



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:03 AM UTC

PDB ID : 1MZJ / pdb_00001mzj
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

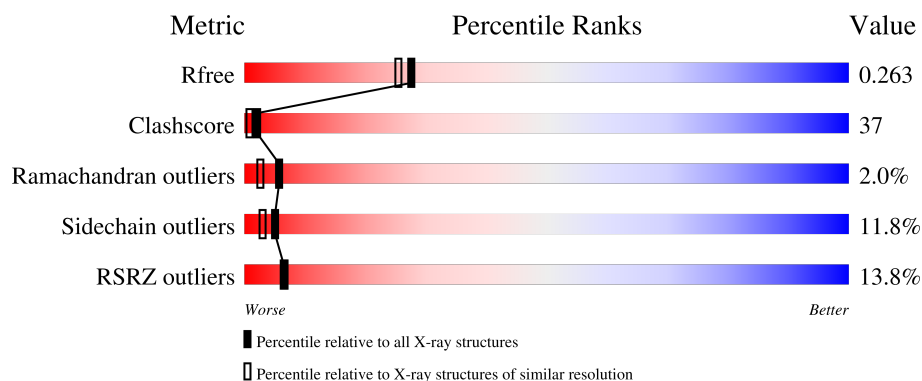
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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	-	X	-
2	COA	B	501	X	X	X	-
3	ACE	A	502	-	-	X	-

2 Entry composition ⓘ

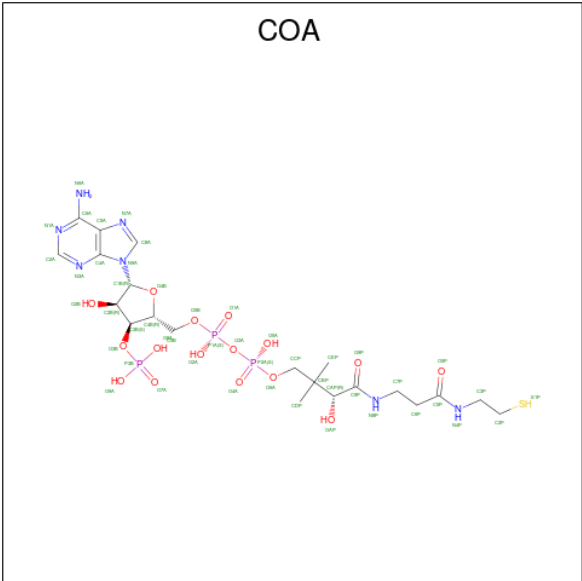
There are 4 unique types of molecules in this entry. The entry contains 5388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

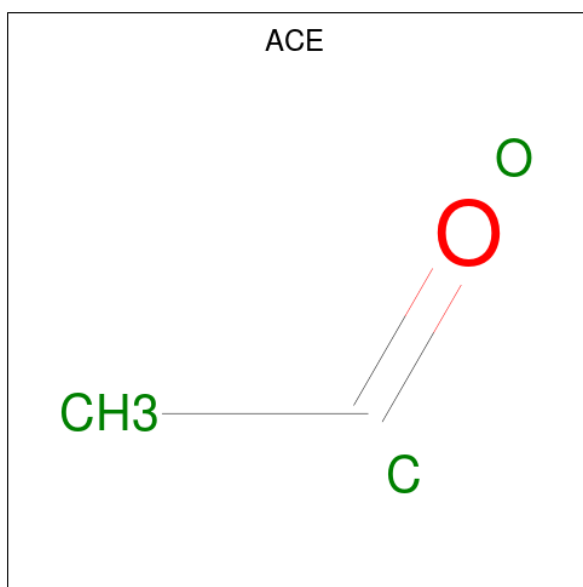
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2453	1530	443	471	9			
1	B	334	Total	C	N	O	S	0	0	0
			2454	1532	443	470	9			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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 (CCD ID: ACE) (formula: C₂H₄O).



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		

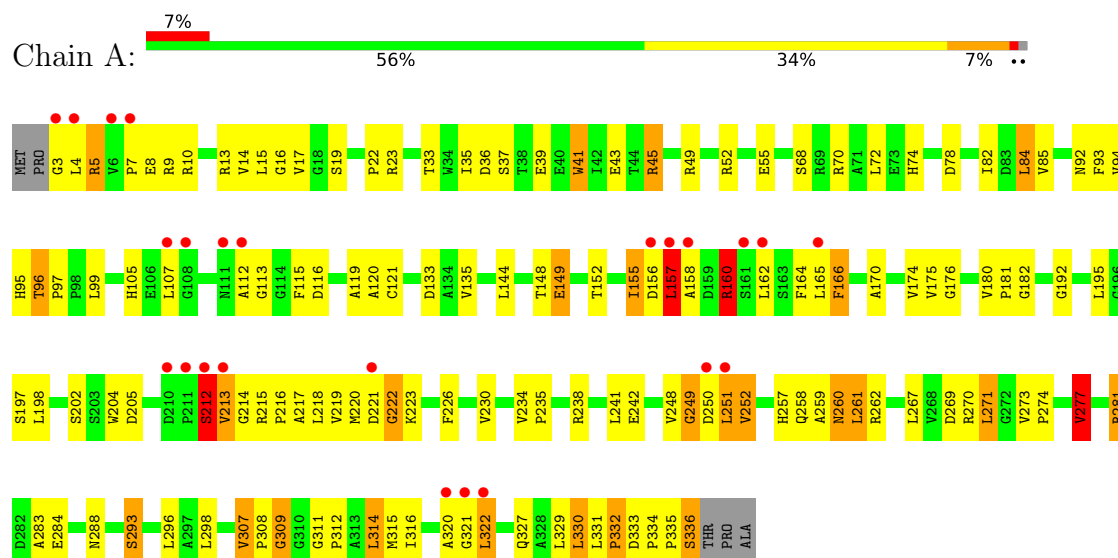
- Molecule 4 is water.

