



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 10:46 AM EDT

PDB ID : 1MZJ  
Title : Crystal Structure of the Priming beta-Ketosynthase from the R1128 Polyketide Biosynthetic Pathway  
Authors : Pan, H.; Tsai, S.C.; Meadows, E.S.; Miercke, L.J.W.; Keatinge-Clay, A.; O'Connell, J.; Khosla, C.; Stroud, R.M.  
Deposited on : 2002-10-08  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

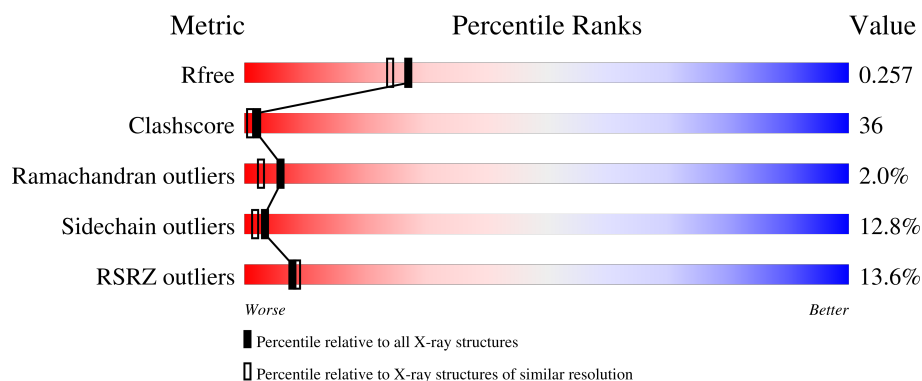
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	

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
2	COA	A	500	X	-	-	-
2	COA	B	501	X	-	X	-
3	ACE	A	502	-	-	X	-

## 2 Entry composition [i](#)

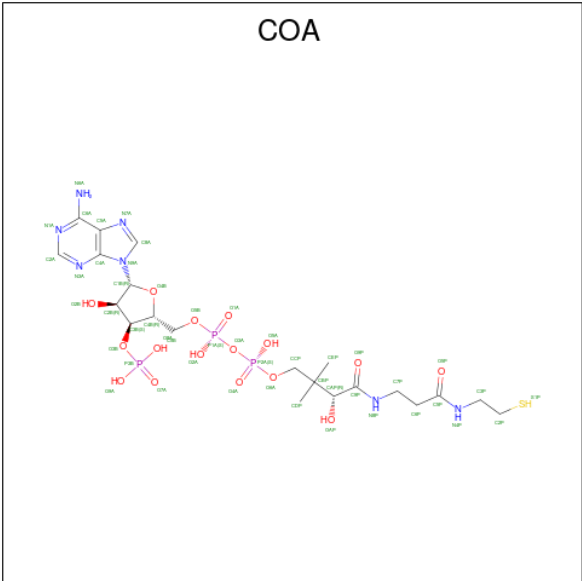
There are 4 unique types of molecules in this entry. The entry contains 5388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-ketoacylsynthase III.

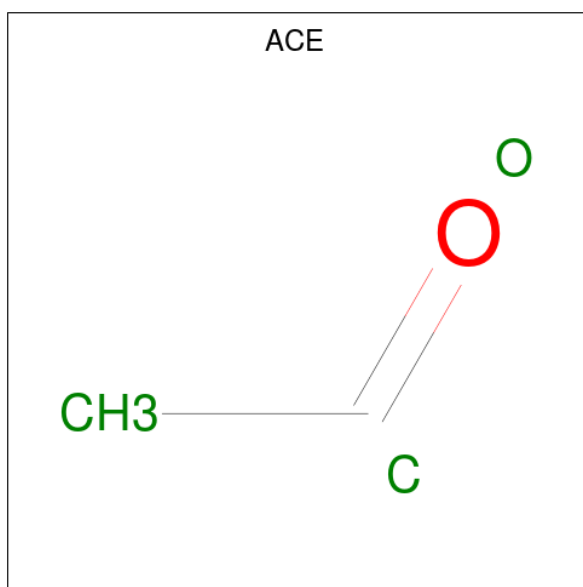
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2453	1530	443	471	9			
1	B	334	Total	C	N	O	S	0	0	0
			2454	1532	443	470	9			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	B	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

- Molecule 3 is ACETYL GROUP (three-letter code: ACE) (formula: C<sub>2</sub>H<sub>4</sub>O).



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

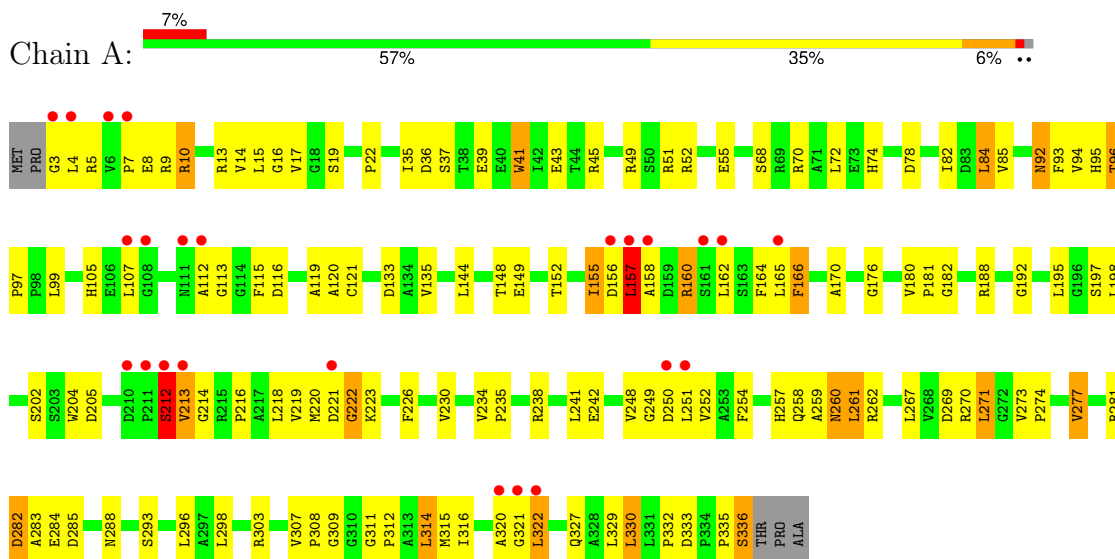
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	152	Total	O	0	0
			152	152		

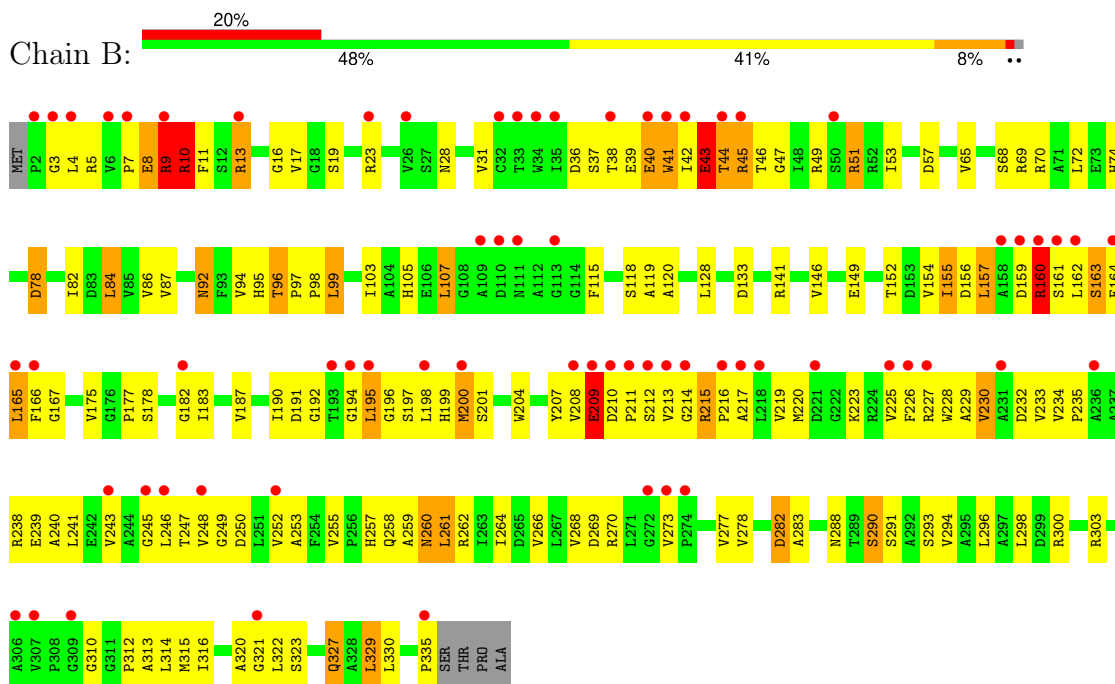
### 3 Residue-property plots [i](#)

