



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:03 PM UTC

PDB ID : 9J6E / pdb_00009j6e
Title : Crystal structure of BioZ from Agrobacterium tumefaciens in complex with galutaryl-CoA
Authors : Zhang, L.; Zhang, L.
Deposited on : 2024-08-15
Resolution : 2.15 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

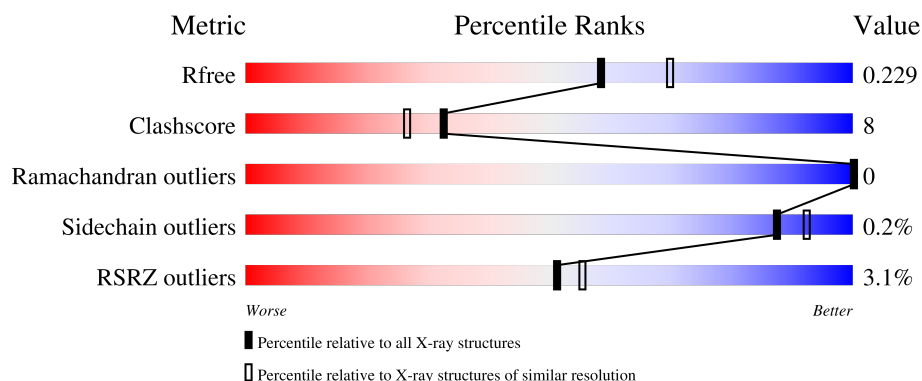
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	328	0% 87% 12% .
1	B	328	5% 87% 12% .
1	C	328	2% 91% 9% .
1	D	328	4% 85% 13% .

2 Entry composition [i](#)

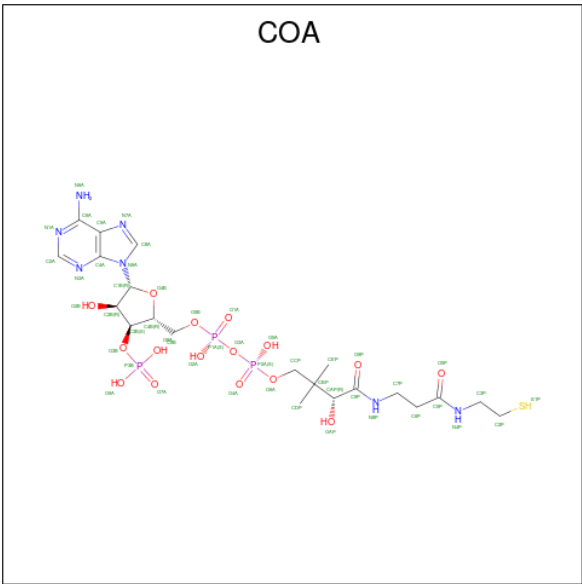
There are 3 unique types of molecules in this entry. The entry contains 10114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxopimeloyl-[acyl-carrier-protein] synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2391	1481	437	461	12			
1	B	327	Total	C	N	O	S	0	0	0
			2391	1481	437	461	12			
1	C	327	Total	C	N	O	S	0	0	0
			2391	1481	437	461	12			
1	D	327	Total	C	N	O	S	0	0	0
			2391	1481	437	461	12			

- 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		

Continued on next page...

Continued from previous page...

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

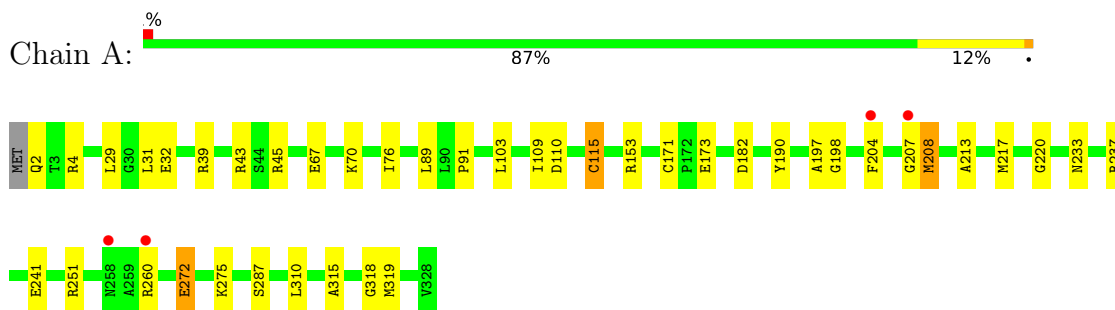
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	84	Total	O	0	0
			84	84		
3	C	86	Total	O	0	0
			86	86		
3	D	105	Total	O	0	0
			105	105		

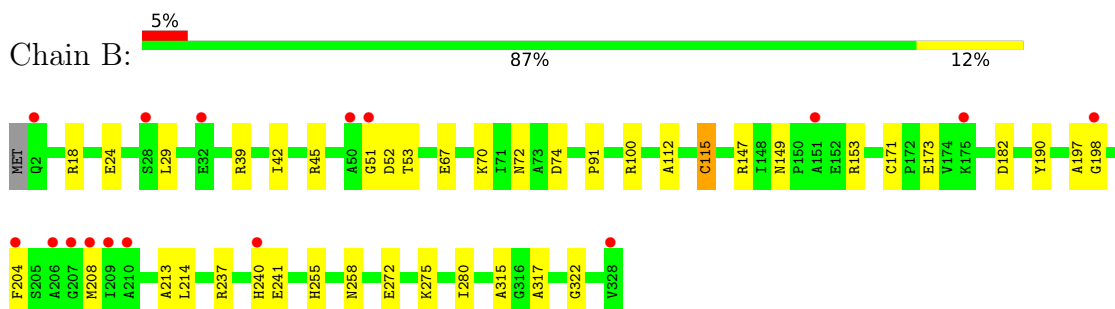
3 Residue-property plots

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.