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

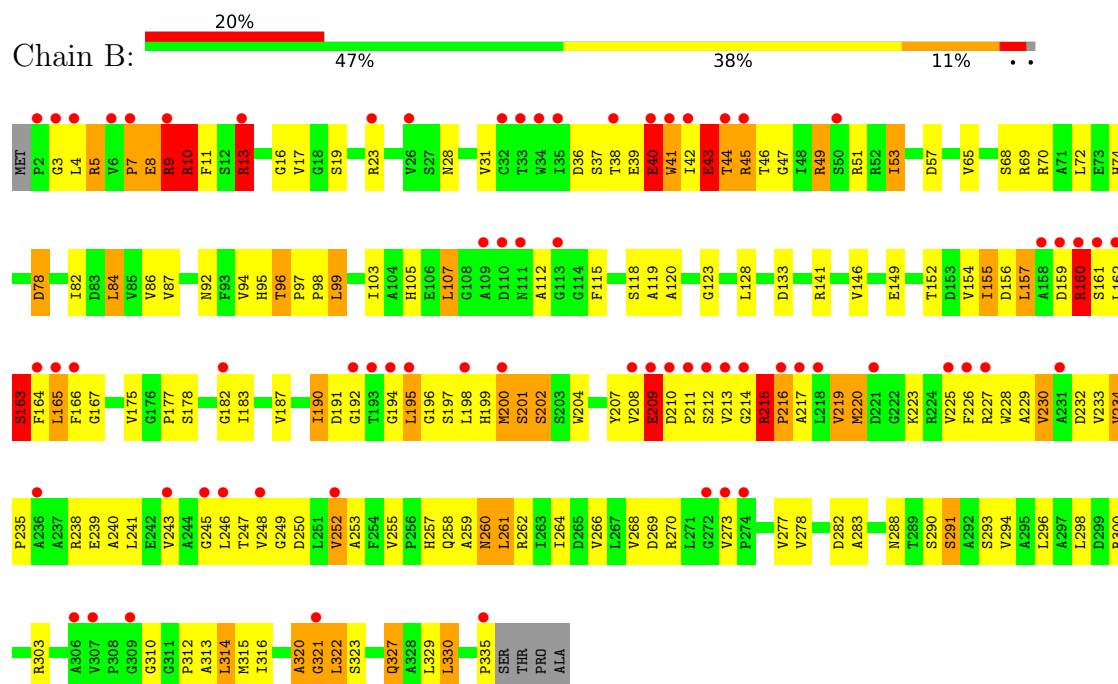
3 Residue-property plots

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.224 , 0.263	Depositor DCC
R_{free} test set	2112 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: 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	1.05	1/2499 (0.0%)	1.38	26/3407 (0.8%)
1	B	0.83	2/2501 (0.1%)	1.24	26/3410 (0.8%)
All	All	0.95	3/5000 (0.1%)	1.31	52/6817 (0.8%)