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: Beta-ketoacylsynthase III



#### • Molecule 1: Beta-ketoacylsynthase III



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.00Å 96.00Å 72.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 2.10 83.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (500.00-2.10) 96.0 (83.14-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.251 0.219 , 0.257	Depositor DCC
$R_{free}$ test set	2112 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.031 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.86	2/2499 (0.1%)	1.03	8/3407 (0.2%)
1	B	0.64	1/2501 (0.0%)	0.87	1/3410 (0.0%)
All	All	0.76	3/5000 (0.1%)	0.95	9/6817 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	TRP	NE1-CE2	8.66	1.48	1.37
1	B	41	TRP	NE1-CE2	8.54	1.48	1.37
1	A	254	PHE	CE1-CZ	5.66	1.48	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	285	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	212	SER	CB-CA-C	-6.09	98.52	110.10
1	A	282	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	303	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	107	LEU	C-N-CA	-5.42	110.91	122.30
1	A	282	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	166	PHE	CA-C-N	-5.08	106.04	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	PHE	O-C-N	5.08	131.83	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	115	PHE	Mainchain

## 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	2453	0	2435	149	0
1	B	2454	0	2438	221	0
2	A	48	0	31	20	0
2	B	48	0	31	23	0
3	A	3	0	3	2	0
3	B	3	0	3	0	0
4	A	227	0	0	11	0
4	B	152	0	0	8	0
All	All	5388	0	4941	363	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 36.