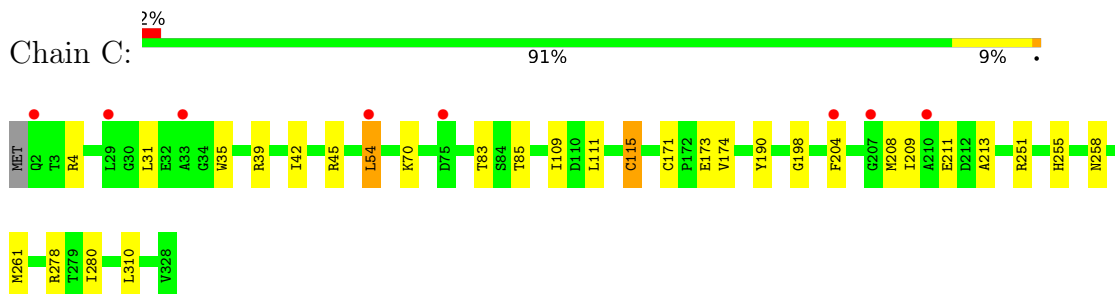
- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase



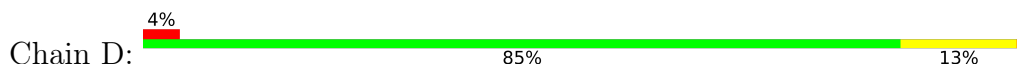
- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase

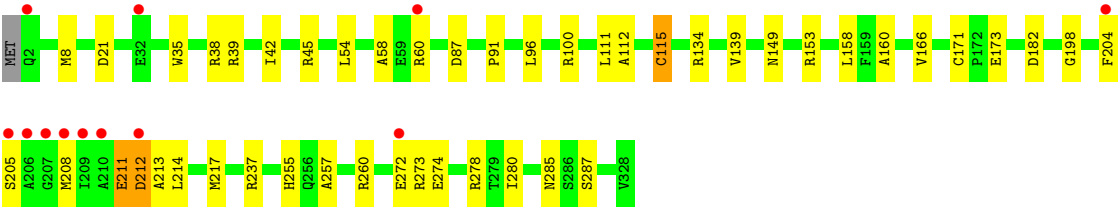


- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase



- Molecule 1: 3-oxopimeloyl-[acyl-carrier-protein] synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.68Å 126.69Å 84.86Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	53.54 – 2.15 53.54 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.5 (53.54-2.15) 95.5 (53.54-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.191 , 0.231 0.191 , 0.229	Depositor DCC
R_{free} test set	3083 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10114	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: COA, A1ECI

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	0.40	0/2409	0.68	6/3268 (0.2%)
1	B	0.37	0/2409	0.66	0/3268
1	C	0.39	0/2409	0.66	1/3268 (0.0%)
1	D	0.43	0/2409	0.77	12/3268 (0.4%)
All	All	0.40	0/9636	0.69	19/13072 (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	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	MET	CB-CG-SD	-11.23	79.00	112.70
1	D	60	ARG	CG-CD-NE	-8.56	93.17	112.00
1	D	260	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	A	43	ARG	CG-CD-NE	-7.07	96.44	112.00
1	D	211	GLU	CA-C-N	-6.74	108.47	121.94
1	D	211	GLU	C-N-CA	-6.74	108.47	121.94
1	D	260	ARG	CA-CB-CG	6.50	127.09	114.10
1	C	54	LEU	CD1-CG-CD2	-6.34	96.86	110.80
1	D	260	ARG	NE-CZ-NH1	-6.32	115.19	121.50
1	D	260	ARG	CB-CG-CD	-6.22	97.00	111.30
1	D	260	ARG	CB-CA-C	6.04	122.61	109.99
1	D	260	ARG	N-CA-CB	-6.03	100.57	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	ARG	CA-CB-CG	5.78	125.65	114.10
1	A	272	GLU	CA-CB-CG	-5.77	102.56	114.10
1	A	207	GLY	CA-C-N	-5.67	112.42	122.74
1	A	207	GLY	C-N-CA	-5.67	112.42	122.74
1	D	60	ARG	CB-CA-C	5.47	119.54	110.90
1	A	4	ARG	CA-CB-CG	5.45	125.00	114.10
1	D	60	ARG	N-CA-CB	-5.26	102.44	110.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ARG	Sidechain

