



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:33 pm BST

PDB ID : 2WPX
Title : Tandem GNAT protein from the clavulanic acid biosynthesis pathway (with AcCoA)
Authors : Iqbal, A.; Arunlanantham, H.; McDonough, M.A.; Chowdhury, R.; Clifton, I.J.
Deposited on : 2009-08-11
Resolution : 2.31 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 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

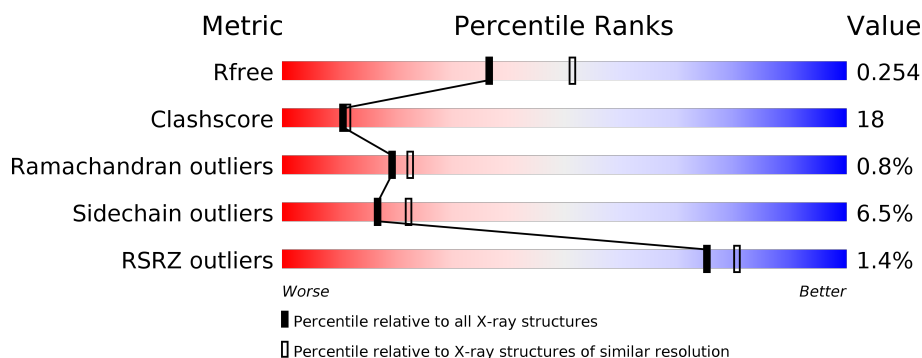
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 ≥ 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	<div> <div>%</div> <div> </div> <div>71% 22% . . .</div> </div>
1	B	339	<div> <div>%</div> <div> </div> <div>72% 20% . . .</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
3	GOL	A	1339	-	-	X	-

2 Entry composition [i](#)

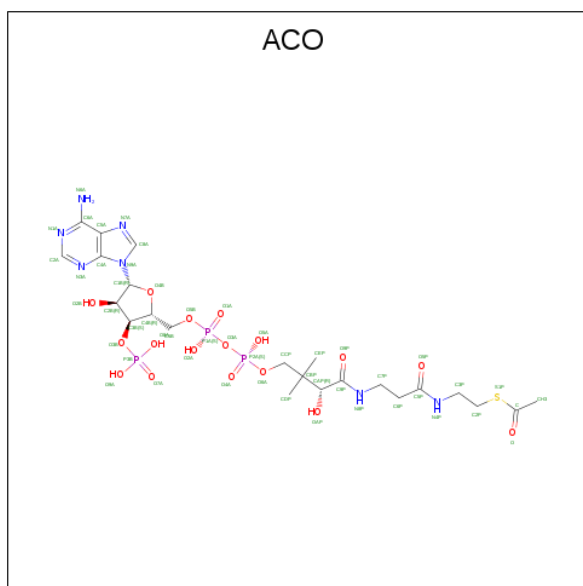
There are 4 unique types of molecules in this entry. The entry contains 5646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ORF14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2471	1546	460	458	7			
1	B	326	Total	C	N	O	S	0	0	0
			2471	1546	460	458	7			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	295	Total	O	0	0
			295	295		

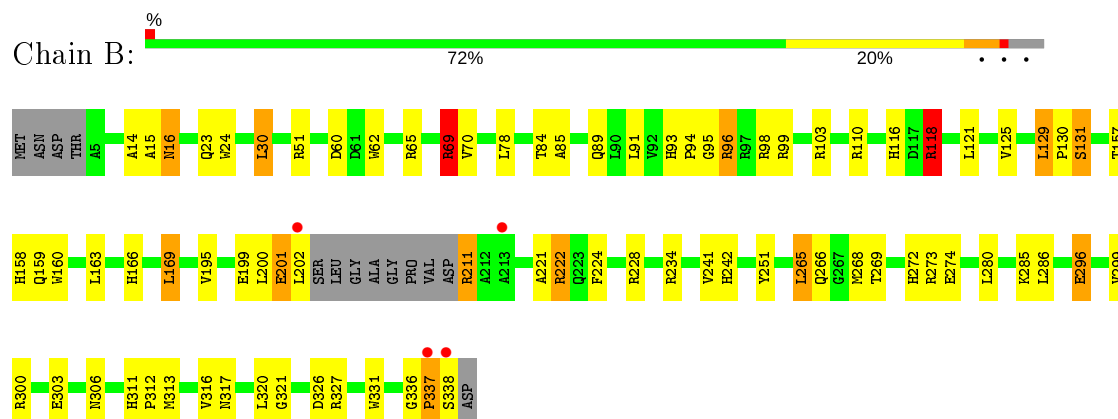
3 Residue-property plots

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: ORF14



• Molecule 1: ORF14



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.99 Å 70.09 Å 106.29 Å 90.00° 134.38° 90.00°	Depositor
Resolution (Å)	31.82 – 2.31 31.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.3 (31.82-2.31) 96.3 (31.82-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.188 , 0.253 0.191 , 0.254	Depositor DCC
R_{free} test set	1720 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h-2*k,l,h+1 0.022 for -h,-k,h+1 0.459 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5646	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: GOL, ACO