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	10.33	1.48	1.37
1	B	41	TRP	NE1-CE2	10.19	1.48	1.37
1	B	234	VAL	CA-CB	5.27	1.57	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	VAL	CA-C-N	9.47	129.41	119.85
1	A	307	VAL	C-N-CA	9.47	129.41	119.85
1	B	252	VAL	N-CA-C	-8.58	104.54	112.43
1	B	321	GLY	N-CA-C	-8.38	104.77	115.42
1	A	166	PHE	O-C-N	7.59	131.83	123.10
1	B	123	GLY	N-CA-C	7.21	121.62	112.83
1	B	107	LEU	CA-C-N	-6.91	110.91	122.25
1	B	107	LEU	C-N-CA	-6.91	110.91	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ALA	CA-C-N	-6.79	114.61	122.83
1	B	112	ALA	C-N-CA	-6.79	114.61	122.83
1	B	163	SER	CA-C-N	6.70	131.37	122.06
1	B	163	SER	C-N-CA	6.70	131.37	122.06
1	A	277	VAL	N-CA-C	6.43	117.84	108.58
1	B	190	ILE	CA-C-N	6.42	132.05	123.00
1	B	190	ILE	C-N-CA	6.42	132.05	123.00
1	A	252	VAL	N-CA-C	-6.24	106.12	113.42
1	A	249	GLY	N-CA-C	6.13	121.58	113.37
1	A	174	VAL	CA-C-N	-6.10	114.64	123.06
1	A	174	VAL	C-N-CA	-6.10	114.64	123.06
1	A	212	SER	CB-CA-C	-6.09	98.52	110.10
1	A	149	GLU	N-CA-C	6.00	118.41	108.99
1	A	331	LEU	CA-C-N	5.88	125.79	119.85
1	A	331	LEU	C-N-CA	5.88	125.79	119.85
1	B	49	ARG	N-CA-C	-5.88	106.23	113.41
1	A	160	ARG	O-C-N	-5.68	115.00	122.39
1	A	217	ALA	O-C-N	-5.64	116.30	123.24
1	A	33	THR	N-CA-C	-5.63	106.07	113.17
1	B	7	PRO	N-CA-CB	5.60	108.23	103.35
1	B	220	MET	N-CA-C	5.53	117.80	109.23
1	A	23	ARG	N-CA-C	5.43	117.96	111.71
1	B	320	ALA	N-CA-C	5.42	117.94	110.35
1	A	160	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	A	293	SER	N-CA-C	5.35	116.80	111.07
1	A	309	GLY	N-CA-C	-5.35	105.70	112.54
1	B	216	PRO	N-CA-CB	5.23	108.31	103.39
1	A	215	ARG	CD-NE-CZ	-5.19	117.14	124.40
1	A	332	PRO	N-CA-CB	5.13	108.10	103.33
1	B	202	SER	O-C-N	-5.13	118.16	123.29
1	B	5	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	A	5	ARG	CD-NE-CZ	-5.12	117.24	124.40
1	A	45	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	B	160	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	281	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	A	5	ARG	O-C-N	-5.05	115.87	122.59
1	B	10	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	B	291	SER	O-C-N	-5.05	116.31	122.22
1	B	9	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	B	13	ARG	CD-NE-CZ	-5.03	117.35	124.40
1	A	334	PRO	N-CA-C	-5.03	105.64	110.47
1	B	215	ARG	CD-NE-CZ	-5.01	117.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	GLU	CA-C-N	5.01	127.40	120.29
1	B	40	GLU	C-N-CA	5.01	127.40	120.29

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 ⓘ

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	155	0
1	B	2454	0	2438	225	0
2	A	48	0	31	21	0
2	B	48	0	31	24	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	373	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 37.

All (373) 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:A:315:MET:HE3	1:A:329:LEU:HD21	1.28	1.15
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:220:MET:HE3	1:A:222:GLY:HA2	1.53	0.90
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:315:MET:HE3	1:A:329:LEU:CD2	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:17:VAL:H	1:A:74:HIS:HD2	1.30	0.78
1:A:221:ASP:O	1:A:222:GLY:C	2.26	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:B:38:THR:C	1:B:40:GLU:H	1.93	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:320:ALA:C	1:B:322:LEU:H	1.94	0.74
1:A:315:MET:CE	1:A:329:LEU:HD21	2.13	0.73
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: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
1:B:156:ASP:HB3	1:B:159:ASP:CG	2.14	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:B:214:GLY:O	1:B:215:ARG:C	2.33	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: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:A:298:LEU:HD13	1:A:315:MET:CE	2.23	0.68
1:A:298:LEU:HD22	1:A:315:MET:HE1	1.75	0.68
1:B:13:ARG:HB3	1:B:182:GLY:HA3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:199:HIS:CE1	1:B:219:VAL:CG2	2.81	0.63
1:B:8:GLU:O	1:B:8:GLU:HG2	1.98	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
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: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: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:38:THR:C	1:B:40:GLU:N	2.59	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:298:LEU:HD22	1:B:315:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:O	1:B:8:GLU:CG	2.48	0.60
1:B:252:VAL:HG22	1:B:312:PRO:O	2.01	0.60
1:A:220:MET:HE3	1:A:222:GLY:CA	2.28	0.60
1:A:260:ASN:ND2	1:A:262:ARG:H	1.99	0.60
1:B:315:MET:HE3	1:B:329:LEU:HD21	1.82	0.60
1:A:298:LEU:CD2	1:A:315:MET:HE1	2.32	0.59
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:B:232:ASP:C	1:B:235:PRO:HD2	2.27	0.59
1:A:220:MET:HE1	2:A:500:COA:H71	1.85	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
1:B:194:GLY:O	1:B:195:LEU:C	2.46	0.58
2:B:501:COA:H132	2:B:501:COA:O4A	2.04	0.58
1:B:298:LEU:HD13	1:B:315:MET:HE2	1.86	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ALA:C	1:B:322:LEU:N	2.64	0.55
1:B:46:THR:OG1	1:B:47:GLY:N	2.38	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
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:210:ASP:CG	1:B:212:SER:HB3	2.32	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: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:B:194:GLY:C	1:B:196:GLY:N	2.67	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:A:92:ASN:HD22	1:A:92:ASN:C	2.18	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:A:13:ARG:NH2	4:A:599:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:HB3	1:B:283:ALA:HB2	1.92	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:A:298:LEU:HD13	1:A:315:MET:HE2	1.92	0.50
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: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:A:220:MET:CE	1:A:222:GLY:HA2	2.35	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:B:216:PRO:O	1:B:217:ALA:HB2	2.11	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: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: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:298:LEU:HD13	1:A:315:MET:HE1	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:B:247:THR:HG22	1:B:250:ASP:CG	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:PHE:HB2	1:B:178:SER:O	2.14	0.47
1:A:221:ASP:C	1:A:221:ASP:OD2	2.57	0.47
1:B:207:TYR:HD2	1:B:214:GLY:CA	2.28	0.47
1:B:211:PRO:O	1:B:212:SER:C	2.58	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:23:ARG:HH22	1:B:57:ASP:CG	2.23	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
1:A:148:THR:C	1:A:149:GLU:HG2	2.40	0.47
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: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:B:159:ASP:C	1:B:161:SER:N	2.74	0.46
1:B:128:LEU:HD23	1:B:327:GLN:CD	2.41	0.46
1:A:84:LEU:HD22	1:A:85:VAL:N	2.30	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:315:MET:HE3	1:B:329:LEU:HD11	1.98	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:A:92:ASN:C	1:A:92:ASN:ND2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:SER:HB2	1:B:322: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:A:298:LEU:CD1	1:A:315:MET:HE1	2.47	0.44
1:B:160:ARG:O	1:B:161:SER:C	2.60	0.44
1:B:165:LEU:O	1:B:288:ASN:HB3	2.17	0.44
1:B:220:MET:HE1	2:B:501:COA:HN4	1.83	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:200:MET:O	1:B:201:SER:C	2.60	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: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:B:245:GLY:C	1:B:246:LEU:HG	2.43	0.43
1:A:15:LEU:HD11	1:A:176:GLY:HA3	2.00	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: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: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:322:LEU:HD12	1:A:322:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:315:MET:HE3	1:A:329:LEU:CG	2.49	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: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
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:198:LEU:CD1	1:B:225:VAL:HG21	2.51	0.41
1:A:226:PHE:C	1:A:226:PHE:CD2	2.98	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:248:VAL:HG23	1:B:249:GLY:N	2.35	0.41
1:A:4:LEU:O	1:A:5:ARG:HB2	2.20	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:200:MET:C	1:B:202:SER:N	2.78	0.40
1:B:262:ARG:O	1:B:266:VAL:HG23	2.21	0.40
1:B:303:ARG:HG2	1:B:335:PRO:HG3	2.03	0.40
1:B:314:LEU:HD23	1:B:314:LEU:C	2.46	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	10
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	2