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	2391	0	2395	41	0
1	B	2391	0	2395	45	0
1	C	2391	0	2395	34	0
1	D	2391	0	2395	44	0
2	A	48	0	32	7	0
2	B	48	0	32	7	0
2	C	48	0	31	10	0
2	D	48	0	32	10	0
3	A	83	0	0	2	0
3	B	84	0	0	7	0
3	C	86	0	0	3	0
3	D	105	0	0	3	0
All	All	10114	0	9707	154	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 8.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:MET:HE1	2:A:401:COA:H62	1.53	0.90
1:C:111:LEU:HD22	1:D:111:LEU:HD22	1.54	0.88
1:D:274:GLU:N	1:D:274:GLU:OE1	2.12	0.83
1:D:205:SER:HB2	1:D:208:MET:HE3	1.62	0.81
1:B:115:A1ECI:SG	2:B:401:COA:H31	2.25	0.77
1:A:198:GLY:HA2	1:A:204:PHE:CD2	2.21	0.76
1:C:54:LEU:HD23	1:C:85:THR:O	1.86	0.75
1:C:198:GLY:HA2	1:C:204:PHE:CD2	2.22	0.74
1:C:204:PHE:CD2	1:D:204:PHE:CD2	2.76	0.74
1:C:39:ARG:NH2	2:C:401:COA:O7A	2.24	0.69
1:B:240:HIS:CD2	3:B:503:HOH:O	2.44	0.69
1:B:315:ALA:O	2:B:401:COA:H22	1.95	0.67
1:A:204:PHE:CD2	1:B:204:PHE:CD2	2.83	0.66
1:B:198:GLY:HA2	1:B:204:PHE:CD2	2.31	0.66
1:A:237:ARG:O	1:A:241:GLU:HG3	1.97	0.65
1:D:198:GLY:HA3	1:D:204:PHE:CE2	2.32	0.65
1:D:134:ARG:NH1	3:D:503:HOH:O	2.29	0.64
1:D:211:GLU:N	1:D:211:GLU:OE1	2.29	0.64
1:B:204:PHE:HD1	1:B:208:MET:SD	2.22	0.63
1:A:115:A1ECI:SG	2:A:401:COA:H31	2.40	0.61
1:B:100:ARG:NH1	3:B:504:HOH:O	2.33	0.61
1:B:67:GLU:O	1:B:70:LYS:HD3	2.00	0.61
1:C:54:LEU:HD12	1:C:54:LEU:O	2.01	0.60
1:B:198:GLY:HA3	1:B:204:PHE:CE2	2.36	0.60
1:A:39:ARG:O	1:A:260:ARG:HD3	2.01	0.59
1:D:205:SER:HB2	1:D:208:MET:CE	2.33	0.59
1:B:29:LEU:HD13	1:B:153:ARG:HG3	1.85	0.59
1:A:197:ALA:HB1	1:A:208:MET:HE1	1.86	0.58
1:A:45:ARG:NE	3:A:501:HOH:O	2.31	0.57
1:B:240:HIS:NE2	3:B:503:HOH:O	2.32	0.57
2:C:401:COA:O1A	2:C:401:COA:H8A	2.04	0.57
1:A:204:PHE:CD2	1:B:204:PHE:CE2	2.92	0.57
1:A:220:GLY:HA3	2:A:401:COA:H132	1.86	0.56
1:C:255:HIS:NE2	2:C:401:COA:H31	2.20	0.56
1:B:42:ILE:HG12	1:B:280:ILE:HG12	1.88	0.56
1:D:39:ARG:NH2	2:D:401:COA:O7A	2.38	0.56
1:D:171:CYS:SG	1:D:173:GLU:HG2	2.46	0.56
1:D:217:MET:SD	2:D:401:COA:OAP	2.64	0.55
1:C:54:LEU:HD21	1:C:83:THR:OG1	2.07	0.55
1:A:182:ASP:OD2	1:A:237:ARG:HD2	2.06	0.55
1:D:217:MET:CE	2:D:401:COA:O5P	2.55	0.54
1:D:21:ASP:CG	3:D:502:HOH:O	2.51	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:NE	2:C:401:COA:O7A	2.39	0.54
1:D:198:GLY:HA2	1:D:204:PHE:CD2	2.43	0.54
1:D:255:HIS:CD2	2:D:401:COA:H21	2.43	0.54
1:B:204:PHE:CD1	1:B:208:MET:SD	3.01	0.54
1:B:198:GLY:CA	1:B:204:PHE:CE2	2.91	0.53
1:A:29:LEU:HB2	1:A:31:LEU:HG	1.91	0.53
1:C:258:ASN:ND2	2:C:401:COA:H143	2.24	0.53
1:B:147:ARG:HG3	3:B:524:HOH:O	2.09	0.53
1:A:233:ASN:O	1:A:237:ARG:HG2	2.09	0.52
1:B:237:ARG:O	1:B:241:GLU:HG3	2.09	0.51
1:D:217:MET:HE2	2:D:401:COA:O5P	2.09	0.51
1:A:197:ALA:CB	1:A:208:MET:HE1	2.40	0.51
1:A:272:GLU:OE1	1:A:275:LYS:HG3	2.10	0.51
1:A:67:GLU:O	1:A:70:LYS:HD2	2.11	0.51
1:A:251:ARG:HB2	1:A:310:LEU:HD13	1.93	0.51
1:B:204:PHE:HE1	1:B:213:ALA:HB2	1.77	0.50
1:C:115:A1ECI:C5	2:C:401:COA:H32	2.41	0.50
1:A:204:PHE:CE2	1:B:204:PHE:CD2	3.00	0.50
1:A:110:ASP:HB2	1:B:112:ALA:HB3	1.93	0.50
1:A:198:GLY:CA	1:A:204:PHE:CE2	2.94	0.50
2:A:401:COA:O5A	2:A:401:COA:H142	2.12	0.50
1:B:53:THR:HA	3:B:533:HOH:O	2.11	0.50
1:B:272:GLU:CD	1:B:275:LYS:HD3	2.37	0.50
1:B:45:ARG:NE	3:B:506:HOH:O	2.43	0.50
1:D:272:GLU:H	1:D:272:GLU:CD	2.19	0.50
1:D:96:LEU:O	1:D:100:ARG:HG3	2.12	0.49
1:C:198:GLY:CA	1:C:204:PHE:CE2	2.95	0.49
1:D:182:ASP:OD2	1:D:237:ARG:HD2	2.12	0.49
1:C:198:GLY:HA2	1:C:204:PHE:CE2	2.47	0.49
1:A:204:PHE:HE1	1:A:213:ALA:HB2	1.77	0.49
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.78	0.49
1:C:278:ARG:HH11	1:C:278:ARG:HG3	1.78	0.49
1:B:197:ALA:HB1	1:B:208:MET:HE1	1.95	0.49
1:D:204:PHE:CE1	1:D:213:ALA:HB2	2.48	0.49
1:B:115:A1ECI:SG	2:B:401:COA:C3P	3.00	0.48
1:A:251:ARG:HB2	1:A:310:LEU:CD1	2.44	0.48
1:C:204:PHE:CD2	1:D:204:PHE:CE2	3.01	0.48
1:C:171:CYS:SG	1:C:173:GLU:HG2	2.52	0.48
1:C:204:PHE:HD1	1:C:208:MET:SD	2.37	0.48
1:D:285:ASN:HD21	2:D:401:COA:C3P	2.27	0.48
1:C:204:PHE:CD1	1:C:208:MET:SD	3.07	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:COA:O5A	2:C:401:COA:H142	2.13	0.47