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	0.88	1/2534 (0.0%)	0.98	7/3465 (0.2%)
1	B	0.86	0/2534	0.94	9/3465 (0.3%)
All	All	0.87	1/5068 (0.0%)	0.96	16/6930 (0.2%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TRP	CB-CG	-5.13	1.41	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	A	97	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	118	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	A	69	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	A	69	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	A	97	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	222	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	222	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	222	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	69	ARG	NE-CZ-NH1	6.52	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	69	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	118	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	118	ARG	CG-CD-NE	5.20	122.72	111.80
1	B	222	ARG	CD-NE-CZ	5.08	130.72	123.60
1	A	222	ARG	CG-CD-NE	-5.00	101.29	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	SER	Peptide
1	A	211	ARG	Peptide

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	2471	0	2409	96	0
1	B	2471	0	2409	86	0
2	A	51	0	34	3	0
2	B	51	0	34	2	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
4	A	295	0	0	28	0
4	B	295	0	0	16	0
All	All	5646	0	4902	182	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 18.

All (182) 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:285:LYS:HE2	1:B:317:ASN:HD21	1.12	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LYS:HE2	1:A:317:ASN:OD1	1.54	1.07
1:B:201:GLU:OE2	1:B:201:GLU:N	1.93	1.02
1:A:55:PRO:O	1:A:57:THR:HG23	1.60	1.00
1:B:129:LEU:HD13	1:B:327:ARG:HB2	1.47	0.96
1:A:84:THR:HG21	4:A:2118:HOH:O	1.65	0.94
1:B:69:ARG:HD2	4:B:2077:HOH:O	1.66	0.93
1:A:272:HIS:HD2	1:A:274:GLU:H	1.17	0.92
1:A:69:ARG:HD2	4:A:2067:HOH:O	1.68	0.92
1:B:93:HIS:HD2	1:B:95:GLY:H	1.18	0.91
1:B:16:ASN:H	1:B:16:ASN:HD22	1.20	0.90
1:A:93:HIS:HD2	1:A:95:GLY:H	1.16	0.89
1:A:272:HIS:CD2	1:A:274:GLU:H	1.92	0.86
1:A:89:GLN:HA	3:A:1339:GOL:H11	1.58	0.85
1:B:16:ASN:HD22	1:B:16:ASN:N	1.72	0.84
1:A:189:THR:HB	4:A:2179:HOH:O	0.66	0.83
1:B:265:LEU:HD13	1:B:265:LEU:C	1.99	0.82
1:B:285:LYS:HE2	1:B:317:ASN:ND2	1.94	0.82
1:B:24:TRP:HE1	1:B:89:GLN:HE22	1.26	0.81
1:A:24:TRP:HE1	1:A:89:GLN:HE22	1.30	0.80
1:A:19:GLU:OE1	4:A:2014:HOH:O	1.99	0.80
1:A:189:THR:HG21	1:A:220:TYR:CZ	2.17	0.79
1:A:131:SER:HB2	4:A:2128:HOH:O	1.82	0.79
1:A:30:LEU:CD1	1:A:94:PRO:HG2	2.11	0.79
1:B:84:THR:HG21	4:B:2129:HOH:O	1.82	0.79
1:A:337:PRO:O	1:A:338:SER:HB2	1.83	0.79
1:A:308:GLU:OE2	4:A:2262:HOH:O	2.00	0.79
1:B:30:LEU:HD13	1:B:94:PRO:HG2	1.65	0.78
1:B:200:LEU:C	1:B:201:GLU:OE2	2.21	0.78
1:A:55:PRO:O	1:A:57:THR:CG2	2.33	0.77
1:B:16:ASN:H	1:B:16:ASN:ND2	1.81	0.75
1:B:159:GLN:HE22	1:B:306:ASN:HD22	1.35	0.75
1:A:108:HIS:HD2	4:A:2109:HOH:O	1.70	0.74
1:A:272:HIS:HD2	1:A:274:GLU:N	1.85	0.73
1:B:93:HIS:CD2	1:B:95:GLY:H	2.05	0.73
1:B:285:LYS:CE	1:B:317:ASN:HD21	1.98	0.73
1:A:200:LEU:CD1	4:A:2212:HOH:O	2.38	0.72
1:B:51:ARG:NH2	4:B:2062:HOH:O	2.22	0.71
1:B:96:ARG:HA	1:B:99:ARG:HH21	1.55	0.71