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 [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	258/262 (98%)	231 (90%)	27 (10%)	6	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	258/262 (98%)	224 (87%)	34 (13%)	4	2
All	All	516/524 (98%)	455 (88%)	61 (12%)	5	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	70	ARG
1	A	78	ASP
1	A	84	LEU
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	175	VAL
1	A	195	LEU
1	A	205	ASP
1	A	212	SER
1	A	219	VAL
1	A	250	ASP
1	A	251	LEU
1	A	260	ASN
1	A	261	LEU
1	A	271	LEU
1	A	277	VAL
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	13	ARG
1	B	40	GLU
1	B	43	GLU
1	B	44	THR
1	B	45	ARG
1	B	53	ILE
1	B	70	ARG
1	B	78	ASP

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Mol	Chain	Res	Type
1	B	84	LEU
1	B	96	THR
1	B	99	LEU
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	219	VAL
1	B	230	VAL
1	B	241	LEU
1	B	260	ASN
1	B	261	LEU
1	B	291	SER
1	B	314	LEU
1	B	322	LEU
1	B	327	GLN
1	B	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	92	ASN
1	A	95	HIS
1	A	111	ASN
1	A	257	HIS
1	A	260	ASN
1	B	28	ASN
1	B	74	HIS
1	B	92	ASN
1	B	95	HIS
1	B	111	ASN
1	B	142	HIS
1	B	199	HIS

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Mol	Chain	Res	Type
1	B	257	HIS
1	B	260	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	B	501	3	47,50,50	2.92	19 (40%)	69,75,75	4.06	38 (55%)
3	ACE	A	502	1,2	1,2,2	1.03	0	0,1,1	-	-
2	COA	A	500	3	47,50,50	3.87	23 (48%)	69,75,75	3.29	30 (43%)
3	ACE	B	503	1,2	1,2,2	1.06	0	0,1,1	-	-

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	B	501	3	1/1/11/13	25/48/64/64	0/3/3/3
2	COA	A	500	3	1/1/11/13	13/48/64/64	0/3/3/3