All (363) 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:B:13:ARG:HD2	4:B:619:HOH:O	1.25	1.32
1:B:41:TRP:CZ3	1:B:164:PHE:CZ	2.20	1.30
1:B:41:TRP:HZ3	1:B:164:PHE:CE2	1.60	1.20
1:B:41:TRP:CH2	1:B:164:PHE:CZ	2.35	1.14
1:B:45:ARG:HH12	2:B:501:COA:C5B	1.58	1.14
1:B:45:ARG:HH12	2:B:501:COA:H52A	0.97	1.09
2:A:500:COA:H8A	4:A:688:HOH:O	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:TRP:CZ3	1:B:164:PHE:CE2	2.40	1.08
1:A:156:ASP:O	1:A:157:LEU:HB2	1.54	1.06
1:B:164:PHE:O	1:B:164:PHE:CD2	2.09	1.05
2:B:501:COA:H132	2:B:501:COA:P2A	1.98	1.03
1:B:41:TRP:HZ3	1:B:164:PHE:CZ	1.66	1.01
1:B:45:ARG:NH1	2:B:501:COA:H52A	1.77	1.00
1:A:298:LEU:HD13	1:A:315:MET:HE2	1.43	0.99
1:B:97:PRO:HG2	4:B:516:HOH:O	1.62	0.99
1:B:41:TRP:HE1	1:B:45:ARG:CZ	1.75	0.98
1:A:259:ALA:HB1	2:A:500:COA:H61	1.44	0.98
1:A:223:LYS:HE2	2:A:500:COA:O4A	1.64	0.98
1:A:5:ARG:O	1:A:7:PRO:HD3	1.63	0.98
1:B:37:SER:HB2	2:B:501:COA:H61A	1.29	0.95
1:A:204:TRP:HE1	1:B:95:HIS:HE1	1.06	0.95
1:B:155:ILE:HD13	1:B:166:PHE:CD1	2.03	0.93
1:B:40:GLU:O	1:B:44:THR:HG23	1.68	0.93
1:A:95:HIS:HE1	1:B:204:TRP:HE1	0.96	0.93
1:B:41:TRP:CH2	1:B:164:PHE:HZ	1.81	0.92
1:A:95:HIS:CE1	1:B:204:TRP:HE1	1.87	0.92
1:A:165:LEU:HD21	2:A:500:COA:O5P	1.72	0.89
1:B:41:TRP:HH2	1:B:164:PHE:HZ	1.17	0.87
1:B:214:GLY:O	1:B:215:ARG:O	1.93	0.85
2:A:500:COA:N3A	2:A:500:COA:O2B	2.09	0.84
1:B:207:TYR:CD2	1:B:215:ARG:N	2.45	0.84
1:A:251:LEU:HD11	1:A:314:LEU:HB2	1.59	0.84
1:B:37:SER:HB2	2:B:501:COA:N6A	1.94	0.83
1:B:37:SER:CB	2:B:501:COA:N6A	2.42	0.83
2:B:501:COA:N3A	2:B:501:COA:O2B	2.12	0.82
1:A:36:ASP:O	1:A:160:ARG:HD2	1.79	0.82
1:A:204:TRP:HE1	1:B:95:HIS:CE1	1.95	0.81
1:B:155:ILE:CD1	1:B:166:PHE:CD1	2.64	0.81
1:A:165:LEU:CD2	2:A:500:COA:O5P	2.29	0.81
1:B:41:TRP:NE1	1:B:45:ARG:NE	2.30	0.80
1:A:13:ARG:HD3	4:A:617:HOH:O	1.82	0.80
1:B:41:TRP:NE1	1:B:45:ARG:CZ	2.45	0.79
1:B:9:ARG:O	1:B:10:ARG:HB3	1.81	0.79
1:B:268:VAL:HG13	1:B:273:VAL:HB	1.65	0.79
1:B:41:TRP:CE2	1:B:45:ARG:HD2	2.17	0.79
1:A:315:MET:CE	1:A:329:LEU:HD21	2.13	0.79
1:B:259:ALA:HB1	2:B:501:COA:O5P	1.84	0.79
1:B:160:ARG:HG3	2:B:501:COA:C2A	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:H	1:A:74:HIS:HD2	1.30	0.78
1:B:223:LYS:O	1:B:227:ARG:HG3	1.82	0.78
1:A:156:ASP:O	1:A:157:LEU:CB	2.30	0.77
1:B:45:ARG:NH1	2:B:501:COA:C5B	2.43	0.77
1:A:105:HIS:CG	1:B:192:GLY:HA3	2.20	0.77
1:B:156:ASP:HB3	1:B:159:ASP:OD1	1.85	0.75
1:B:37:SER:CB	2:B:501:COA:H61A	1.98	0.75
1:A:261:LEU:HD13	1:A:283:ALA:HB3	1.69	0.75
1:B:210:ASP:OD2	1:B:212:SER:HB3	1.86	0.74
1:B:38:THR:O	1:B:40:GLU:N	2.21	0.73
1:A:335:PRO:O	1:A:336:SER:HB2	1.86	0.73
1:A:260:ASN:HD22	1:A:262:ARG:H	1.36	0.73
1:A:221:ASP:O	1:A:222:GLY:C	2.26	0.73
1:A:238:ARG:O	1:A:242:GLU:HG3	1.88	0.73
1:B:226:PHE:O	1:B:230:VAL:HG12	1.89	0.73
1:B:42:ILE:O	1:B:43:GLU:HB2	1.87	0.73
1:A:269:ASP:OD2	4:A:569:HOH:O	2.06	0.72
1:A:166:PHE:CZ	2:A:500:COA:H21	2.23	0.72
1:B:41:TRP:CZ2	1:B:45:ARG:HD2	2.24	0.72
2:A:500:COA:O9A	2:A:500:COA:H4B	1.88	0.72
1:B:13:ARG:CD	4:B:619:HOH:O	2.02	0.72
1:B:190:ILE:HG22	1:B:323:SER:HB3	1.73	0.71
1:A:166:PHE:HZ	2:A:500:COA:H21	1.55	0.71
1:A:298:LEU:CD1	1:A:315:MET:HE2	2.20	0.71
1:B:194:GLY:O	1:B:197:SER:N	2.21	0.71
2:A:500:COA:O2B	2:A:500:COA:C4A	2.39	0.70
1:B:17:VAL:H	1:B:74:HIS:HD2	1.39	0.70
1:B:38:THR:C	1:B:40:GLU:H	1.93	0.70
1:B:28:ASN:HD21	1:B:49:ARG:HA	1.56	0.70
1:B:247:THR:HG22	1:B:250:ASP:OD2	1.92	0.70
1:A:112:ALA:O	1:B:190:ILE:HG12	1.90	0.70
1:B:36:ASP:HB3	1:B:160:ARG:NH2	2.06	0.70
1:B:164:PHE:O	1:B:164:PHE:CG	2.45	0.70
1:B:298:LEU:HD13	1:B:315:MET:HE2	1.73	0.69
1:B:320:ALA:C	1:B:322:LEU:H	1.94	0.69
1:B:156:ASP:HB3	1:B:159:ASP:CG	2.14	0.68
1:B:13:ARG:HB3	1:B:182:GLY:HA3	1.76	0.68
1:A:4:LEU:HD21	1:B:330:LEU:HD21	1.74	0.67
1:A:259:ALA:HB1	2:A:500:COA:C6P	2.22	0.67
1:A:321:GLY:HA2	1:A:322:LEU:HD12	1.75	0.67
1:A:248:VAL:O	1:A:251:LEU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ALA:HB2	1:B:320:ALA:HB3	1.75	0.67
1:A:120:ALA:HB1	3:A:502:ACE:O	1.95	0.67
1:B:40:GLU:O	1:B:44:THR:CG2	2.41	0.67
1:B:78:ASP:HB3	4:B:620:HOH:O	1.94	0.67
1:B:5:ARG:O	1:B:7:PRO:HD3	1.94	0.67
2:B:501:COA:O2B	2:B:501:COA:C4A	2.42	0.67
1:B:155:ILE:HD13	1:B:166:PHE:HD1	1.59	0.66
1:B:214:GLY:O	1:B:215:ARG:C	2.33	0.66
1:B:194:GLY:O	1:B:196:GLY:N	2.28	0.66
1:B:128:LEU:HD21	1:B:329:LEU:HD23	1.78	0.66
1:B:194:GLY:HA3	1:B:322:LEU:HD23	1.78	0.66
1:A:95:HIS:HE1	1:B:204:TRP:NE1	1.81	0.66
1:B:228:TRP:CE3	1:B:322:LEU:HD12	2.30	0.65
1:B:37:SER:OG	2:B:501:COA:N6A	2.29	0.65
1:A:315:MET:HE3	1:A:329:LEU:HD21	1.77	0.65
1:A:182:GLY:HA2	1:A:330:LEU:HD22	1.79	0.64
1:B:36:ASP:O	1:B:160:ARG:NH2	2.21	0.64
1:A:248:VAL:HG12	1:A:274:PRO:HD3	1.79	0.64
1:B:8:GLU:O	1:B:8:GLU:HG2	1.98	0.64
1:B:199:HIS:CE1	1:B:219:VAL:CG2	2.81	0.63
1:B:234:VAL:HB	1:B:235:PRO:HD3	1.80	0.63
1:A:16:GLY:HA2	1:A:74:HIS:CD2	2.33	0.63
1:B:10:ARG:HG3	1:B:11:PHE:N	2.12	0.63
1:A:298:LEU:HD13	1:A:315:MET:CE	2.23	0.63
2:B:501:COA:P2A	2:B:501:COA:CDP	2.83	0.63
1:B:13:ARG:HG2	1:B:178:SER:HB2	1.80	0.63
1:A:223:LYS:HG2	4:A:683:HOH:O	1.98	0.63
1:A:315:MET:HE1	1:A:329:LEU:HD21	1.81	0.63
1:B:235:PRO:O	1:B:238:ARG:HG2	1.98	0.63
1:B:199:HIS:CE1	1:B:219:VAL:HG22	2.34	0.62
1:A:320:ALA:HB1	1:B:97:PRO:HB3	1.81	0.62
1:A:105:HIS:ND1	1:B:192:GLY:HA3	2.15	0.62
1:A:220:MET:HE3	1:A:222:GLY:HA2	1.81	0.62
1:A:267:LEU:O	1:A:271:LEU:HB2	2.00	0.62
1:A:181:PRO:HG2	1:B:3:GLY:O	2.00	0.61
1:A:220:MET:SD	2:A:500:COA:H31	2.40	0.61
1:B:228:TRP:CD2	1:B:322:LEU:HD12	2.35	0.61
1:A:198:LEU:HD23	1:A:218:LEU:HD11	1.81	0.61
1:B:261:LEU:HD12	1:B:264:ILE:HD12	1.82	0.61
1:A:120:ALA:CB	1:A:320:ALA:HB3	2.31	0.61
1:B:8:GLU:O	1:B:8:GLU:CG	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG22	1:B:312:PRO:O	2.01	0.60
1:A:260:ASN:ND2	1:A:262:ARG:H	1.99	0.60
1:B:120:ALA:CB	1:B:320:ALA:HB3	2.31	0.59
2:B:501:COA:O9P	2:B:501:COA:CEP	2.48	0.59
2:B:501:COA:C4A	2:B:501:COA:HO2A	2.16	0.59
1:A:96:THR:HG22	1:B:200:MET:SD	2.42	0.59
1:A:204:TRP:NE1	1:B:95:HIS:HE1	1.90	0.59
1:B:17:VAL:H	1:B:74:HIS:CD2	2.21	0.58
1:B:204:TRP:CE2	1:B:216:PRO:CG	2.86	0.58
2:A:500:COA:O9A	2:A:500:COA:C4B	2.51	0.58
1:B:68:SER:CB	1:B:107:LEU:HD11	2.33	0.58
1:A:198:LEU:CD2	1:A:218:LEU:HD11	2.33	0.58
1:A:249:GLY:HA2	1:A:274:PRO:HG2	1.86	0.58
2:B:501:COA:H132	2:B:501:COA:O4A	2.04	0.58
1:B:207:TYR:HD2	1:B:214:GLY:HA2	1.69	0.57
1:B:208:VAL:O	1:B:209:GLU:HB2	2.04	0.57
1:B:215:ARG:HG2	1:B:215:ARG:HH11	1.69	0.57
1:A:41:TRP:CE2	1:A:45:ARG:HG3	2.39	0.57
1:A:309:GLY:HA3	1:A:333:ASP:OD2	2.05	0.57
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.69	0.57
1:B:28:ASN:ND2	1:B:49:ARG:HA	2.20	0.57
1:B:282:ASP:OD1	1:B:300:ARG:HD2	2.04	0.57
1:B:46:THR:OG1	1:B:47:GLY:N	2.38	0.56
1:A:220:MET:CE	1:A:222:GLY:HA2	2.35	0.56
1:B:41:TRP:CD1	2:B:501:COA:C8A	2.87	0.56
1:A:72:LEU:HD21	1:A:82:ILE:HD11	1.87	0.56
2:A:500:COA:H141	2:A:500:COA:O9P	2.05	0.56
1:B:41:TRP:HE1	1:B:45:ARG:NH2	2.01	0.56
1:A:223:LYS:CE	2:A:500:COA:O4A	2.48	0.56
1:B:159:ASP:O	1:B:163:SER:HB3	2.06	0.56
1:B:68:SER:HB3	1:B:107:LEU:HD11	1.88	0.56
1:A:133:ASP:HB3	1:B:133:ASP:HB3	1.88	0.56
1:B:182:GLY:HA2	1:B:330:LEU:HD22	1.87	0.56
1:A:198:LEU:HD11	2:A:500:COA:H32	1.87	0.56
1:B:253:ALA:HA	1:B:278:VAL:O	2.06	0.55
1:A:92:ASN:HD22	1:A:93:PHE:N	2.04	0.55
1:A:82:ILE:O	1:A:112:ALA:HB2	2.06	0.55
1:A:261:LEU:CD1	1:A:283:ALA:HB3	2.34	0.55
1:B:96:THR:OG1	1:B:97:PRO:HA	2.07	0.55
1:A:155:ILE:HG12	1:A:162:LEU:HD13	1.89	0.55
1:A:241:LEU:CD1	1:A:248:VAL:HG22	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASP:CB	1:B:159:ASP:OD1	2.54	0.55
1:A:213:VAL:CG1	1:A:214:GLY:N	2.69	0.54
1:B:232:ASP:C	1:B:235:PRO:HD2	2.27	0.54
1:B:253:ALA:N	1:B:277:VAL:HG23	2.22	0.54
1:B:160:ARG:HG3	2:B:501:COA:H2A	1.87	0.54
1:B:204:TRP:CE2	1:B:216:PRO:HG2	2.43	0.54
1:B:207:TYR:CD2	1:B:214:GLY:HA2	2.42	0.54
1:B:315:MET:CE	1:B:329:LEU:HD21	2.37	0.54
1:B:207:TYR:CE2	1:B:215:ARG:N	2.55	0.54
1:A:17:VAL:H	1:A:74:HIS:CD2	2.18	0.53
1:B:160:ARG:O	1:B:164:PHE:HE1	1.92	0.53
1:B:194:GLY:O	1:B:195:LEU:C	2.46	0.53
1:B:215:ARG:HH11	1:B:215:ARG:CG	2.21	0.53
1:A:212:SER:O	1:A:213:VAL:HB	2.08	0.53
1:B:41:TRP:CE2	1:B:45:ARG:CD	2.90	0.53