1:A:93:HIS:CD2	1:A:95:GLY:H	2.05	0.71
1:A:90:LEU:H	3:A:1339:GOL:H12	1.55	0.70
1:A:108:HIS:CD2	4:A:2109:HOH:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD11	1:A:248:LEU:O	1.93	0.69
1:A:98:ARG:NH1	2:A:401:ACO:O8A	2.25	0.69
1:A:30:LEU:CD1	1:A:94:PRO:CG	2.69	0.69
1:B:84:THR:HG22	1:B:85:ALA:N	2.06	0.69
1:B:110:ARG:HH21	1:B:336:GLY:HA3	1.58	0.69
1:A:90:LEU:H	3:A:1339:GOL:C1	2.06	0.67
1:B:110:ARG:NH2	1:B:336:GLY:HA3	2.10	0.67
1:B:16:ASN:ND2	1:B:16:ASN:N	2.42	0.66
1:B:268:MET:HG3	4:B:2236:HOH:O	1.95	0.66
1:B:211:ARG:HH11	1:B:211:ARG:HB2	1.61	0.66
1:A:256:LYS:HD3	1:A:296:GLU:HG2	1.77	0.66
1:B:129:LEU:O	1:B:131:SER:N	2.29	0.66
1:B:299:VAL:O	1:B:300:ARG:HD2	1.97	0.65
1:A:190:PRO:HG2	1:B:51:ARG:HH21	1.61	0.65
1:B:265:LEU:CD1	1:B:265:LEU:C	2.66	0.62
1:A:228:ARG:HG2	4:A:2216:HOH:O	1.98	0.62
1:A:106:TRP:CD1	1:A:146:MET:HE3	2.34	0.62
1:B:269:THR:HB	1:B:313:MET:HE2	1.83	0.61
1:B:296:GLU:HG3	4:B:2232:HOH:O	2.00	0.61
1:A:55:PRO:HG3	1:A:223:GLN:HB3	1.83	0.60
1:B:129:LEU:CD1	1:B:327:ARG:HB2	2.26	0.60
1:B:265:LEU:HD13	1:B:266:GLN:N	2.15	0.60
1:B:234:ARG:HD3	4:B:2212:HOH:O	2.01	0.60
1:B:200:LEU:HD13	4:B:2223:HOH:O	2.02	0.60
1:A:131:SER:OG	4:A:2127:HOH:O	1.92	0.60
1:B:224:PHE:HB3	1:B:228:ARG:HH12	1.66	0.60
1:B:202:LEU:HG	1:B:273:ARG:HG2	1.82	0.59
1:B:195:VAL:O	1:B:199:GLU:HG2	2.03	0.58
1:B:84:THR:CG2	1:B:85:ALA:N	2.67	0.58
1:A:316:VAL:O	1:A:320:LEU:HD13	2.03	0.58
1:A:296:GLU:HG3	4:A:2224:HOH:O	2.03	0.58
1:B:129:LEU:C	1:B:131:SER:H	2.07	0.58
1:A:308:GLU:HG3	4:A:2262:HOH:O	2.03	0.57
1:A:337:PRO:O	1:A:338:SER:CB	2.51	0.57
1:B:266:GLN:NE2	1:B:285:LYS:HE2	2.19	0.57
1:B:158:HIS:HE1	1:B:303:GLU:OE1	1.87	0.57
1:A:93:HIS:HD2	1:A:95:GLY:N	1.96	0.57
1:B:296:GLU:HB3	1:B:299:VAL:HG23	1.87	0.56
1:A:30:LEU:HD11	1:A:94:PRO:HG2	1.87	0.56
1:B:272:HIS:CE1	1:B:274:GLU:HB2	2.41	0.56
1:B:118:ARG:N	1:B:118:ARG:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:HG2	1:B:338:SER:H	1.72	0.54
1:B:336:GLY:HA2	4:B:2117:HOH:O	2.06	0.54
1:B:93:HIS:HD2	1:B:95:GLY:N	1.97	0.54
1:A:65:ARG:HD3	4:A:2065:HOH:O	2.08	0.54
1:A:53:ALA:HB1	1:A:54:PRO:HD2	1.89	0.54
1:A:272:HIS:NE2	1:A:274:GLU:HG3	2.23	0.54
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.73	0.54
1:A:27:LEU:HD21	1:A:91:LEU:HD22	1.90	0.53
1:A:106:TRP:HB3	1:A:146:MET:HE2	1.89	0.53
1:A:160:TRP:CZ3	1:A:303:GLU:HB3	2.44	0.53
1:A:189:THR:CG2	1:A:220:TYR:CZ	2.91	0.53
1:B:15:ALA:HB3	1:B:51:ARG:HH11	1.73	0.53
1:B:311:HIS:N	1:B:312:PRO:CD	2.72	0.52
1:A:189:THR:HG22	1:A:225:GLU:OE1	2.09	0.52
1:A:189:THR:HG21	1:A:220:TYR:CE2	2.44	0.52
1:B:158:HIS:CE1	1:B:303:GLU:OE1	2.63	0.51
1:A:57:THR:HG21	4:A:2085:HOH:O	2.10	0.51
1:A:96:ARG:HA	1:A:99:ARG:HH21	1.74	0.51
1:A:16:ASN:OD1	1:A:16:ASN:N	2.31	0.51
1:B:221:ALA:HB3	1:B:224:PHE:CD2	2.46	0.51
1:A:266:GLN:NE2	1:A:285:LYS:HE3	2.26	0.51
1:A:153:ILE:HB	1:A:154:PRO:HD2	1.93	0.50
1:B:78:LEU:HB3	1:B:118:ARG:NH1	2.27	0.50
1:B:201:GLU:OE2	1:B:201:GLU:CA	2.60	0.49
1:A:311:HIS:N	1:A:312:PRO:CD	2.75	0.49
1:A:97:ARG:HG3	2:A:401:ACO:O4A	2.12	0.49
1:B:98:ARG:NH1	2:B:401:ACO:O8A	2.47	0.48
1:A:299:VAL:O	4:A:2255:HOH:O	2.20	0.48
1:B:228:ARG:HD3	4:B:2225:HOH:O	2.11	0.48
1:A:97:ARG:HG2	4:A:2287:HOH:O	2.14	0.48
1:B:224:PHE:HB3	1:B:228:ARG:NH1	2.29	0.48