1:D:35:TRP:CZ2	1:D:153:ARG:HD3	2.48	0.47
1:C:70:LYS:NZ	3:C:502:HOH:O	2.36	0.47
1:D:158:LEU:HD13	2:D:401:COA:H62	1.96	0.47
1:A:2:GLN:HG3	3:A:527:HOH:O	2.14	0.47
1:A:76:ILE:HG21	1:A:103:LEU:HD13	1.97	0.47
1:C:31:LEU:HD13	1:C:35:TRP:CE3	2.50	0.47
1:D:182:ASP:CG	1:D:237:ARG:HD2	2.40	0.47
1:D:42:ILE:HG12	1:D:280:ILE:HG12	1.97	0.47
1:A:315:ALA:O	2:A:401:COA:H22	2.15	0.46
1:B:171:CYS:SG	1:B:173:GLU:HG2	2.56	0.46
1:A:190:TYR:CD1	1:B:91:PRO:HG2	2.51	0.46
1:D:54:LEU:HB3	1:D:87:ASP:OD1	2.16	0.46
1:A:115:A1ECI:SG	2:A:401:COA:C3P	3.03	0.46
2:B:401:COA:O5A	2:B:401:COA:H142	2.16	0.46
1:B:18:ARG:NH2	1:B:24:GLU:OE2	2.49	0.45
1:D:198:GLY:CA	1:D:204:PHE:CD2	2.99	0.45
1:A:115:A1ECI:C5	2:A:401:COA:H32	2.45	0.45
1:D:257:ALA:HB1	2:D:401:COA:H31	1.98	0.45
1:A:198:GLY:HA3	1:A:204:PHE:CE2	2.52	0.45
1:D:273:ARG:HG2	1:D:278:ARG:CZ	2.47	0.45
1:A:198:GLY:HA2	1:A:204:PHE:CE2	2.51	0.45
1:C:45:ARG:NE	3:C:504:HOH:O	2.49	0.45
1:B:255:HIS:CD2	2:B:401:COA:H21	2.51	0.45
1:A:204:PHE:CD1	1:A:208:MET:CE	3.00	0.44
1:B:204:PHE:CE1	1:B:213:ALA:HB2	2.52	0.44
1:B:72:ASN:OD1	1:B:74:ASP:HB2	2.17	0.44
1:D:35:TRP:CH2	1:D:153:ARG:HD3	2.53	0.44
1:B:258:ASN:ND2	2:B:401:COA:H143	2.32	0.44
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.82	0.44
1:A:91:PRO:HG2	1:B:190:TYR:CD1	2.53	0.44
1:D:285:ASN:HD21	2:D:401:COA:H32	1.83	0.44
1:D:38:ARG:NH2	3:D:509:HOH:O	2.49	0.43
1:D:8:MET:HG2	1:D:166:VAL:HG21	1.99	0.43
1:C:42:ILE:HG12	1:C:280:ILE:HG12	2.01	0.43
1:B:51:GLY:O	1:B:52:ASP:C	2.61	0.43
1:B:182:ASP:O	1:B:322:GLY:HA2	2.18	0.43
1:C:211:GLU:HG2	3:C:554:HOH:O	2.17	0.43
1:A:190:TYR:CE1	1:B:91:PRO:HG2	2.54	0.43
1:C:109:ILE:HG13	1:D:112:ALA:O	2.19	0.43
1:C:208:MET:HE1	1:C:213:ALA:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:HB2	1:C:310:LEU:HD22	2.01	0.42
1:B:72:ASN:OD1	1:B:72:ASN:C	2.61	0.42
1:D:58:ALA:HB1	1:D:139:VAL:HG11	2.00	0.42
1:C:4:ARG:HD3	1:C:174:VAL:CG1	2.48	0.42
1:C:39:ARG:CZ	2:C:401:COA:O7A	2.67	0.42
1:A:171:CYS:SG	1:A:173:GLU:HG2	2.60	0.42
1:C:190:TYR:CE1	1:D:91:PRO:HG2	2.54	0.42
2:C:401:COA:O7A	2:C:401:COA:H4B	2.17	0.42
1:C:209:ILE:H	1:C:209:ILE:HD12	1.85	0.42
1:A:91:PRO:HB3	1:B:317:ALA:HB1	2.02	0.42
1:D:149:ASN:HA	1:D:214:LEU:HD13	2.02	0.42
1:B:149:ASN:HA	1:B:214:LEU:HD13	2.02	0.42
1:B:198:GLY:CA	1:B:204:PHE:CD2	3.02	0.41
1:D:198:GLY:CA	1:D:204:PHE:CE2	3.00	0.41
1:B:115:A1ECL:C5	2:B:401:COA:H32	2.51	0.41
1:C:278:ARG:HG3	1:C:278:ARG:NH1	2.35	0.41
1:D:217:MET:HE1	2:D:401:COA:O5P	2.20	0.41
1:C:39:ARG:HH21	2:C:401:COA:P3B	2.42	0.41
1:A:109:ILE:HG13	1:B:112:ALA:O	2.21	0.41
1:D:115:A1ECL:SG	1:D:287:SER:HA	2.60	0.41
1:A:115:A1ECL:SG	1:A:287:SER:HA	2.60	0.41
1:A:318:GLY:N	1:A:319:MET:HE2	2.36	0.41
1:B:147:ARG:NH2	3:B:507:HOH:O	2.46	0.41
1:C:45:ARG:HH11	1:C:45:ARG:HG2	1.86	0.41
1:A:182:ASP:CG	1:A:237:ARG:HD2	2.46	0.40
1:D:212:ASP:N	1:D:212:ASP:OD1	2.54	0.40
1:C:261:MET:HE3	1:C:261:MET:HB2	1.82	0.40
1:A:89:LEU:HD11	1:B:204:PHE:HE2	1.87	0.40
1:D:45:ARG:HB2	1:D:160:ALA:HB2	2.03	0.40
1:D:204:PHE:HE1	1:D:213:ALA:HB2	1.86	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	323/328 (98%)	312 (97%)	11 (3%)	0	100	100
1	B	323/328 (98%)	313 (97%)	10 (3%)	0	100	100
1	C	323/328 (98%)	312 (97%)	11 (3%)	0	100	100
1	D	323/328 (98%)	315 (98%)	8 (2%)	0	100	100
All	All	1292/1312 (98%)	1252 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	239/240 (100%)	238 (100%)	1 (0%)	84	89
1	B	239/240 (100%)	239 (100%)	0	100	100
1	C	239/240 (100%)	239 (100%)	0	100	100
1	D	239/240 (100%)	238 (100%)	1 (0%)	84	89
All	All	956/960 (100%)	954 (100%)	2 (0%)	87	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	D	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	D	99	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	A1ECI	C	115	1	12,13,14	2.39	2 (16%)	11,15,17	3.72	3 (27%)
1	A1ECI	A	115	1	12,13,14	2.67	2 (16%)	11,15,17	4.27	3 (27%)
1	A1ECI	B	115	1	12,13,14	2.34	2 (16%)	11,15,17	5.16	5 (45%)
1	A1ECI	D	115	1	12,13,14	2.48	2 (16%)	11,15,17	4.18	4 (36%)