1:A:41:TRP:CZ3	1:A:164:PHE:CZ	2.96	0.53
1:A:45:ARG:NH1	2:A:500:COA:O5A	2.38	0.53
1:A:162:LEU:HD21	1:A:218:LEU:O	2.09	0.53
1:A:119:ALA:HA	1:B:98:PRO:HG3	1.90	0.53
1:A:3:GLY:HA2	1:B:246:LEU:HD11	1.90	0.52
1:B:31:VAL:HG21	1:B:51:ARG:CZ	2.39	0.52
1:A:45:ARG:HD2	2:A:500:COA:O5A	2.09	0.52
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.25	0.52
1:B:149:GLU:HG3	1:B:290:SER:HB3	1.92	0.52
1:A:166:PHE:HA	1:A:288:ASN:O	2.10	0.52
1:A:213:VAL:HG13	1:A:214:GLY:O	2.09	0.52
1:B:3:GLY:O	1:B:4:LEU:HB2	2.09	0.51
1:B:42:ILE:O	1:B:43:GLU:CB	2.55	0.51
1:B:99:LEU:HD22	1:B:103:ILE:HG13	1.92	0.51
1:B:261:LEU:HD13	1:B:283:ALA:HB3	1.92	0.51
1:A:170:ALA:O	1:A:296:LEU:HD21	2.10	0.51
1:B:38:THR:C	1:B:40:GLU:N	2.59	0.51
1:A:13:ARG:NH2	4:A:599:HOH:O	2.42	0.51
1:B:258:GLN:HB3	1:B:283:ALA:HB2	1.92	0.51
1:B:216:PRO:O	1:B:217:ALA:HB2	2.11	0.51
1:A:41:TRP:HZ3	1:A:164:PHE:CZ	2.29	0.51
1:A:155:ILE:CG1	1:A:162:LEU:HD13	2.41	0.51
1:B:9:ARG:H	1:B:9:ARG:HD3	1.76	0.51
1:B:155:ILE:HD11	1:B:166:PHE:CE1	2.46	0.50
1:A:252:VAL:HG22	1:A:312:PRO:O	2.11	0.50
1:B:315:MET:HE3	1:B:329:LEU:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TRP:CZ2	1:B:216:PRO:HG2	2.45	0.50
1:B:167:GLY:N	1:B:288:ASN:O	2.38	0.50
1:B:210:ASP:CG	1:B:212:SER:HB3	2.32	0.50
1:A:68:SER:HB3	1:A:107:LEU:HD21	1.92	0.49
1:B:41:TRP:CZ2	1:B:45:ARG:CD	2.95	0.49
1:A:55:GLU:HG3	4:A:523:HOH:O	2.12	0.49
1:A:113:GLY:HA2	1:B:190:ILE:HG23	1.94	0.49
1:A:230:VAL:CG1	1:A:270:ARG:NH2	2.75	0.49
1:A:260:ASN:HD21	1:A:262:ARG:HB2	1.75	0.49
1:B:257:HIS:HD2	1:B:293:SER:HB3	1.78	0.49
1:B:248:VAL:HG13	4:B:600:HOH:O	2.12	0.49
1:A:68:SER:CB	1:A:107:LEU:HD21	2.43	0.48
1:A:5:ARG:HB3	4:A:659:HOH:O	2.12	0.48
1:B:194:GLY:C	1:B:196:GLY:N	2.67	0.48
1:B:204:TRP:CH2	1:B:216:PRO:HD2	2.47	0.48
1:A:120:ALA:HB2	1:A:320:ALA:HB3	1.94	0.48
1:A:248:VAL:HG23	4:A:532:HOH:O	2.12	0.48
1:B:84:LEU:HD13	1:B:86:VAL:HG23	1.96	0.48
1:B:239:GLU:O	1:B:243:VAL:HG23	2.14	0.48
1:A:92:ASN:HD22	1:A:92:ASN:C	2.18	0.48
1:A:321:GLY:HA2	1:A:322:LEU:CD1	2.41	0.48
1:A:274:PRO:O	1:A:277:VAL:HG13	2.13	0.48
1:B:9:ARG:HD3	1:B:9:ARG:N	2.29	0.48
1:B:229:ALA:O	1:B:233:VAL:HB	2.14	0.47
1:A:14:VAL:HG12	1:A:332:PRO:HG3	1.96	0.47
1:A:316:ILE:HG23	1:A:316:ILE:O	2.14	0.47
1:B:190:ILE:HG22	1:B:323:SER:CB	2.41	0.47
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.69	0.47
2:B:501:COA:O4A	2:B:501:COA:CAP	2.62	0.47
1:B:41:TRP:CZ3	1:B:164:PHE:CE1	2.97	0.47
1:A:96:THR:OG1	1:A:97:PRO:HA	2.14	0.47
1:A:202:SER:O	1:A:216:PRO:HB3	2.14	0.47
1:A:251:LEU:CD1	1:A:314:LEU:HB2	2.35	0.47
1:B:11:PHE:HB2	1:B:178:SER:O	2.14	0.47
1:B:207:TYR:HD2	1:B:214:GLY:CA	2.28	0.47
1:B:321:GLY:O	1:B:322:LEU:HB2	2.15	0.47
1:A:260:ASN:ND2	1:A:262:ARG:N	2.63	0.47
1:B:16:GLY:HA2	1:B:74:HIS:CD2	2.49	0.47
1:B:298:LEU:HD22	1:B:315:MET:HE1	1.96	0.47
1:B:13:ARG:CB	1:B:182:GLY:HA3	2.44	0.47
1:B:13:ARG:HA	1:B:183:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASP:O	1:B:235:PRO:HD2	2.15	0.47
1:B:207:TYR:HD2	1:B:215:ARG:N	2.07	0.46
1:B:315:MET:HE1	1:B:329:LEU:HD21	1.97	0.46
1:B:245:GLY:O	1:B:246:LEU:HG	2.15	0.46
1:B:9:ARG:N	1:B:9:ARG:CD	2.79	0.46
1:B:87:VAL:HA	1:B:146:VAL:O	2.15	0.46
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.76	0.46
1:A:197:SER:O	1:A:220:MET:HA	2.15	0.46
1:A:84:LEU:HD22	1:A:85:VAL:N	2.30	0.46
1:A:298:LEU:HD22	1:A:315:MET:HE1	1.98	0.46
1:A:321:GLY:CA	4:A:540:HOH:O	2.64	0.46
1:A:121:CYS:N	3:A:502:ACE:O	2.39	0.45
1:A:307:VAL:HA	1:A:308:PRO:HD3	1.65	0.45
1:B:199:HIS:CE1	1:B:219:VAL:HG21	2.50	0.45
1:B:87:VAL:HG21	1:B:103:ILE:HD12	1.97	0.45
1:A:8:GLU:HA	4:A:704:HOH:O	2.15	0.45
1:A:19:SER:HB2	1:A:296:LEU:HD23	1.99	0.45
1:B:198:LEU:HD23	1:B:220:MET:HB2	1.98	0.45
1:A:10:ARG:NH1	1:A:135:VAL:HG13	2.32	0.45
1:B:19:SER:HB2	1:B:296:LEU:HD23	1.97	0.45
1:B:92:ASN:ND2	1:B:94:VAL:H	2.14	0.45
1:B:229:ALA:HA	1:B:233:VAL:HG23	1.97	0.45
1:B:314:LEU:HD23	1:B:315:MET:N	2.32	0.45
1:A:248:VAL:CG1	1:A:274:PRO:HD3	2.47	0.45
1:A:230:VAL:HG11	1:A:270:ARG:NH2	2.32	0.44
1:A:248:VAL:HG11	1:A:273:VAL:HA	1.99	0.44
1:A:257:HIS:HD2	1:A:293:SER:CB	2.30	0.44
1:B:9:ARG:HB3	1:B:10:ARG:H	1.54	0.44
1:B:197:SER:HB2	1:B:322:LEU:HD21	1.99	0.44
1:B:320:ALA:C	1:B:322:LEU:N	2.64	0.44
1:B:315:MET:HE3	1:B:329:LEU:HD21	1.99	0.44
1:A:35:ILE:HG22	1:A:158:ALA:O	2.17	0.44
1:B:322:LEU:HD13	1:B:322:LEU:HA	1.75	0.44
1:B:43:GLU:O	1:B:47:GLY:HA2	2.17	0.44
1:B:165:LEU:O	1:B:288:ASN:HB3	2.17	0.44
1:A:321:GLY:HA2	1:A:322:LEU:HA	1.73	0.44
1:B:53:ILE:HG23	1:B:152:THR:HG21	1.99	0.44
1:B:207:TYR:CD2	1:B:214:GLY:CA	3.00	0.44
1:A:204:TRP:CE2	1:A:216:PRO:HG2	2.53	0.43
1:A:115:PHE:HB3	1:B:119:ALA:HB2	2.00	0.43
1:A:315:MET:HE3	1:A:329:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:CG	1:B:215:ARG:NH1	2.75	0.43
1:A:115:PHE:CB	1:B:119:ALA:HB2	2.49	0.43
1:B:37:SER:CB	2:B:501:COA:H62A	2.26	0.43
1:B:68:SER:HB2	1:B:107:LEU:HD11	2.00	0.43
1:B:257:HIS:HD2	1:B:293:SER:CB	2.32	0.43
1:A:321:GLY:HA3	4:A:540:HOH:O	2.18	0.43
1:B:187:VAL:HG21	1:B:240:ALA:HB2	1.99	0.43
1:A:257:HIS:HD2	1:A:293:SER:HB3	1.82	0.43
1:B:235:PRO:HA	1:B:238:ARG:HG2	2.01	0.43
1:B:255:VAL:HB	1:B:315:MET:HG2	2.01	0.43
1:A:222:GLY:CA	2:A:500:COA:H141	2.49	0.43
1:A:15:LEU:HD11	1:A:176:GLY:HA3	2.00	0.42
1:B:247:THR:HG22	1:B:250:ASP:CG	2.39	0.42
1:A:72:LEU:CD2	1:A:82:ILE:HD11	2.49	0.42
1:B:215:ARG:HA	1:B:216:PRO:HD2	1.87	0.42
1:A:92:ASN:ND2	1:A:94:VAL:H	2.17	0.42
1:B:154:VAL:O	1:B:217:ALA:HA	2.20	0.42
1:B:211:PRO:HA	4:B:618:HOH:O	2.19	0.42
1:B:315:MET:CE	1:B:329:LEU:HD11	2.49	0.42
1:A:221:ASP:C	1:A:221:ASP:OD2	2.57	0.42
1:A:234:VAL:N	1:A:235:PRO:CD	2.83	0.42
1:A:314:LEU:HD22	1:A:315:MET:N	2.34	0.42
1:B:23:ARG:HH22	1:B:57:ASP:CG	2.23	0.42
1:B:211:PRO:O	1:B:212:SER:C	2.58	0.42
1:B:155:ILE:CD1	1:B:166:PHE:CE1	3.02	0.42
1:A:116:ASP:HB2	1:B:118:SER:HB3	2.01	0.42
1:B:273:VAL:HG13	1:B:277:VAL:HG11	2.01	0.42
1:A:37:SER:CB	2:A:500:COA:H62A	2.33	0.42
1:A:43:GLU:OE1	1:A:49:ARG:HD2	2.18	0.42
1:A:148:THR:C	1:A:149:GLU:HG2	2.40	0.42
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.75	0.42
1:B:40:GLU:HB2	4:B:645:HOH:O	2.19	0.42
1:B:141:ARG:O	1:B:177:PRO:HD3	2.19	0.42
1:A:192:GLY:HA3	1:B:105:HIS:CG	2.55	0.42
1:B:166:PHE:HA	1:B:288:ASN:O	2.20	0.42
1:B:23:ARG:NH2	1:B:57:ASP:OD2	2.53	0.41
1:A:4:LEU:O	1:A:5:ARG:HB2	2.20	0.41
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.87	0.41
1:B:294:VAL:CG1	1:B:315:MET:SD	3.08	0.41
1:A:320:ALA:HA	1:A:321:GLY:HA2	1.67	0.41
1:B:266:VAL:O	1:B:269:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:HB3	1:B:329:LEU:HD12	2.03	0.41
1:A:281:ARG:HH11	1:A:281:ARG:HD3	1.62	0.41
1:B:65:VAL:O	1:B:69:ARG:HG3	2.19	0.41
1:B:159:ASP:C	1:B:161:SER:N	2.74	0.41
1:B:198:LEU:CD1	1:B:225:VAL:HG21	2.51	0.41
1:A:273:VAL:HA	1:A:274:PRO:HD3	1.97	0.41
1:B:277:VAL:O	1:B:277:VAL:HG13	2.20	0.41
2:B:501:COA:H132	2:B:501:COA:O5A	2.20	0.41
1:A:9:ARG:NH1	4:B:555:HOH:O	2.52	0.41
1:A:311:GLY:HA2	1:A:312:PRO:HD3	1.89	0.41
1:B:72:LEU:HD21	1:B:82:ILE:HD11	2.03	0.41
1:B:234:VAL:HG11	1:B:270:ARG:HB3	2.02	0.41
1:B:260:ASN:HD22	1:B:260:ASN:HA	1.54	0.41
1:A:17:VAL:N	1:A:74:HIS:HD2	2.08	0.41
1:A:180:VAL:HB	1:A:181:PRO:HD2	2.02	0.41
1:B:37:SER:OG	1:B:38:THR:N	2.53	0.41
1:B:128:LEU:HD23	1:B:327:GLN:CD	2.41	0.41
1:B:248:VAL:HG23	1:B:249:GLY:N	2.35	0.41
1:A:22:PRO:O	1:A:52:ARG:HD3	2.21	0.41
1:A:259:ALA:O	1:A:260:ASN:HB3	2.20	0.41
1:A:258:GLN:HB3	1:A:283:ALA:HB2	2.02	0.40
1:B:166:PHE:HA	1:B:288:ASN:HB3	2.02	0.40
1:B:329:LEU:HD12	1:B:329:LEU:O	2.21	0.40
1:A:97:PRO:HB3	1:B:321:GLY:N	2.35	0.40
1:B:262:ARG:O	1:B:266:VAL:HG23	2.21	0.40
1:B:298:LEU:HD22	1:B:315:MET:CE	2.51	0.40
1:B:303:ARG:HG2	1:B:335:PRO:HG3	2.03	0.40
1:A:49:ARG:HG3	1:A:284:GLU:HG3	2.02	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	332/339 (98%)	308 (93%)	21 (6%)	3 (1%)	14	11
1	B	332/339 (98%)	295 (89%)	27 (8%)	10 (3%)	3	1
All	All	664/678 (98%)	603 (91%)	48 (7%)	13 (2%)	6	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	VAL
1	B	9	ARG
1	B	39	GLU
1	B	43	GLU
1	B	195	LEU
1	B	209	GLU
1	B	215	ARG
1	A	222	GLY
1	B	10	ARG
1	B	310	GLY
1	A	157	LEU
1	B	160	ARG
1	B	316	ILE