1:B:228:ARG:CD	4:B:2209:HOH:O	2.61	0.48
1:B:99:ARG:CB	4:B:2110:HOH:O	2.61	0.48
1:A:308:GLU:CG	4:A:2262:HOH:O	2.59	0.47
1:B:157:THR:HG21	4:B:2166:HOH:O	2.14	0.47
1:A:200:LEU:HD12	4:A:2212:HOH:O	2.10	0.47
1:A:311:HIS:HB2	1:A:312:PRO:HD3	1.94	0.47
1:A:56:ALA:C	1:A:57:THR:CG2	2.83	0.47
1:B:51:ARG:CZ	4:B:2061:HOH:O	2.63	0.47
1:B:158:HIS:HB3	1:B:326:ASP:OD2	2.15	0.47
1:A:200:LEU:HD13	4:A:2212:HOH:O	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD12	1:A:94:PRO:HG2	1.93	0.47
1:A:75:ARG:HG3	1:A:89:GLN:HB3	1.97	0.47
1:A:56:ALA:O	1:A:57:THR:HG22	2.15	0.46
1:A:30:LEU:HD12	1:A:94:PRO:CG	2.43	0.46
1:A:30:LEU:HD13	1:A:94:PRO:HG3	1.96	0.46
1:A:290:GLU:OE1	4:A:2245:HOH:O	2.20	0.46
1:A:231:ARG:NH1	4:A:2202:HOH:O	2.42	0.46
1:A:91:LEU:HD23	1:A:91:LEU:C	2.36	0.46
1:B:266:GLN:NE2	1:B:285:LYS:CE	2.78	0.45
1:A:196:PRO:HA	1:A:199:GLU:HG2	1.98	0.45
1:B:160:TRP:HB2	4:B:2276:HOH:O	2.16	0.45
1:A:11:VAL:HG13	1:A:63:VAL:HG23	1.98	0.45
1:B:316:VAL:O	1:B:320:LEU:HD13	2.16	0.45
1:B:125:VAL:CG2	1:B:331:TRP:CD1	3.00	0.45
1:A:265:LEU:HD22	1:A:303:GLU:HG3	1.99	0.45
1:B:78:LEU:HD22	1:B:78:LEU:N	2.32	0.45
1:A:30:LEU:CD1	1:A:94:PRO:HG3	2.46	0.44
1:B:211:ARG:NH1	1:B:211:ARG:HB2	2.29	0.44
1:B:23:GLN:NE2	1:B:70:VAL:H	2.15	0.44
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.32	0.44
1:B:211:ARG:HD3	1:B:211:ARG:HA	1.83	0.44
1:A:184:THR:CG2	4:A:2208:HOH:O	2.64	0.44
1:B:14:ALA:HB1	1:B:16:ASN:HD21	1.81	0.44
1:A:184:THR:HG22	4:A:2208:HOH:O	2.17	0.44
1:A:158:HIS:HB3	1:A:326:ASP:OD2	2.18	0.44
1:A:103:ARG:N	2:A:401:ACO:O1A	2.46	0.44
1:B:129:LEU:C	1:B:131:SER:N	2.69	0.44
1:B:200:LEU:HD12	1:B:200:LEU:HA	1.83	0.43
1:A:189:THR:CG2	1:A:220:TYR:CE2	3.01	0.43
1:A:166:HIS:HD2	1:A:321:GLY:HA3	1.84	0.43
1:A:173:VAL:HA	1:A:174:PRO:HD3	1.87	0.43
1:B:241:VAL:HG12	1:B:242:HIS:N	2.33	0.43
1:A:261:PRO:HA	4:A:2219:HOH:O	2.19	0.43
1:B:116:HIS:O	1:B:118:ARG:CD	2.67	0.43
1:B:169:LEU:CD1	1:B:286:LEU:HD22	2.48	0.43
1:A:166:HIS:CD2	1:A:321:GLY:HA3	2.54	0.43
1:A:114:ARG:CZ	1:A:338:SER:HA	2.49	0.42
1:B:60:ASP:OD1	1:B:62:TRP:NE1	2.47	0.42
1:B:166:HIS:CD2	1:B:321:GLY:HA3	2.54	0.42
1:B:99:ARG:N	4:B:2110:HOH:O	2.45	0.42
1:A:221:ALA:HB3	1:A:224:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:MET:HG3	4:A:2228:HOH:O	2.19	0.42
1:A:93:HIS:HE1	4:A:2025:HOH:O	2.02	0.42
1:B:51:ARG:NH1	4:B:2061:HOH:O	2.53	0.41
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.20	0.41
1:B:14:ALA:CB	1:B:16:ASN:HD21	2.34	0.41
1:B:160:TRP:CZ3	1:B:303:GLU:HB3	2.55	0.41
3:A:1339:GOL:H2	4:A:2295:HOH:O	2.20	0.41
1:A:265:LEU:CD2	1:A:303:GLU:HG3	2.50	0.41
1:A:91:LEU:HD23	1:A:92:VAL:N	2.35	0.41
1:B:159:GLN:HE22	1:B:306:ASN:ND2	2.12	0.41
1:B:65:ARG:HA	1:B:69:ARG:O	2.21	0.41
1:B:69:ARG:H	1:B:69:ARG:HG3	1.64	0.41
1:A:211:ARG:CZ	1:A:211:ARG:HB2	2.50	0.41
1:A:272:HIS:CD2	1:A:272:HIS:C	2.95	0.41
1:B:103:ARG:N	2:B:401:ACO:O1A	2.48	0.41
1:A:299:VAL:O	1:A:300:ARG:HD2	2.21	0.41
1:A:272:HIS:CD2	1:A:274:GLU:N	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	322/339 (95%)	314 (98%)	6 (2%)	2 (1%)	25	30
1	B	322/339 (95%)	314 (98%)	5 (2%)	3 (1%)	17	19
All	All	644/678 (95%)	628 (98%)	11 (2%)	5 (1%)	19	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	SER