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
1	A1ECI	C	115	1	-	3/11/13/15	-
1	A1ECI	A	115	1	-	2/11/13/15	-
1	A1ECI	B	115	1	-	4/11/13/15	-
1	A1ECI	D	115	1	-	3/11/13/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	A1ECI	C5-SG	-6.34	1.61	1.76
1	D	115	A1ECI	C5-SG	-6.19	1.61	1.76
1	A	115	A1ECI	C5-SG	-6.14	1.61	1.76
1	B	115	A1ECI	C5-SG	-6.03	1.62	1.76
1	A	115	A1ECI	C4-C5	5.57	1.56	1.50
1	D	115	A1ECI	C4-C5	4.60	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	A1ECI	C4-C5	4.21	1.55	1.50
1	C	115	A1ECI	C4-C5	4.09	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	A1ECI	CB-SG-C5	14.87	121.20	100.76
1	A	115	A1ECI	CB-SG-C5	12.55	118.01	100.76
1	D	115	A1ECI	CB-SG-C5	12.10	117.39	100.76
1	C	115	A1ECI	CB-SG-C5	10.77	115.56	100.76
1	B	115	A1ECI	O3-C5-SG	6.24	130.62	122.68
1	D	115	A1ECI	O3-C5-SG	4.79	128.78	122.68
1	A	115	A1ECI	O3-C5-SG	4.67	128.62	122.68
1	C	115	A1ECI	O3-C5-SG	4.17	127.98	122.68
1	B	115	A1ECI	O3-C5-C4	-3.93	119.45	123.98
1	A	115	A1ECI	C4-C5-SG	-3.36	109.40	113.40
1	D	115	A1ECI	O3-C5-C4	-3.05	120.46	123.98
1	B	115	A1ECI	C4-C5-SG	-2.92	109.92	113.40
1	C	115	A1ECI	O3-C5-C4	-2.73	120.83	123.98
1	B	115	A1ECI	C3-C2-C1	-2.24	108.65	114.51
1	D	115	A1ECI	C4-C5-SG	-2.23	110.74	113.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	115	A1ECI	C2-C3-C4-C5
1	B	115	A1ECI	C2-C3-C4-C5
1	C	115	A1ECI	C2-C3-C4-C5
1	D	115	A1ECI	C2-C3-C4-C5
1	B	115	A1ECI	C1-C2-C3-C4
1	C	115	A1ECI	C1-C2-C3-C4
1	A	115	A1ECI	O2-C1-C2-C3
1	B	115	A1ECI	O2-C1-C2-C3
1	D	115	A1ECI	O2-C1-C2-C3
1	B	115	A1ECI	O1-C1-C2-C3
1	D	115	A1ECI	O1-C1-C2-C3
1	C	115	A1ECI	O2-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	115	A1ECI	1	0
1	A	115	A1ECI	4	0
1	B	115	A1ECI	3	0
1	D	115	A1ECI	1	0