### 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	258/262 (98%)	228 (88%)	30 (12%)	4	2
1	B	258/262 (98%)	222 (86%)	36 (14%)	3	1
All	All	516/524 (98%)	450 (87%)	66 (13%)	3	2

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	39	GLU
1	A	51	ARG

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Mol	Chain	Res	Type
1	A	70	ARG
1	A	78	ASP
1	A	84	LEU
1	A	92	ASN
1	A	96	THR
1	A	99	LEU
1	A	144	LEU
1	A	152	THR
1	A	155	ILE
1	A	157	LEU
1	A	160	ARG
1	A	195	LEU
1	A	205	ASP
1	A	212	SER
1	A	219	VAL
1	A	226	PHE
1	A	250	ASP
1	A	260	ASN
1	A	261	LEU
1	A	271	LEU
1	A	277	VAL
1	A	282	ASP
1	A	314	LEU
1	A	322	LEU
1	A	327	GLN
1	A	330	LEU
1	A	336	SER
1	B	8	GLU
1	B	9	ARG
1	B	10	ARG
1	B	13	ARG
1	B	40	GLU
1	B	43	GLU
1	B	44	THR
1	B	45	ARG
1	B	51	ARG
1	B	70	ARG
1	B	78	ASP
1	B	84	LEU
1	B	92	ASN
1	B	96	THR
1	B	99	LEU