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Mol	Chain	Res	Type
1	B	337	PRO
1	A	212	ALA
1	B	130	PRO
1	A	337	PRO

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	246/256 (96%)	231 (94%)	15 (6%)	18	25
1	B	246/256 (96%)	229 (93%)	17 (7%)	15	20
All	All	492/512 (96%)	460 (94%)	32 (6%)	17	22

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	57	THR
1	A	69	ARG
1	A	121	LEU
1	A	131	SER
1	A	202	LEU
1	A	211	ARG
1	A	222	ARG
1	A	228	ARG
1	A	251	TYR
1	A	280	LEU
1	A	293	LEU
1	A	294	ARG
1	A	296	GLU
1	A	300	ARG
1	B	16	ASN
1	B	30	LEU
1	B	69	ARG
1	B	91	LEU

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Mol	Chain	Res	Type
1	B	96	ARG
1	B	118	ARG
1	B	121	LEU
1	B	129	LEU
1	B	163	LEU
1	B	169	LEU
1	B	201	GLU
1	B	211	ARG
1	B	222	ARG
1	B	251	TYR
1	B	265	LEU
1	B	280	LEU
1	B	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	93	HIS
1	A	108	HIS
1	A	135	GLN
1	A	260	ASN
1	A	266	GLN
1	A	272	HIS
1	A	288	ASN
1	B	16	ASN
1	B	23	GLN
1	B	89	GLN
1	B	93	HIS
1	B	108	HIS
1	B	135	GLN
1	B	158	HIS
1	B	266	GLN
1	B	306	ASN
1	B	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	ACO	B	401	-	45,53,53	1.56	3 (6%)	56,79,79	3.62	21 (37%)
2	ACO	A	401	-	45,53,53	1.65	5 (11%)	56,79,79	3.65	19 (33%)
3	GOL	A	1339	-	5,5,5	0.73	0	5,5,5	1.35	1 (20%)
3	GOL	B	1339	-	5,5,5	0.88	0	5,5,5	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	B	401	-	-	19/47/67/67	0/3/3/3
2	ACO	A	401	-	-	13/47/67/67	0/3/3/3
3	GOL	A	1339	-	-	2/4/4/4	-
3	GOL	B	1339	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ACO	O4B-C1B	6.49	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ACO	P3B-O7A	5.40	1.68	1.50
2	B	401	ACO	O4B-C1B	4.73	1.47	1.41
2	A	401	ACO	P3B-O7A	4.11	1.63	1.50
2	A	401	ACO	O5B-C5B	-3.96	1.29	1.44
2	B	401	ACO	O5B-C5B	-3.43	1.31	1.44
2	A	401	ACO	P1A-O1A	2.73	1.60	1.50
2	A	401	ACO	CEP-CBP	-2.19	1.49	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ACO	CEP-CBP-CCP	-13.50	86.21	108.23
2	A	401	ACO	CEP-CBP-CCP	-12.39	88.03	108.23
2	A	401	ACO	CDP-CBP-CCP	-12.17	88.38	108.23
2	B	401	ACO	C5B-C4B-C3B	-9.60	82.60	114.40
2	A	401	ACO	C5B-C4B-C3B	-9.31	83.54	114.40
2	B	401	ACO	CEP-CBP-CAP	8.52	123.58	108.82
2	B	401	ACO	CDP-CBP-CCP	-7.83	95.46	108.23
2	A	401	ACO	CEP-CBP-CAP	7.61	122.01	108.82
2	A	401	ACO	O9A-P3B-O8A	-7.53	78.85	107.64
2	A	401	ACO	CDP-CBP-CAP	7.30	121.47	108.82
2	B	401	ACO	O9A-P3B-O7A	-7.01	83.23	110.68
2	A	401	ACO	O9A-P3B-O7A	-6.87	83.77	110.68
2	B	401	ACO	O9A-P3B-O8A	-5.56	86.37	107.64
2	B	401	ACO	O9A-P3B-O3B	-5.27	82.37	105.99
2	B	401	ACO	O8A-P3B-O7A	5.14	130.79	110.68
2	B	401	ACO	CEP-CBP-CDP	5.08	119.53	109.17
2	A	401	ACO	O9A-P3B-O3B	-5.04	83.43	105.99
2	B	401	ACO	N3A-C2A-N1A	-4.85	121.09	128.68
2	B	401	ACO	CDP-CBP-CAP	4.65	116.89	108.82
2	B	401	ACO	C6P-C7P-N8P	-4.39	103.04	111.90
2	B	401	ACO	O4B-C4B-C5B	3.57	121.12	109.37
2	A	401	ACO	CEP-CBP-CDP	3.41	116.12	109.17
2	A	401	ACO	C6P-C7P-N8P	-3.34	105.15	111.90
2	B	401	ACO	O3B-C3B-C4B	-3.21	98.49	110.08
2	A	401	ACO	O4B-C4B-C5B	3.07	119.46	109.37
2	B	401	ACO	C6P-C5P-N4P	-3.05	111.28	116.42
2	A	401	ACO	O5A-P2A-O6A	3.03	121.82	107.75
2	B	401	ACO	O5A-P2A-O6A	2.94	121.40	107.75
2	A	401	ACO	N3A-C2A-N1A	-2.89	124.16	128.68
2	A	401	ACO	O8A-P3B-O7A	2.83	121.77	110.68
2	B	401	ACO	O2A-P1A-O5B	2.81	120.80	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ACO	O6A-CCP-CBP	2.52	114.60	110.55
2	B	401	ACO	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	401	ACO	O3B-C3B-C4B	-2.47	101.16	110.08
2	A	401	ACO	O2A-P1A-O5B	2.46	119.18	107.75
2	A	401	ACO	C1B-N9A-C4A	2.45	130.95	126.64
2	B	401	ACO	C1B-N9A-C4A	2.44	130.93	126.64
2	A	401	ACO	P2A-O3A-P1A	2.44	141.20	132.83
2	A	401	ACO	O3B-P3B-O7A	2.30	118.28	109.39
2	B	401	ACO	O4B-C1B-C2B	-2.06	103.92	106.93
3	A	1339	GOL	O3-C3-C2	2.05	120.03	110.20