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	401	-	47,50,50	3.29	18 (38%)	69,75,75	1.71	14 (20%)
2	COA	B	401	-	47,50,50	3.19	17 (36%)	69,75,75	1.78	15 (21%)
2	COA	C	401	-	47,50,50	3.26	17 (36%)	69,75,75	1.65	14 (20%)
2	COA	D	401	-	47,50,50	3.29	18 (38%)	69,75,75	1.71	15 (21%)

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	401	-	-	20/48/64/64	0/3/3/3
2	COA	B	401	-	-	23/48/64/64	0/3/3/3
2	COA	C	401	-	-	18/48/64/64	0/3/3/3
2	COA	D	401	-	-	21/48/64/64	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	COA	C2B-C3B	-12.66	1.25	1.53
2	D	401	COA	C2B-C3B	-12.64	1.25	1.53
2	B	401	COA	C2B-C3B	-12.52	1.25	1.53
2	C	401	COA	C2B-C3B	-12.30	1.26	1.53
2	D	401	COA	C9P-N8P	6.83	1.49	1.33
2	C	401	COA	C9P-N8P	6.76	1.49	1.33
2	A	401	COA	C9P-N8P	6.74	1.49	1.33
2	A	401	COA	C5P-N4P	6.73	1.49	1.33
2	B	401	COA	C9P-N8P	6.69	1.49	1.33
2	D	401	COA	P2A-O3A	6.68	1.66	1.59
2	C	401	COA	C5P-N4P	6.63	1.49	1.33
2	A	401	COA	P2A-O3A	6.48	1.66	1.59
2	B	401	COA	C5P-N4P	6.43	1.48	1.33
2	D	401	COA	C5P-N4P	6.42	1.48	1.33
2	A	401	COA	O4B-C1B	-6.06	1.28	1.42
2	C	401	COA	P2A-O3A	6.04	1.66	1.59
2	C	401	COA	O4B-C1B	-5.84	1.28	1.42
2	B	401	COA	O4B-C1B	-5.79	1.28	1.42
2	D	401	COA	O4B-C1B	-5.73	1.28	1.42
2	B	401	COA	P2A-O3A	5.35	1.65	1.59
2	D	401	COA	O4B-C4B	5.03	1.56	1.45
2	B	401	COA	O4B-C4B	4.95	1.56	1.45
2	A	401	COA	O4B-C4B	4.81	1.55	1.45
2	C	401	COA	O4B-C4B	4.74	1.55	1.45
2	A	401	COA	C2B-C1B	4.69	1.68	1.53
2	C	401	COA	C2B-C1B	4.68	1.68	1.53
2	B	401	COA	C5B-C4B	-4.67	1.37	1.51
2	D	401	COA	C2B-C1B	4.63	1.68	1.53
2	B	401	COA	C2B-C1B	4.57	1.67	1.53
2	A	401	COA	C5B-C4B	-4.50	1.38	1.51
2	D	401	COA	P1A-O3A	4.37	1.64	1.59
2	C	401	COA	C6A-N6A	4.28	1.45	1.34
2	C	401	COA	C5B-C4B	-4.27	1.38	1.51
2	B	401	COA	C6A-N6A	4.21	1.45	1.34
2	C	401	COA	P3B-O3B	4.19	1.66	1.59
2	A	401	COA	C6A-N6A	4.17	1.44	1.34
2	D	401	COA	C6A-N6A	4.13	1.44	1.34
2	D	401	COA	C5B-C4B	-4.11	1.39	1.51
2	C	401	COA	P1A-O3A	3.99	1.63	1.59
2	D	401	COA	P3B-O3B	3.78	1.66	1.59
2	A	401	COA	P1A-O3A	3.63	1.63	1.59
2	B	401	COA	P3B-O3B	3.33	1.65	1.59
2	B	401	COA	CCP-CBP	3.30	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	COA	P3B-O3B	3.27	1.65	1.59
2	C	401	COA	OAP-CAP	-3.19	1.36	1.42
2	C	401	COA	CCP-CBP	3.14	1.57	1.52
2	A	401	COA	OAP-CAP	-3.07	1.36	1.42
2	A	401	COA	C8A-N9A	-3.04	1.32	1.37
2	B	401	COA	OAP-CAP	-3.03	1.37	1.42
2	A	401	COA	CCP-CBP	3.03	1.57	1.52
2	B	401	COA	P1A-O3A	2.98	1.62	1.59
2	D	401	COA	CCP-CBP	2.97	1.57	1.52
2	C	401	COA	C8A-N9A	-2.92	1.32	1.37
2	D	401	COA	C8A-N9A	-2.91	1.32	1.37
2	B	401	COA	C8A-N9A	-2.80	1.32	1.37
2	D	401	COA	OAP-CAP	-2.73	1.37	1.42
2	C	401	COA	O3B-C3B	2.50	1.52	1.44
2	D	401	COA	O3B-C3B	2.40	1.52	1.44
2	A	401	COA	O3B-C3B	2.35	1.52	1.44
2	A	401	COA	C5A-N7A	-2.33	1.34	1.39
2	B	401	COA	O3B-C3B	2.31	1.52	1.44
2	C	401	COA	O9P-C9P	-2.24	1.19	1.23
2	C	401	COA	C5A-N7A	-2.23	1.35	1.39
2	D	401	COA	P1A-O5B	2.22	1.68	1.59
2	D	401	COA	C5A-N7A	-2.19	1.35	1.39
2	A	401	COA	P1A-O5B	2.14	1.67	1.59
2	B	401	COA	O9P-C9P	-2.07	1.19	1.23
2	B	401	COA	C5A-N7A	-2.02	1.35	1.39
2	D	401	COA	O9P-C9P	-2.02	1.19	1.23
2	A	401	COA	O9P-C9P	-2.00	1.19	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	COA	C5A-C4A-N3A	-5.21	119.54	126.72
2	D	401	COA	C5A-C4A-N3A	-5.20	119.56	126.72
2	A	401	COA	C5A-C4A-N3A	-5.01	119.82	126.72
2	D	401	COA	C2P-C3P-N4P	-5.00	100.96	112.31
2	B	401	COA	C5A-C4A-N3A	-4.96	119.89	126.72
2	B	401	COA	N3A-C2A-N1A	-4.67	121.51	128.58
2	B	401	COA	C2P-C3P-N4P	-4.56	101.97	112.31
2	D	401	COA	N3A-C2A-N1A	-4.53	121.73	128.58
2	C	401	COA	N3A-C2A-N1A	-4.48	121.81	128.58
2	C	401	COA	C2P-C3P-N4P	-4.44	102.23	112.31
2	A	401	COA	N3A-C2A-N1A	-4.41	121.90	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	COA	C7P-C6P-C5P	-4.16	105.46	112.39
2	A	401	COA	C2P-C3P-N4P	-4.08	103.05	112.31
2	A	401	COA	N3A-C4A-N9A	4.04	134.03	127.17
2	D	401	COA	N3A-C4A-N9A	3.89	133.78	127.17
2	C	401	COA	N3A-C4A-N9A	3.80	133.63	127.17
2	B	401	COA	N3A-C4A-N9A	3.64	133.35	127.17
2	B	401	COA	C2A-N3A-C4A	3.49	120.37	111.83
2	C	401	COA	C2A-N3A-C4A	3.45	120.26	111.83
2	D	401	COA	C2A-N3A-C4A	3.44	120.22	111.83
2	A	401	COA	C2A-N3A-C4A	3.40	120.13	111.83
2	B	401	COA	N9A-C8A-N7A	-3.39	109.13	113.94
2	A	401	COA	N9A-C8A-N7A	-3.27	109.30	113.94
2	B	401	COA	C2B-C3B-C4B	-3.20	97.64	103.24
2	A	401	COA	C4A-N9A-C8A	2.94	108.82	105.74
2	D	401	COA	N9A-C8A-N7A	-2.93	109.78	113.94
2	B	401	COA	C5A-N7A-C8A	2.91	108.03	103.45
2	B	401	COA	C3P-N4P-C5P	-2.90	117.42	122.82
2	C	401	COA	N9A-C8A-N7A	-2.87	109.86	113.94
2	C	401	COA	C4B-O4B-C1B	-2.83	103.23	109.47
2	A	401	COA	C7P-C6P-C5P	-2.82	107.70	112.39
2	D	401	COA	C6P-C7P-N8P	2.80	117.95	112.00
2	B	401	COA	C4A-N9A-C8A	2.79	108.66	105.74
2	B	401	COA	C4A-C5A-N7A	-2.77	107.41	110.58
2	A	401	COA	C5A-N7A-C8A	2.75	107.78	103.45
2	D	401	COA	C5A-N7A-C8A	2.69	107.67	103.45
2	C	401	COA	C5A-N7A-C8A	2.61	107.55	103.45
2	A	401	COA	CEP-CBP-CCP	2.57	112.46	108.22
2	B	401	COA	O3B-C3B-C4B	-2.55	101.05	110.03
2	C	401	COA	C4A-C5A-N7A	-2.52	107.70	110.58
2	D	401	COA	C4A-C5A-N7A	-2.50	107.73	110.58
2	C	401	COA	C7P-C6P-C5P	-2.47	108.28	112.39
2	D	401	COA	C4B-O4B-C1B	-2.47	104.02	109.47
2	A	401	COA	C4B-O4B-C1B	-2.46	104.03	109.47
2	D	401	COA	P3B-O3B-C3B	-2.45	116.89	123.43
2	C	401	COA	C6P-C7P-N8P	2.44	117.19	112.00
2	D	401	COA	C4A-N9A-C8A	2.30	108.16	105.74
2	A	401	COA	C4A-C5A-N7A	-2.29	107.96	110.58
2	D	401	COA	C7P-C6P-C5P	-2.25	108.64	112.39
2	C	401	COA	C4A-N9A-C8A	2.20	108.05	105.74
2	C	401	COA	O4B-C1B-C2B	-2.15	102.01	106.62
2	B	401	COA	C4B-O4B-C1B	-2.10	104.82	109.47
2	A	401	COA	O6A-CCP-CBP	-2.10	107.18	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	COA	O4B-C1B-C2B	-2.09	102.15	106.62
2	A	401	COA	C6P-C7P-N8P	2.06	116.39	112.00
2	C	401	COA	CEP-CBP-CCP	2.03	111.58	108.22
2	D	401	COA	O6A-CCP-CBP	-2.02	107.30	110.55
2	B	401	COA	C6P-C7P-N8P	2.01	116.28	112.00

