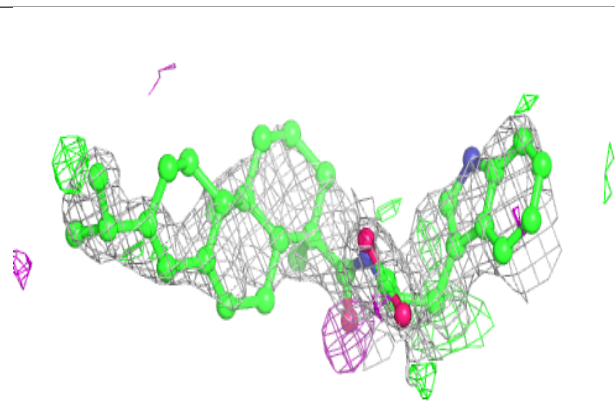
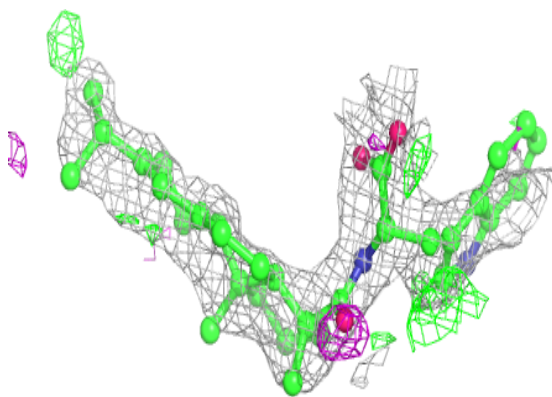
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RUR	B	501	43/43	0.99	0.07	17,20,22,33	0
3	CMO	A	502	2/2	0.99	0.08	18,18,18,24	0
2	RUR	A	501	43/43	1.00	0.09	16,18,22,29	0

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



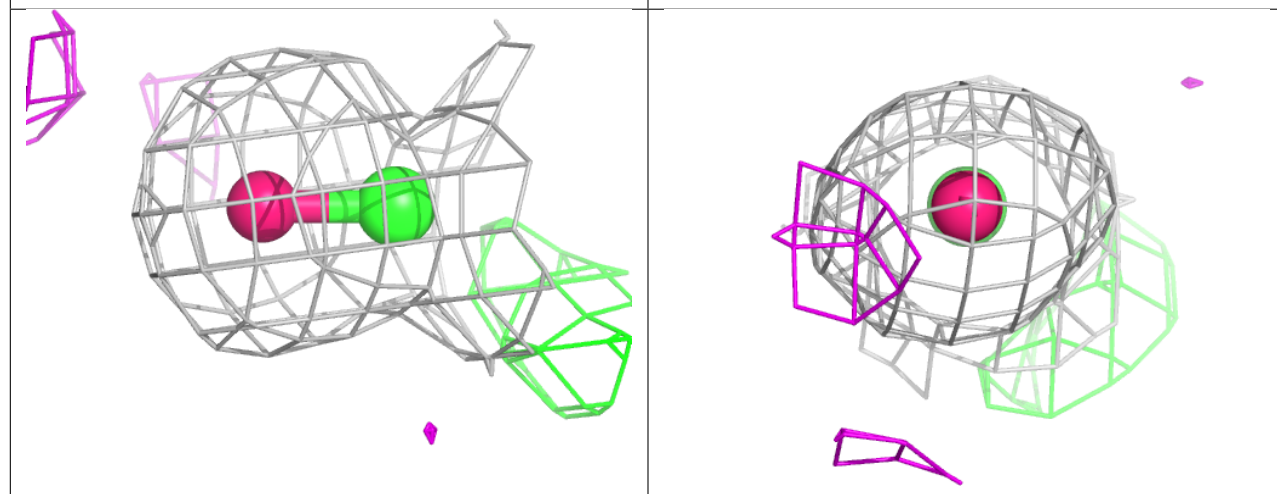
**Electron density around WAA A 509:**

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



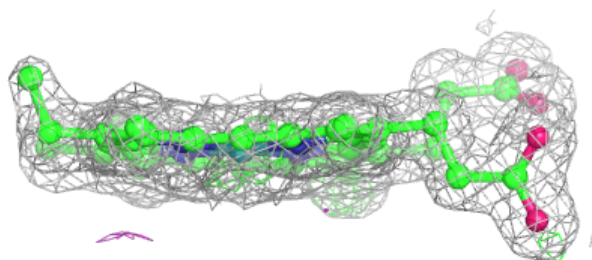
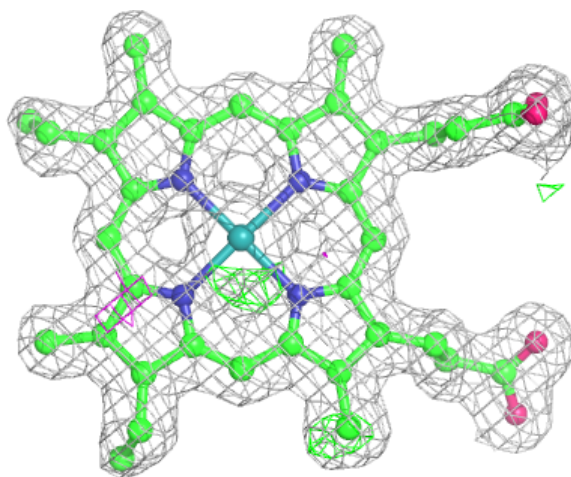
**Electron density around CMO B 502:**