All (42) 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	P3B-O3B	8.51	1.74	1.59
2	A	500	COA	C5A-C4A	7.72	1.52	1.39
2	B	501	COA	P2A-O3A	7.51	1.67	1.59
2	A	500	COA	C8A-N7A	7.19	1.45	1.31
2	A	500	COA	C4A-N3A	7.14	1.47	1.34
2	B	501	COA	C4A-N3A	6.68	1.46	1.34
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	B	501	COA	C8A-N7A	5.67	1.42	1.31
2	B	501	COA	C6A-N6A	5.26	1.47	1.34
2	B	501	COA	P1A-O3A	4.80	1.64	1.59
2	A	500	COA	C6A-N6A	4.48	1.45	1.34
2	A	500	COA	C9P-N8P	4.33	1.43	1.33
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	C2A-N3A	4.07	1.41	1.33
2	B	501	COA	C6A-N1A	3.94	1.46	1.35
2	B	501	COA	C5A-C4A	3.82	1.45	1.39
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	C2A-N3A	3.61	1.40	1.33
2	A	500	COA	P3B-O7A	3.55	1.61	1.50
2	A	500	COA	C6A-N1A	3.10	1.44	1.35
2	A	500	COA	C8A-N9A	3.09	1.42	1.37
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	P1A-O1A	2.24	1.58	1.50
2	A	500	COA	O4B-C1B	2.17	1.47	1.42
2	A	500	COA	C1B-N9A	2.14	1.52	1.46
2	B	501	COA	C8A-N9A	2.13	1.41	1.37
2	A	500	COA	O2B-C2B	2.06	1.48	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	COA	C5A-C4A-N3A	-15.52	105.34	126.72
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	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
2	B	501	COA	N3A-C2A-N1A	-8.73	115.36	128.58
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	CEP-CBP-CAP	7.06	120.81	108.77
2	B	501	COA	C6A-C5A-C4A	6.27	125.74	117.18
2	A	500	COA	O2B-C2B-C1B	-6.13	88.98	110.10
2	A	500	COA	C2A-N1A-C6A	5.89	128.41	118.73
2	B	501	COA	N6A-C6A-N1A	5.80	131.30	118.38
2	A	500	COA	C7P-C6P-C5P	-5.74	102.83	112.39
2	A	500	COA	C5A-C4A-N3A	-5.54	119.09	126.72
2	A	500	COA	C5A-C6A-N6A	5.52	136.96	123.29
2	A	500	COA	O4B-C1B-C2B	-5.40	95.07	106.62
2	A	500	COA	C4A-C5A-N7A	-5.39	104.42	110.58
2	B	501	COA	CDP-CBP-CAP	-5.30	99.74	108.77
2	B	501	COA	N9A-C8A-N7A	-5.26	106.47	113.94
2	A	500	COA	N6A-C6A-N1A	-5.12	106.97	118.38
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	C6A-C5A-C4A	4.86	123.81	117.18
2	A	500	COA	N3A-C2A-N1A	-4.84	121.25	128.58
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	B	501	COA	C7P-C6P-C5P	-4.39	105.08	112.39
2	A	500	COA	C5A-C4A-N9A	4.14	110.32	105.81
2	B	501	COA	C4A-N9A-C8A	4.05	109.99	105.74
2	B	501	COA	CEP-CBP-CDP	-3.85	101.53	109.20
2	A	500	COA	C1B-N9A-C8A	-3.85	118.56	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	COA	C4A-N9A-C1B	3.83	135.59	126.63
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	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	C5A-N7A-C8A	3.36	108.72	103.45
2	B	501	COA	C1B-N9A-C8A	-3.34	119.69	127.09
2	A	500	COA	CDP-CBP-CCP	-3.33	102.72	108.22
2	B	501	COA	C6A-C5A-N7A	-3.32	125.69	132.09
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	C5A-C6A-N1A	-3.06	109.74	117.51
2	B	501	COA	C4A-C5A-N7A	-3.03	107.12	110.58
2	B	501	COA	C5A-N7A-C8A	3.02	108.19	103.45
2	B	501	COA	N3A-C4A-N9A	2.87	132.04	127.17
2	B	501	COA	CEP-CBP-CCP	-2.83	103.55	108.22
2	B	501	COA	C4B-O4B-C1B	-2.79	103.30	109.47
2	A	500	COA	CEP-CBP-CDP	2.76	114.71	109.20
2	B	501	COA	O4B-C1B-C2B	-2.71	100.81	106.62
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	O4B-C1B-N9A	-2.61	103.07	108.09
2	B	501	COA	C2B-C3B-C4B	2.57	107.73	103.24
2	B	501	COA	C5A-C6A-N6A	-2.56	116.95	123.29
2	A	500	COA	C2P-C3P-N4P	-2.48	106.69	112.31
2	B	501	COA	O5B-C5B-C4B	-2.41	100.78	108.99
2	B	501	COA	C5A-C6A-N1A	-2.28	111.74	117.51
2	A	500	COA	C3B-C2B-C1B	2.24	104.82	99.89
2	A	500	COA	N9A-C8A-N7A	-2.12	110.92	113.94
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 (38) torsion outliers are listed below:

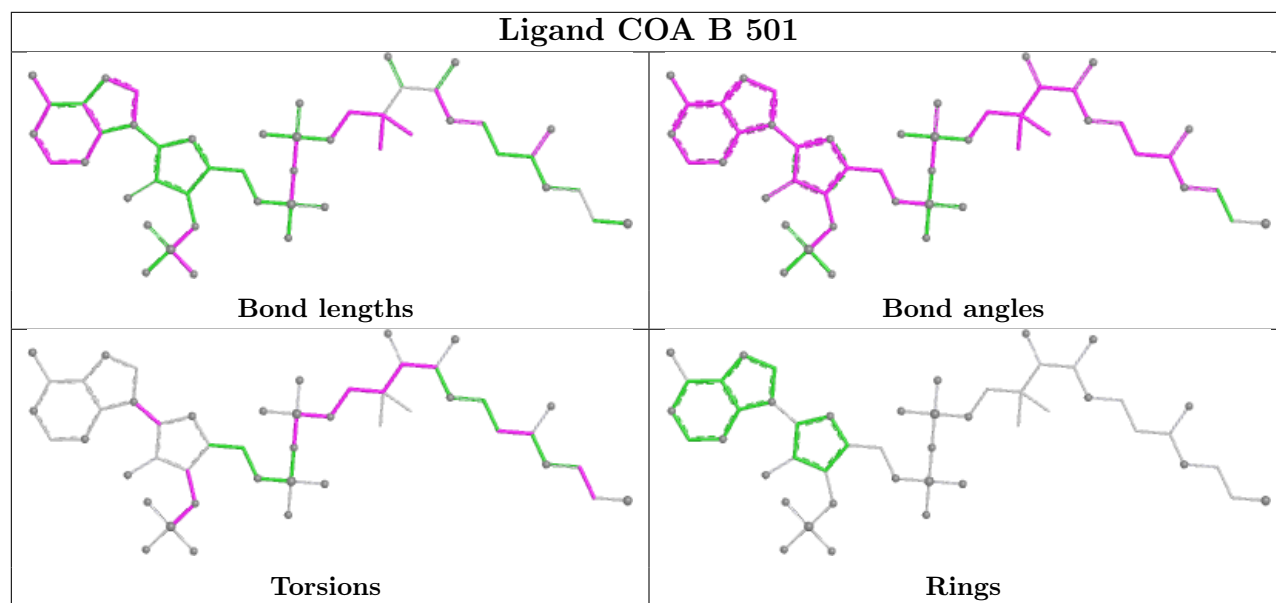
Mol	Chain	Res	Type	Atoms
2	A	500	COA	C4B-C3B-O3B-P3B
2	A	500	COA	CCP-O6A-P2A-O4A
2	A	500	COA	C5P-C6P-C7P-N8P
2	A	500	COA	S1P-C2P-C3P-N4P
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	CCP-O6A-P2A-O4A
2	B	501	COA	CBP-CCP-O6A-P2A
2	B	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CEP-CBP-CCP-O6A
2	B	501	COA	CAP-CBP-CCP-O6A
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
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	A	500	COA	C2B-C1B-N9A-C8A
2	B	501	COA	C2B-C1B-N9A-C8A
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

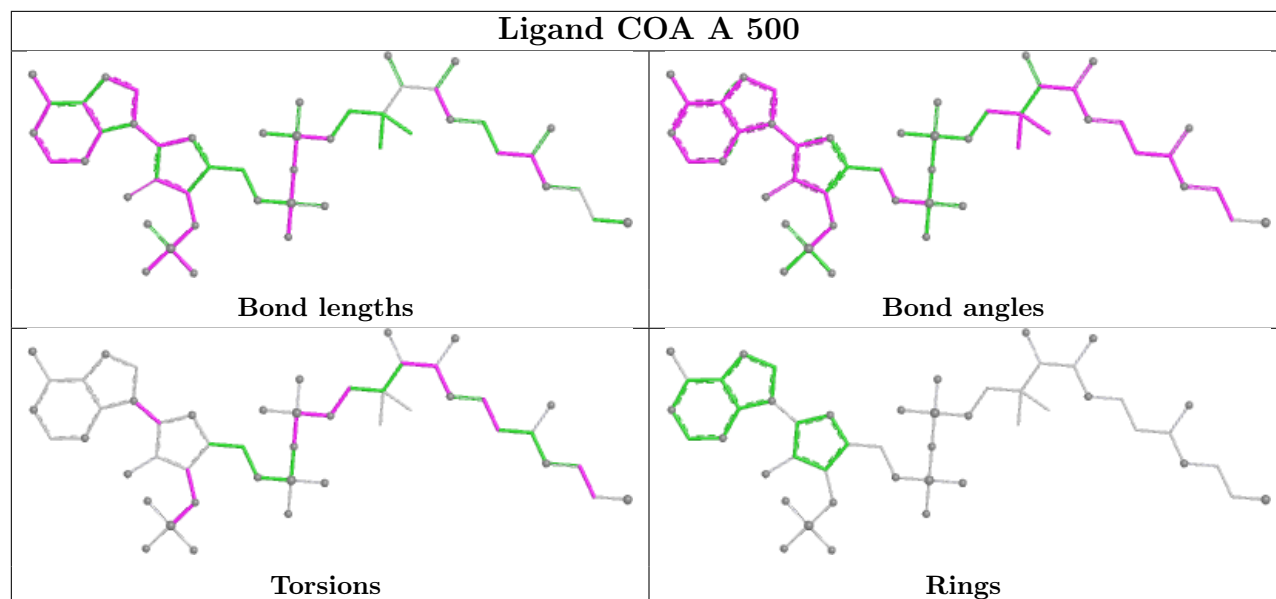
There are no ring outliers.