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Mol	Chain	Res	Type
1	B	155	ILE
1	B	157	LEU
1	B	160	ARG
1	B	162	LEU
1	B	163	SER
1	B	165	LEU
1	B	175	VAL
1	B	191	ASP
1	B	200	MET
1	B	201	SER
1	B	209	GLU
1	B	213	VAL
1	B	230	VAL
1	B	241	LEU
1	B	260	ASN
1	B	261	LEU
1	B	282	ASP
1	B	290	SER
1	B	291	SER
1	B	327	GLN
1	B	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	92	ASN
1	A	95	HIS
1	A	257	HIS
1	A	260	ASN
1	B	74	HIS
1	B	92	ASN
1	B	95	HIS
1	B	142	HIS
1	B	199	HIS
1	B	257	HIS
1	B	260	ASN

### 5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	COA	A	500	3	43,50,50	3.90	19 (44%)	56,75,75	3.49	24 (42%)
3	ACE	A	502	2,1	1,2,2	1.03	0	0,1,1	-	-
3	ACE	B	503	2,1	1,2,2	1.06	0	0,1,1	-	-
2	COA	B	501	3	43,50,50	3.01	17 (39%)	56,75,75	3.91	30 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	A	500	3	1/1/11/13	12/44/64/64	0/3/3/3
2	COA	B	501	3	1/1/11/13	24/44/64/64	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	P1A-O3A	11.41	1.71	1.59
2	A	500	COA	P2A-O3A	11.01	1.71	1.59
2	A	500	COA	C4A-N3A	8.97	1.47	1.35
2	A	500	COA	P3B-O3B	8.51	1.74	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	COA	C4A-N3A	8.33	1.46	1.35
2	B	501	COA	P2A-O3A	7.51	1.67	1.59
2	B	501	COA	P3B-O3B	6.62	1.71	1.59
2	B	501	COA	C7P-N8P	6.15	1.60	1.46
2	A	500	COA	C8A-N7A	5.90	1.45	1.34
2	B	501	COA	C2A-N3A	5.86	1.41	1.32
2	A	500	COA	C2A-N3A	5.33	1.40	1.32
2	B	501	COA	P1A-O3A	4.80	1.64	1.59
2	A	500	COA	O4B-C1B	4.67	1.47	1.40
2	A	500	COA	C9P-N8P	4.33	1.43	1.33
2	B	501	COA	C8A-N7A	4.31	1.42	1.34
2	A	500	COA	O3B-C3B	4.16	1.58	1.44
2	A	500	COA	C6P-C5P	-4.13	1.43	1.51
2	B	501	COA	C6A-N6A	3.79	1.47	1.34
2	A	500	COA	P2A-O6A	3.77	1.74	1.59
2	A	500	COA	C2A-N1A	3.75	1.40	1.33
2	A	500	COA	P3B-O7A	3.55	1.61	1.50
2	A	500	COA	C6A-N6A	3.23	1.45	1.34
2	B	501	COA	O6A-CCP	3.05	1.53	1.43
2	B	501	COA	C2A-N1A	2.85	1.39	1.33
2	B	501	COA	P3B-O7A	2.60	1.58	1.50
2	B	501	COA	C6A-N1A	2.59	1.46	1.36
2	A	500	COA	P3B-O8A	2.56	1.64	1.54
2	B	501	COA	CDP-CBP	2.54	1.59	1.53
2	B	501	COA	CEP-CBP	2.52	1.58	1.53
2	A	500	COA	C5P-N4P	2.49	1.39	1.33
2	B	501	COA	CCP-CBP	2.39	1.56	1.52
2	A	500	COA	C2B-C3B	2.32	1.58	1.53
2	B	501	COA	C9P-N8P	2.30	1.39	1.33
2	B	501	COA	O5P-C5P	2.28	1.27	1.23
2	A	500	COA	P1A-O1A	2.24	1.58	1.50
2	A	500	COA	O2B-C2B	2.06	1.48	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	COA	C5A-C6A-N6A	10.93	136.96	120.31
2	B	501	COA	C7P-N8P-C9P	-10.00	104.58	122.55
2	A	500	COA	O5P-C5P-C6P	-9.82	104.22	122.02
2	B	501	COA	N3A-C2A-N1A	-9.81	115.36	128.67
2	A	500	COA	C6P-C5P-N4P	9.43	133.53	116.34
2	B	501	COA	CDP-CBP-CCP	-9.08	93.24	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	COA	CAP-C9P-N8P	8.62	132.84	116.48
2	B	501	COA	C3P-N4P-C5P	-7.41	109.03	122.82
2	B	501	COA	C4B-O4B-C1B	-7.23	103.30	109.92
2	B	501	COA	CEP-CBP-CAP	7.06	120.81	108.77
2	B	501	COA	N6A-C6A-N1A	6.07	131.30	118.33
2	A	500	COA	C7P-C6P-C5P	-5.74	102.83	112.39
2	A	500	COA	N3A-C2A-N1A	-5.47	121.25	128.67
2	A	500	COA	N6A-C6A-N1A	-5.32	106.97	118.33
2	B	501	COA	CDP-CBP-CAP	-5.30	99.74	108.77
2	A	500	COA	C1B-N9A-C4A	5.09	135.59	126.64
2	A	500	COA	C3P-N4P-C5P	-4.97	113.57	122.82
2	B	501	COA	O9P-C9P-CAP	-4.88	107.26	120.89
2	A	500	COA	C4A-C5A-N7A	-4.66	104.42	109.34
2	A	500	COA	O9P-C9P-CAP	-4.53	108.25	120.89
2	B	501	COA	O2B-C2B-C3B	-4.52	98.54	111.19
2	B	501	COA	O6A-CCP-CBP	4.51	117.81	110.55
2	A	500	COA	C5A-C6A-N1A	-4.40	109.74	120.23
2	B	501	COA	C7P-C6P-C5P	-4.39	105.08	112.39
2	A	500	COA	C4B-O4B-C1B	-4.35	105.94	109.92
2	B	501	COA	O4B-C1B-N9A	-4.28	103.07	108.75
2	B	501	COA	C6A-C5A-C4A	4.03	125.74	117.90
2	B	501	COA	CEP-CBP-CDP	-3.85	101.53	109.20
2	B	501	COA	O5P-C5P-C6P	3.79	128.89	122.02
2	B	501	COA	OAP-CAP-C9P	-3.78	93.60	109.38
2	A	500	COA	P3B-O3B-C3B	-3.58	113.86	123.43
2	A	500	COA	P1A-O5B-C5B	-3.57	100.92	121.35
2	B	501	COA	C5A-C6A-N1A	-3.56	111.74	120.23
2	A	500	COA	C7P-N8P-C9P	-3.46	116.34	122.55
2	A	500	COA	O2B-C2B-C3B	-3.44	101.56	111.19
2	A	500	COA	CDP-CBP-CCP	-3.33	102.72	108.22
2	A	500	COA	CEP-CBP-CCP	3.31	113.69	108.22
2	B	501	COA	P3B-O3B-C3B	3.29	132.23	123.43
2	B	501	COA	P1A-O5B-C5B	-3.15	103.32	121.35
2	A	500	COA	C6A-C5A-C4A	3.04	123.81	117.90
2	A	500	COA	O4B-C1B-N9A	-3.03	104.72	108.75
2	B	501	COA	CEP-CBP-CCP	-2.83	103.55	108.22
2	A	500	COA	CEP-CBP-CDP	2.76	114.71	109.20
2	B	501	COA	O5A-P2A-O3A	-2.68	100.02	107.27
2	B	501	COA	O4B-C4B-C3B	-2.68	99.27	104.92
2	B	501	COA	O5P-C5P-N4P	-2.61	117.90	123.03
2	B	501	COA	C2B-C3B-C4B	2.57	107.73	103.24
2	A	500	COA	C2P-C3P-N4P	-2.48	106.69	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	COA	O5B-C5B-C4B	-2.41	100.78	108.99
2	A	500	COA	C3B-C2B-C1B	2.24	104.82	99.89
2	B	501	COA	C5A-C6A-N6A	-2.21	116.95	120.31
2	B	501	COA	C4A-C5A-N7A	-2.10	107.12	109.34
2	A	500	COA	C6P-C7P-N8P	-2.01	107.72	112.00
2	B	501	COA	OAP-CAP-CBP	-2.01	105.53	110.18