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	COA	C4B-C5B-O5B-P1A
2	A	401	COA	CCP-O6A-P2A-O4A
2	A	401	COA	CCP-O6A-P2A-O5A
2	A	401	COA	CBP-CCP-O6A-P2A
2	A	401	COA	CDP-CBP-CCP-O6A
2	A	401	COA	CEP-CBP-CCP-O6A
2	A	401	COA	CAP-CBP-CCP-O6A
2	A	401	COA	C5P-C6P-C7P-N8P
2	B	401	COA	P2A-O3A-P1A-O5B
2	B	401	COA	CBP-CCP-O6A-P2A
2	B	401	COA	CDP-CBP-CCP-O6A
2	B	401	COA	CEP-CBP-CCP-O6A
2	B	401	COA	CAP-CBP-CCP-O6A
2	B	401	COA	OAP-CAP-CBP-CCP
2	B	401	COA	C9P-CAP-CBP-CCP
2	B	401	COA	OAP-CAP-CBP-CDP
2	B	401	COA	C9P-CAP-CBP-CDP
2	B	401	COA	OAP-CAP-CBP-CEP
2	B	401	COA	C9P-CAP-CBP-CEP
2	B	401	COA	C5P-C6P-C7P-N8P
2	C	401	COA	C4B-C3B-O3B-P3B
2	C	401	COA	C5B-O5B-P1A-O1A
2	C	401	COA	C5B-O5B-P1A-O2A
2	C	401	COA	C5B-O5B-P1A-O3A
2	C	401	COA	CCP-O6A-P2A-O3A
2	C	401	COA	CCP-O6A-P2A-O5A
2	C	401	COA	CBP-CCP-O6A-P2A
2	C	401	COA	CDP-CBP-CCP-O6A
2	C	401	COA	CEP-CBP-CCP-O6A
2	C	401	COA	CAP-CBP-CCP-O6A
2	C	401	COA	C5P-C6P-C7P-N8P
2	D	401	COA	C5B-O5B-P1A-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	401	COA	C5B-O5B-P1A-O2A
2	D	401	COA	C5B-O5B-P1A-O3A
2	D	401	COA	CCP-O6A-P2A-O3A
2	D	401	COA	CCP-O6A-P2A-O4A
2	D	401	COA	CCP-O6A-P2A-O5A
2	D	401	COA	CBP-CCP-O6A-P2A
2	D	401	COA	CDP-CBP-CCP-O6A
2	D	401	COA	CEP-CBP-CCP-O6A
2	D	401	COA	CAP-CBP-CCP-O6A
2	D	401	COA	C6P-C5P-N4P-C3P
2	B	401	COA	C3B-C4B-C5B-O5B
2	D	401	COA	C3B-C4B-C5B-O5B
2	D	401	COA	O5P-C5P-N4P-C3P
2	B	401	COA	O4B-C4B-C5B-O5B
2	D	401	COA	O4B-C4B-C5B-O5B
2	B	401	COA	C2B-C3B-O3B-P3B
2	B	401	COA	C4B-C5B-O5B-P1A
2	B	401	COA	C4B-C3B-O3B-P3B
2	A	401	COA	C3B-C4B-C5B-O5B
2	B	401	COA	P1A-O3A-P2A-O4A
2	D	401	COA	P2A-O3A-P1A-O1A
2	A	401	COA	O9P-C9P-CAP-CBP
2	D	401	COA	O9P-C9P-CAP-CBP
2	A	401	COA	N8P-C9P-CAP-CBP
2	D	401	COA	N8P-C9P-CAP-CBP
2	D	401	COA	N8P-C9P-CAP-OAP
2	B	401	COA	O5P-C5P-C6P-C7P
2	C	401	COA	O5P-C5P-C6P-C7P
2	A	401	COA	P2A-O3A-P1A-O5B
2	C	401	COA	P2A-O3A-P1A-O5B
2	B	401	COA	C3B-O3B-P3B-O7A
2	A	401	COA	C5B-O5B-P1A-O3A
2	A	401	COA	CCP-O6A-P2A-O3A
2	C	401	COA	C4B-C5B-O5B-P1A
2	C	401	COA	N4P-C5P-C6P-C7P
2	B	401	COA	O9P-C9P-CAP-CBP
2	C	401	COA	O9P-C9P-CAP-CBP
2	C	401	COA	C3B-O3B-P3B-O9A
2	B	401	COA	N8P-C9P-CAP-CBP
2	C	401	COA	N8P-C9P-CAP-CBP
2	B	401	COA	N4P-C5P-C6P-C7P
2	A	401	COA	O5P-C5P-C6P-C7P