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



**Electron density around RUR B 501:**

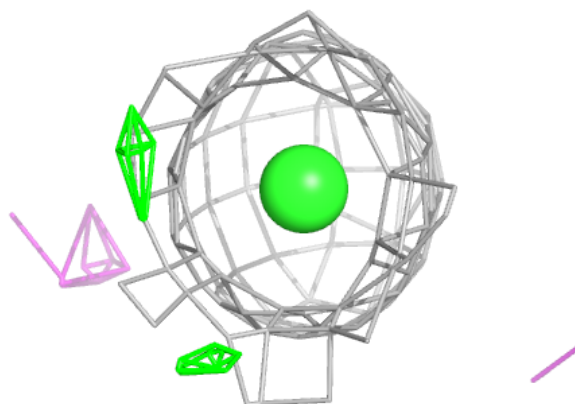
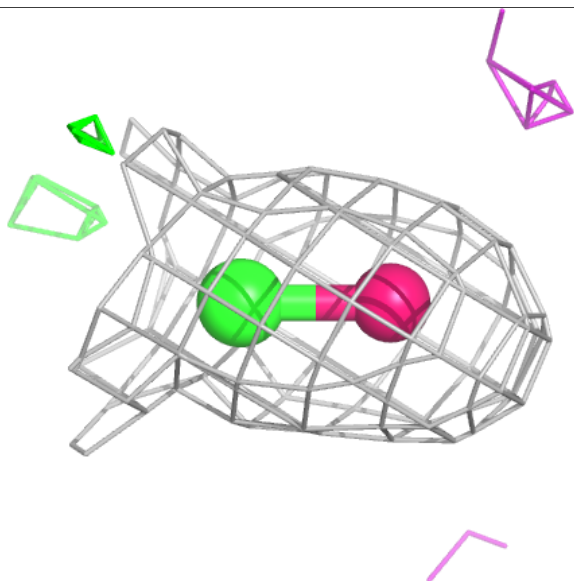
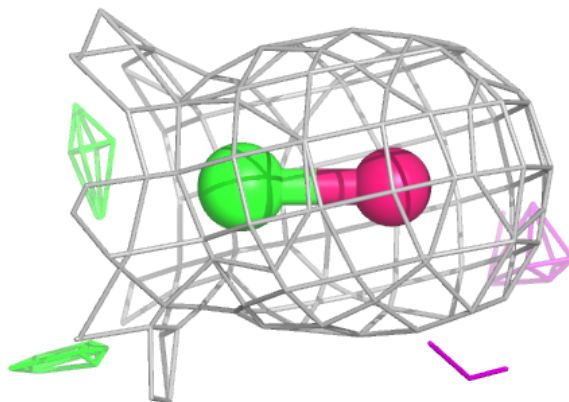
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





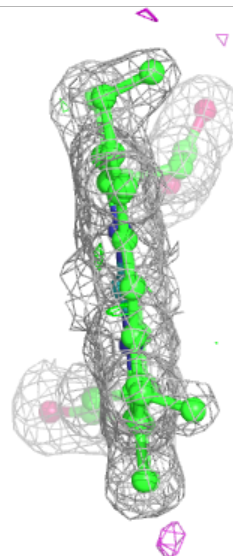
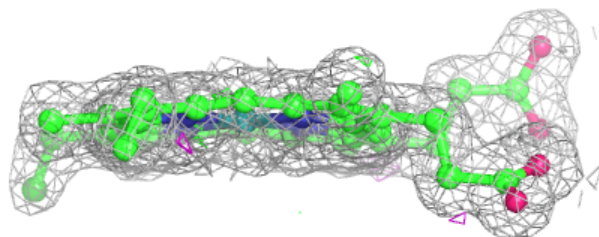
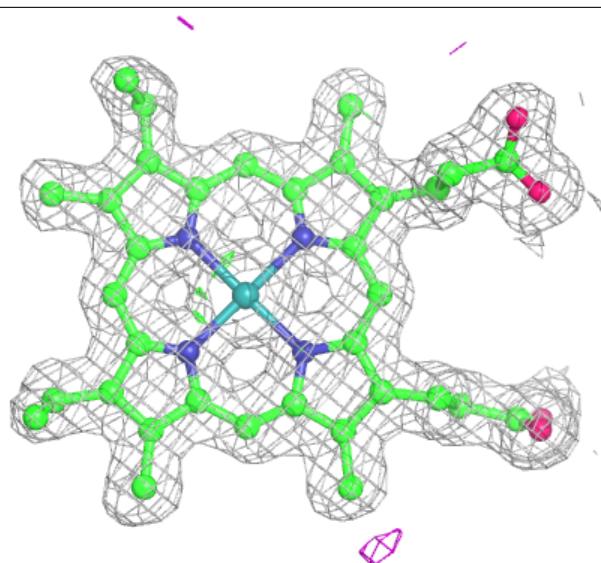
**Electron density around CMO A 502:**

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



**Electron density around RUR A 501:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.