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	ACO	C5B-O5B-P1A-O1A
2	B	401	ACO	C5B-O5B-P1A-O2A
2	B	401	ACO	CCP-O6A-P2A-O4A
2	B	401	ACO	CDP-CBP-CCP-O6A
2	B	401	ACO	CEP-CBP-CCP-O6A
2	B	401	ACO	CAP-CBP-CCP-O6A
2	B	401	ACO	OAP-CAP-CBP-CCP
2	B	401	ACO	C9P-CAP-CBP-CCP
2	B	401	ACO	OAP-CAP-CBP-CEP
2	B	401	ACO	C9P-CAP-CBP-CEP
2	A	401	ACO	C5B-O5B-P1A-O1A
2	A	401	ACO	C5B-O5B-P1A-O2A
2	A	401	ACO	CCP-O6A-P2A-O4A
2	A	401	ACO	CDP-CBP-CCP-O6A
2	A	401	ACO	CEP-CBP-CCP-O6A
2	A	401	ACO	CAP-CBP-CCP-O6A
2	A	401	ACO	OAP-CAP-CBP-CCP
2	A	401	ACO	C9P-CAP-CBP-CCP
2	A	401	ACO	OAP-CAP-CBP-CEP
2	A	401	ACO	C9P-CAP-CBP-CEP
3	A	1339	GOL	C1-C2-C3-O3
3	A	1339	GOL	O2-C2-C3-O3
2	B	401	ACO	OAP-CAP-CBP-CDP
2	B	401	ACO	C3B-C4B-C5B-O5B
2	B	401	ACO	C9P-CAP-CBP-CDP
2	B	401	ACO	P1A-O3A-P2A-O5A
2	A	401	ACO	P1A-O3A-P2A-O5A