3 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	COA	24	0
3	A	502	ACE	2	0
2	A	500	COA	21	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, 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	334/339 (98%)	0.35	24 (7%) 21 23	22, 35, 56, 85	0
1	B	334/339 (98%)	1.11	68 (20%) 3 3	29, 51, 77, 96	0
All	All	668/678 (98%)	0.73	92 (13%) 6 6	22, 42, 73, 96	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PRO	8.3
1	B	164	PHE	6.7
1	A	4	LEU	5.9
1	B	44	THR	5.4
1	B	213	VAL	5.2
1	A	210	ASP	4.7
1	A	321	GLY	4.7
1	B	3	GLY	4.7
1	B	40	GLU	4.2
1	A	213	VAL	4.2
1	A	3	GLY	4.2
1	B	214	GLY	4.2
1	A	212	SER	4.1
1	B	217	ALA	4.1
1	B	195	LEU	3.8
1	B	208	VAL	3.7
1	A	161	SER	3.7
1	B	41	TRP	3.6
1	B	9	ARG	3.6
1	B	42	ILE	3.6
1	A	156	ASP	3.5
1	B	161	SER	3.5
1	A	162	LEU	3.5
1	B	35	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	PRO	3.4
1	A	320	ALA	3.4
1	A	250	ASP	3.3
1	B	200	MET	3.3
1	A	158	ALA	3.2
1	B	109	ALA	3.2
1	A	165	LEU	3.2
1	B	110	ASP	3.2
1	B	272	GLY	3.2
1	B	45	ARG	3.1
1	B	226	PHE	3.0
1	B	225	VAL	2.9
1	B	321	GLY	2.9
1	A	112	ALA	2.9
1	B	210	ASP	2.8
1	B	50	SER	2.8
1	B	2	PRO	2.8
1	B	245	GLY	2.8
1	B	7	PRO	2.8
1	B	198	LEU	2.8
1	B	159	ASP	2.7
1	B	243	VAL	2.7
1	B	335	PRO	2.7
1	B	6	VAL	2.7
1	B	32	CYS	2.7
1	B	34	TRP	2.7
1	B	211	PRO	2.6
1	B	306	ALA	2.6
1	B	246	LEU	2.6
1	B	273	VAL	2.6
1	A	7	PRO	2.6
1	B	113	GLY	2.5
1	B	4	LEU	2.5
1	B	166	PHE	2.5
1	B	309	GLY	2.5
1	B	158	ALA	2.5
1	B	236	ALA	2.5
1	A	322	LEU	2.5
1	B	162	LEU	2.5
1	B	221	ASP	2.4
1	B	274	PRO	2.4
1	B	209	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	26	VAL	2.4
1	B	248	VAL	2.4
1	B	111	ASN	2.4
1	A	221	ASP	2.4
1	B	252	VAL	2.4
1	A	251	LEU	2.4
1	A	6	VAL	2.4
1	B	227	ARG	2.4
1	B	212	SER	2.3
1	B	218	LEU	2.3
1	B	231	ALA	2.3
1	B	38	THR	2.3
1	A	111	ASN	2.3
1	A	108	GLY	2.3
1	B	193	THR	2.2
1	B	307	VAL	2.2
1	B	194	GLY	2.2
1	A	157	LEU	2.2
1	B	23	ARG	2.2
1	B	182	GLY	2.2
1	A	107	LEU	2.2
1	B	165	LEU	2.2
1	B	33	THR	2.2
1	B	160	ARG	2.1
1	B	13	ARG	2.1
1	B	192	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

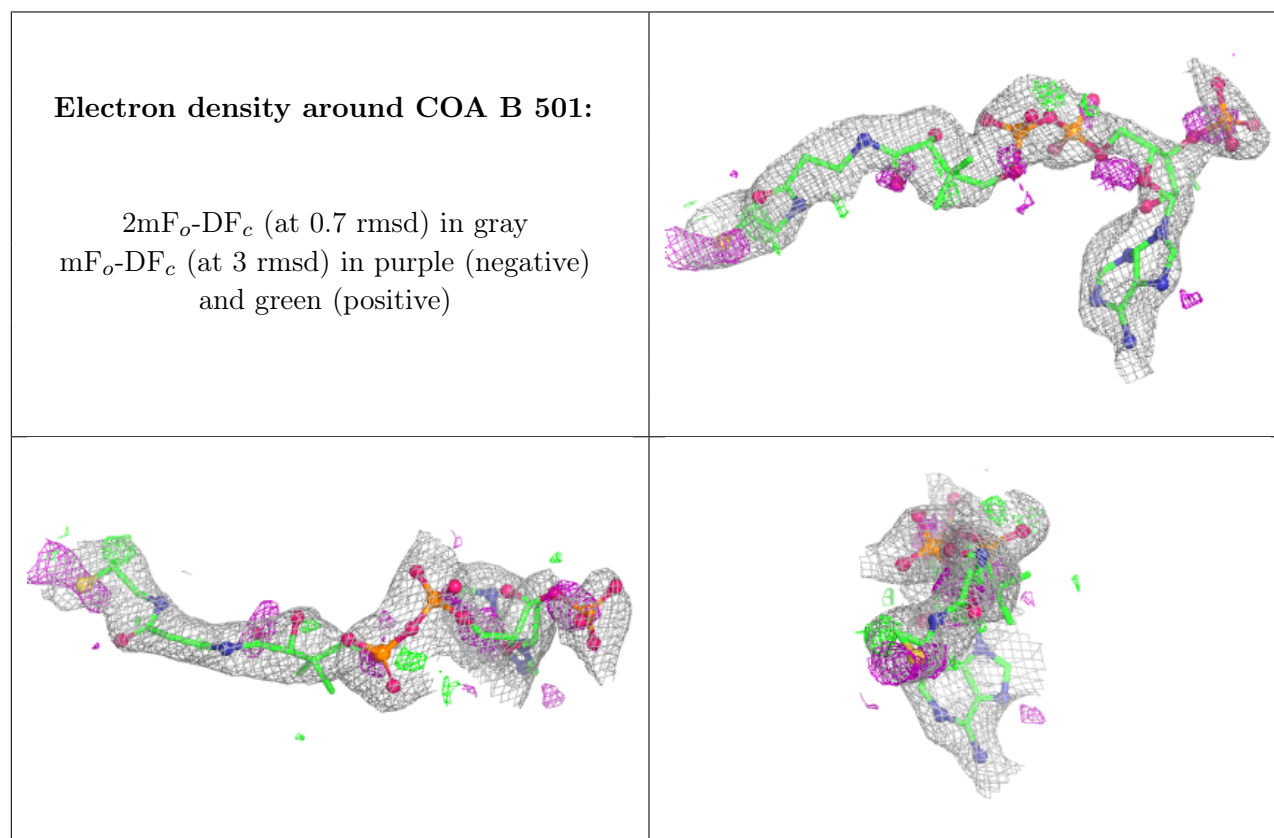
There are no oligosaccharides in this entry.