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	500	COA	C2B
2	B	501	COA	C2B

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	COA	C4B-C3B-O3B-P3B
2	A	500	COA	CCP-O6A-P2A-O4A
2	A	500	COA	C5P-C6P-C7P-N8P
2	A	500	COA	S1P-C2P-C3P-N4P
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	CCP-O6A-P2A-O4A
2	B	501	COA	CBP-CCP-O6A-P2A
2	B	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CEP-CBP-CCP-O6A
2	B	501	COA	CAP-CBP-CCP-O6A
2	B	501	COA	OAP-CAP-CBP-CCP
2	B	501	COA	C9P-CAP-CBP-CCP
2	B	501	COA	OAP-CAP-CBP-CDP
2	B	501	COA	C9P-CAP-CBP-CDP
2	B	501	COA	OAP-CAP-CBP-CEP
2	B	501	COA	C9P-CAP-CBP-CEP
2	B	501	COA	S1P-C2P-C3P-N4P
2	B	501	COA	C4B-C3B-O3B-P3B
2	A	500	COA	O9P-C9P-N8P-C7P
2	B	501	COA	O9P-C9P-CAP-OAP
2	B	501	COA	O5P-C5P-C6P-C7P
2	B	501	COA	O9P-C9P-CAP-CBP
2	A	500	COA	N8P-C9P-CAP-CBP
2	B	501	COA	N4P-C5P-C6P-C7P
2	B	501	COA	P1A-O3A-P2A-O6A
2	A	500	COA	P1A-O3A-P2A-O4A

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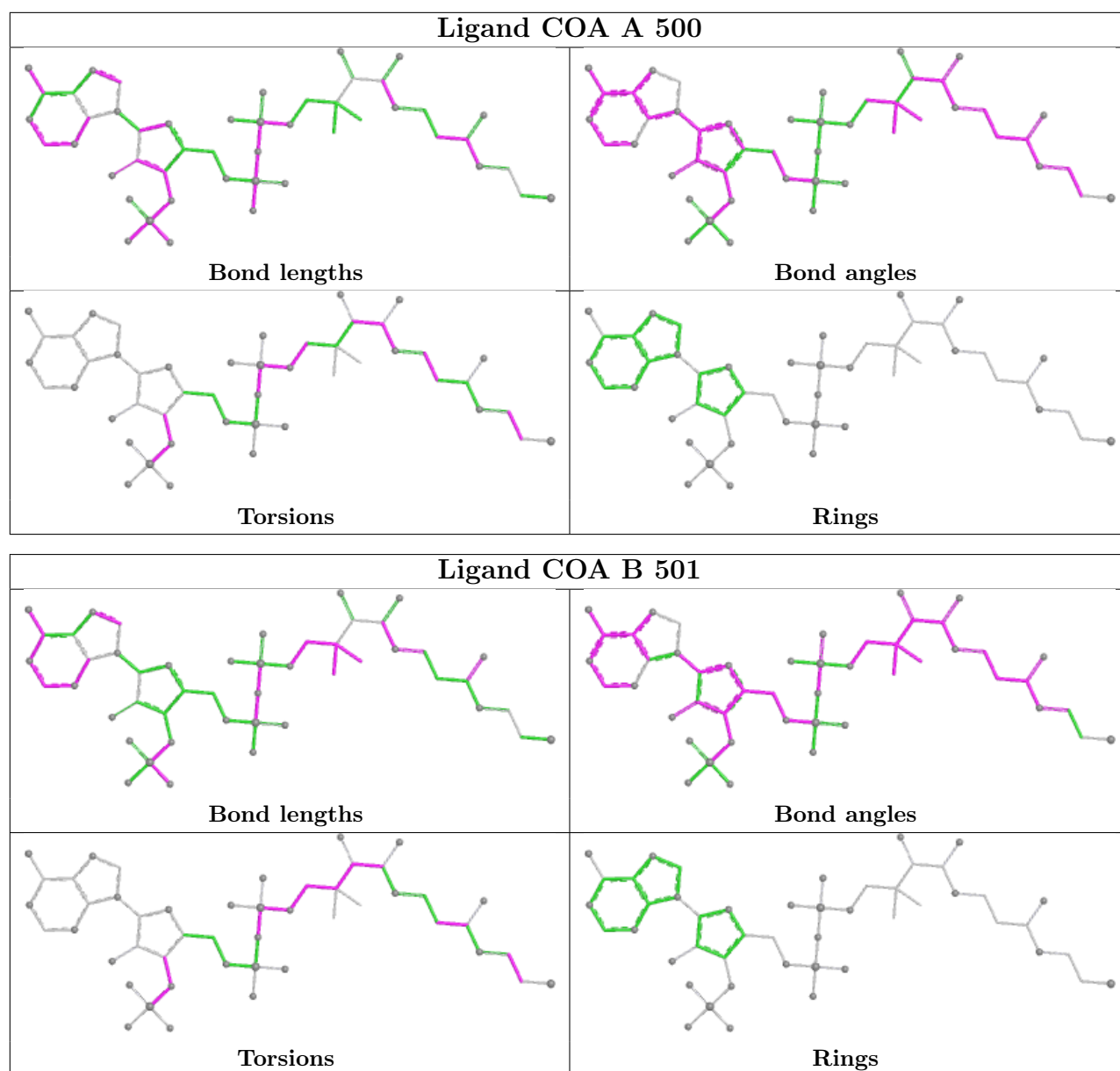
Mol	Chain	Res	Type	Atoms
2	A	500	COA	C3B-O3B-P3B-O7A
2	B	501	COA	CCP-O6A-P2A-O5A
2	B	501	COA	N8P-C9P-CAP-CBP
2	A	500	COA	N8P-C9P-CAP-OAP
2	B	501	COA	N8P-C9P-CAP-OAP
2	B	501	COA	P1A-O3A-P2A-O5A
2	A	500	COA	C3B-O3B-P3B-O9A
2	A	500	COA	CBP-CCP-O6A-P2A
2	B	501	COA	C3B-O3B-P3B-O7A
2	A	500	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

3 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	COA	20	0
3	A	502	ACE	2	0
2	B	501	COA	23	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/339 (98%)	0.24	24 (7%) 23 25	22, 35, 56, 85	0
1	B	334/339 (98%)	1.00	67 (20%) 3 4	29, 51, 77, 96	0
All	All	668/678 (98%)	0.62	91 (13%) 8 9	22, 42, 73, 96	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PRO	8.1
1	B	164	PHE	6.5
1	A	4	LEU	5.7
1	B	44	THR	5.2
1	B	213	VAL	5.0
1	A	210	ASP	4.7
1	A	321	GLY	4.5
1	B	3	GLY	4.5
1	B	40	GLU	4.2
1	A	213	VAL	4.0
1	A	212	SER	4.0
1	A	3	GLY	4.0
1	B	214	GLY	4.0
1	B	217	ALA	3.9
1	B	195	LEU	3.7
1	A	161	SER	3.6
1	B	208	VAL	3.6
1	B	9	ARG	3.6
1	A	156	ASP	3.5
1	B	42	ILE	3.5
1	B	161	SER	3.4
1	B	41	TRP	3.4
1	A	162	LEU	3.3
1	B	35	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	PRO	3.2
1	A	250	ASP	3.2
1	A	320	ALA	3.2
1	B	200	MET	3.2
1	B	110	ASP	3.1
1	B	45	ARG	3.0
1	A	165	LEU	3.0
1	A	158	ALA	3.0
1	B	109	ALA	3.0
1	B	272	GLY	3.0
1	B	226	PHE	2.9
1	B	225	VAL	2.8
1	B	321	GLY	2.8
1	B	210	ASP	2.8
1	B	50	SER	2.7
1	A	112	ALA	2.7
1	B	2	PRO	2.7
1	B	159	ASP	2.7
1	B	7	PRO	2.6
1	B	245	GLY	2.6
1	B	198	LEU	2.6
1	B	243	VAL	2.6
1	B	335	PRO	2.6
1	B	32	CYS	2.5
1	B	6	VAL	2.5
1	B	211	PRO	2.5
1	B	246	LEU	2.5
1	B	34	TRP	2.5
1	B	306	ALA	2.5
1	B	273	VAL	2.5
1	A	7	PRO	2.4
1	B	113	GLY	2.4
1	B	4	LEU	2.4
1	B	166	PHE	2.4
1	B	221	ASP	2.4
1	B	309	GLY	2.4
1	B	209	GLU	2.3
1	A	322	LEU	2.3
1	B	162	LEU	2.3
1	B	158	ALA	2.3
1	B	236	ALA	2.3
1	B	274	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	ASP	2.3
1	B	111	ASN	2.3
1	B	227	ARG	2.3
1	B	26	VAL	2.3
1	B	248	VAL	2.3
1	B	252	VAL	2.2
1	A	251	LEU	2.2
1	B	212	SER	2.2
1	A	6	VAL	2.2
1	B	218	LEU	2.2
1	A	111	ASN	2.2
1	B	38	THR	2.1
1	B	231	ALA	2.1
1	B	23	ARG	2.1
1	A	108	GLY	2.1
1	B	193	THR	2.1
1	B	307	VAL	2.1
1	A	157	LEU	2.1
1	B	194	GLY	2.0
1	B	160	ARG	2.0
1	A	107	LEU	2.0
1	B	33	THR	2.0
1	B	165	LEU	2.0
1	B	182	GLY	2.0
1	B	13	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