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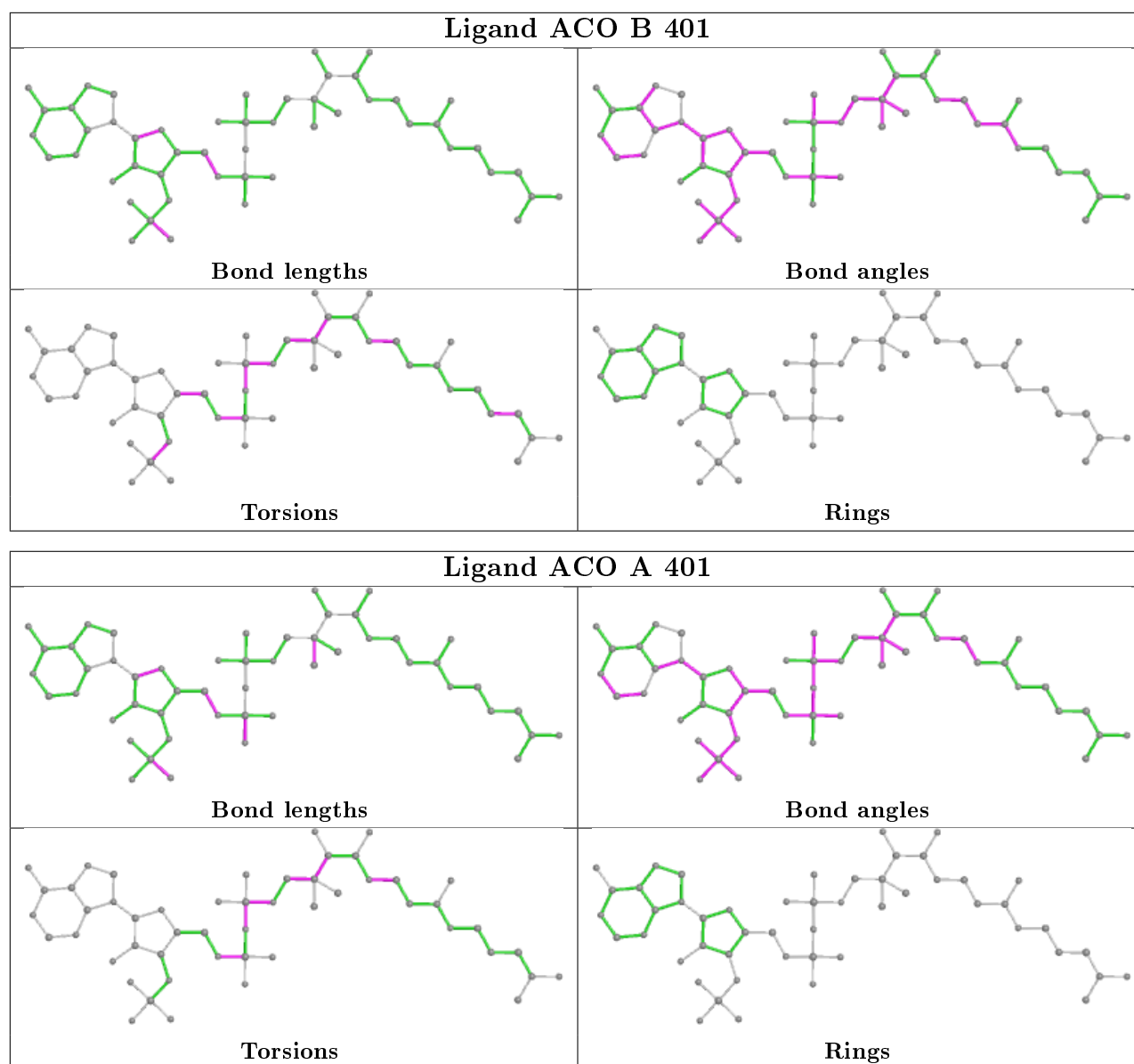
Mol	Chain	Res	Type	Atoms
2	A	401	ACO	C6P-C7P-N8P-C9P
2	B	401	ACO	C6P-C7P-N8P-C9P
2	B	401	ACO	C3P-C2P-S1P-C
2	B	401	ACO	C3B-O3B-P3B-O8A
2	B	401	ACO	C5B-O5B-P1A-O3A
2	A	401	ACO	C5B-O5B-P1A-O3A
2	B	401	ACO	P1A-O3A-P2A-O4A

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ACO	2	0
2	A	401	ACO	3	0
3	A	1339	GOL	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/339 (96%)	-0.55	5 (1%) 73 79	9, 19, 42, 65	2 (0%)
1	B	326/339 (96%)	-0.53	4 (1%) 79 83	11, 19, 40, 63	1 (0%)
All	All	652/678 (96%)	-0.54	9 (1%) 75 80	9, 19, 42, 65	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	SER	4.2
1	A	213	ALA	3.5
1	B	337	PRO	2.7
1	A	337	PRO	2.7
1	B	213	ALA	2.7
1	B	202	LEU	2.5
1	A	338	SER	2.5
1	A	5	ALA	2.4
1	A	212	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