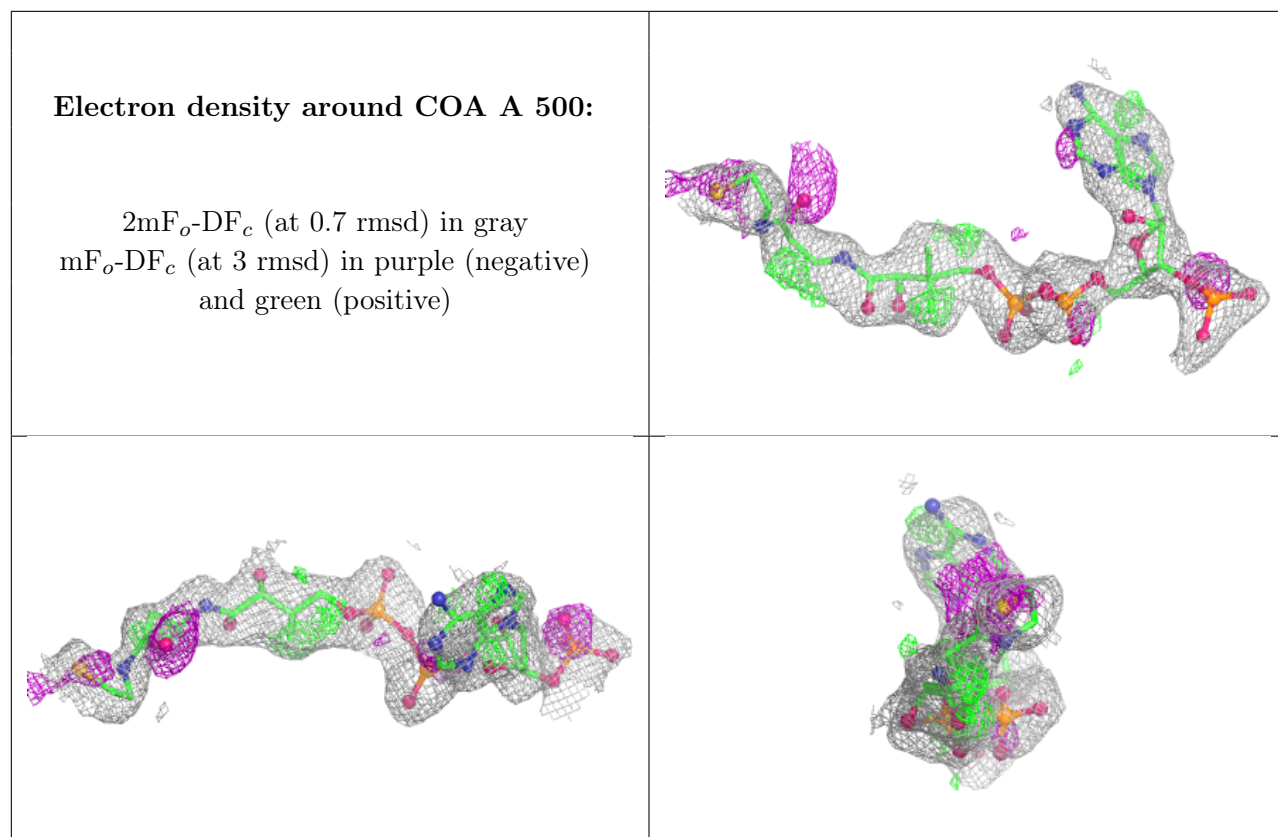
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.