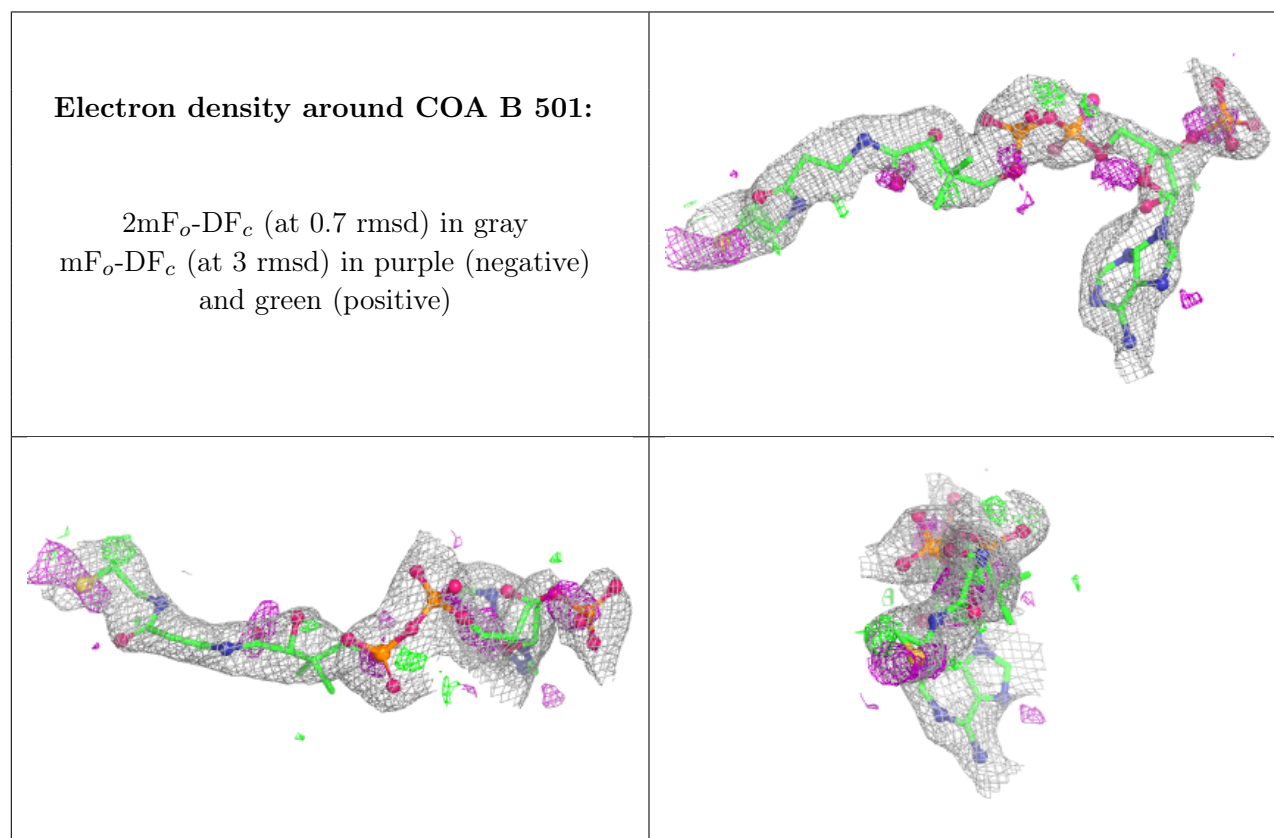
There are no monosaccharides in this entry.

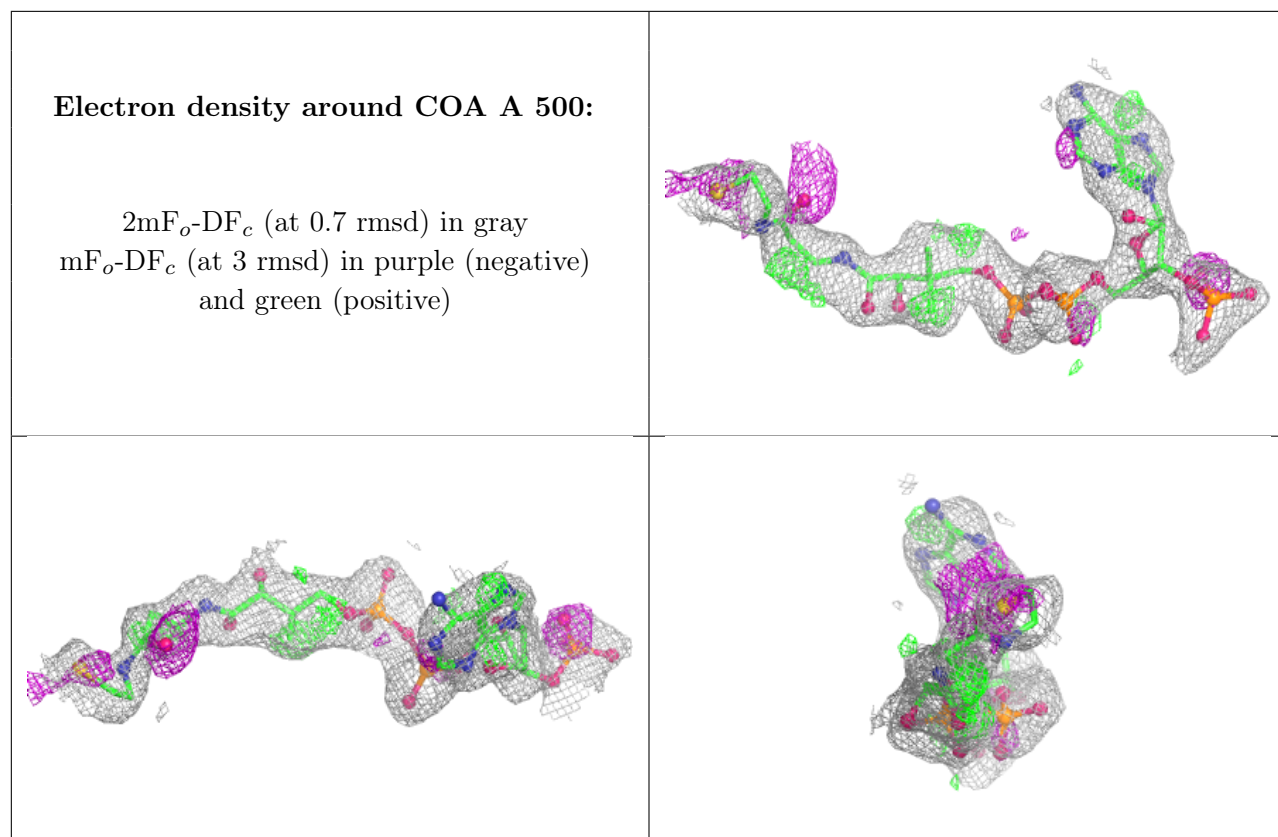
## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	COA	B	501	48/48	0.76	0.16	55,71,78,79	0
2	COA	A	500	48/48	0.77	0.15	46,56,73,75	0
3	ACE	A	502	3/3	0.78	0.20	20,20,20,20	0
3	ACE	B	503	3/3	0.90	0.24	20,20,20,20	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.