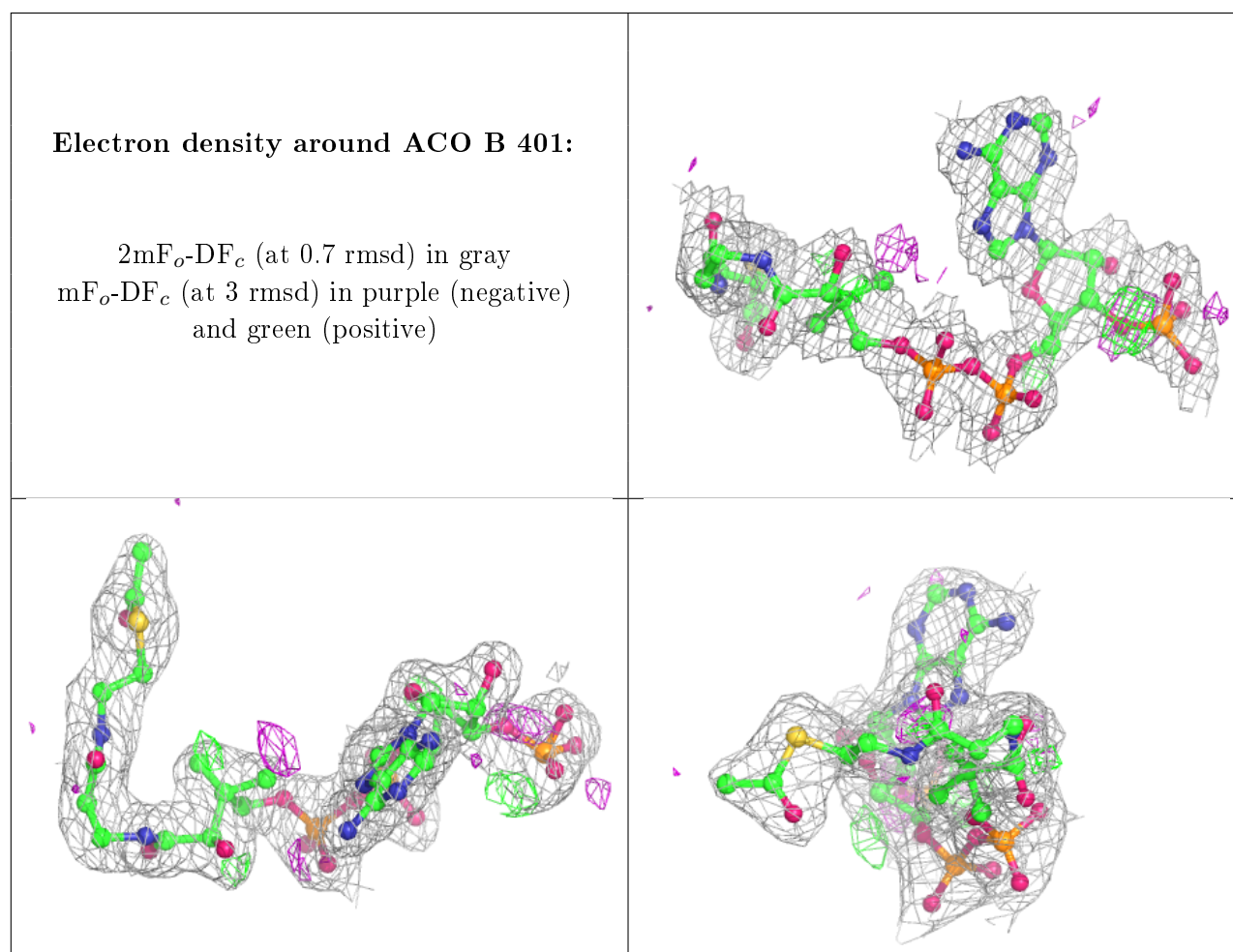
6.4 Ligands [i](#)

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, 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.

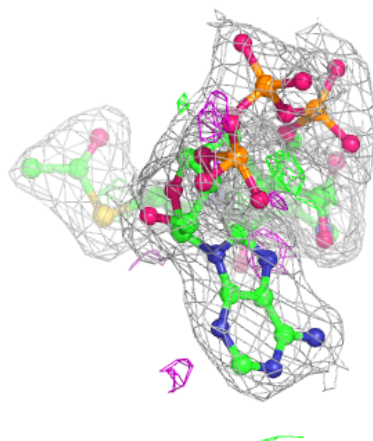
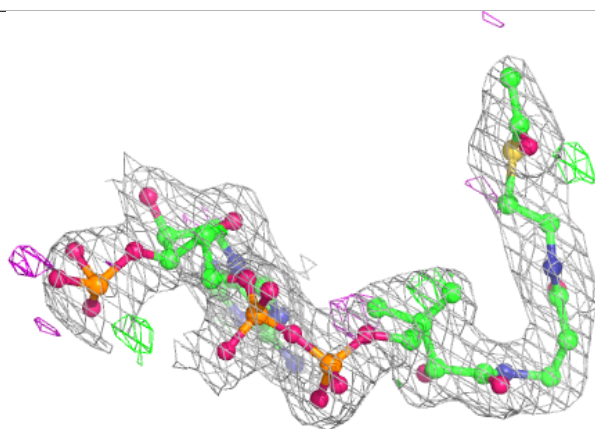
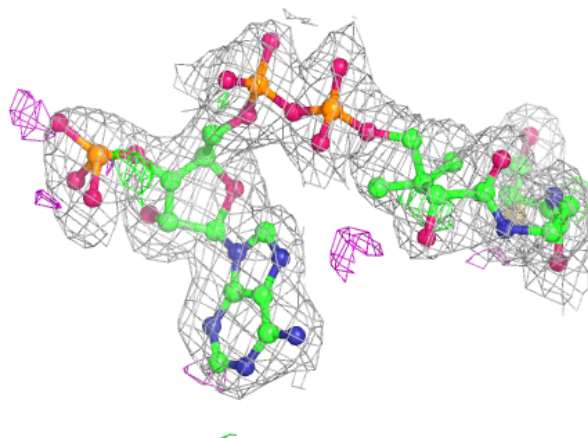
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	1339	6/6	0.88	0.14	31,32,34,35	0
3	GOL	B	1339	6/6	0.91	0.15	29,29,30,31	0
2	ACO	B	401	51/51	0.96	0.12	11,20,28,33	0
2	ACO	A	401	51/51	0.97	0.11	11,20,29,35	0

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 ACO A 401:

$2mF_o-DF_c$ (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.