Continued on next page...

Continued from previous page...

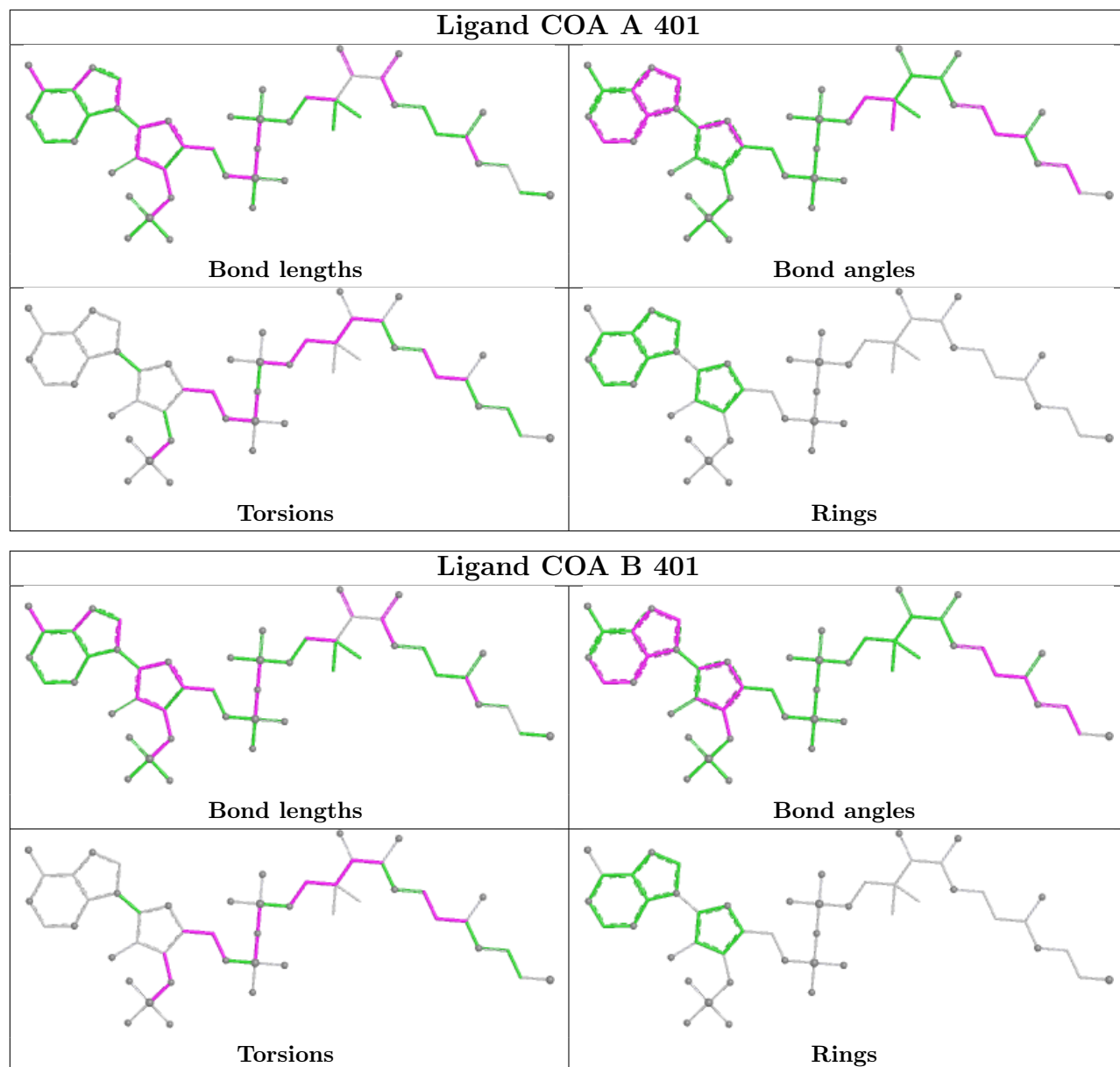
Mol	Chain	Res	Type	Atoms
2	A	401	COA	C3B-O3B-P3B-O7A
2	A	401	COA	P2A-O3A-P1A-O1A
2	D	401	COA	P2A-O3A-P1A-O2A
2	D	401	COA	C4B-C5B-O5B-P1A
2	A	401	COA	N4P-C5P-C6P-C7P
2	A	401	COA	OAP-CAP-CBP-CEP
2	A	401	COA	O4B-C4B-C5B-O5B
2	D	401	COA	P1A-O3A-P2A-O5A

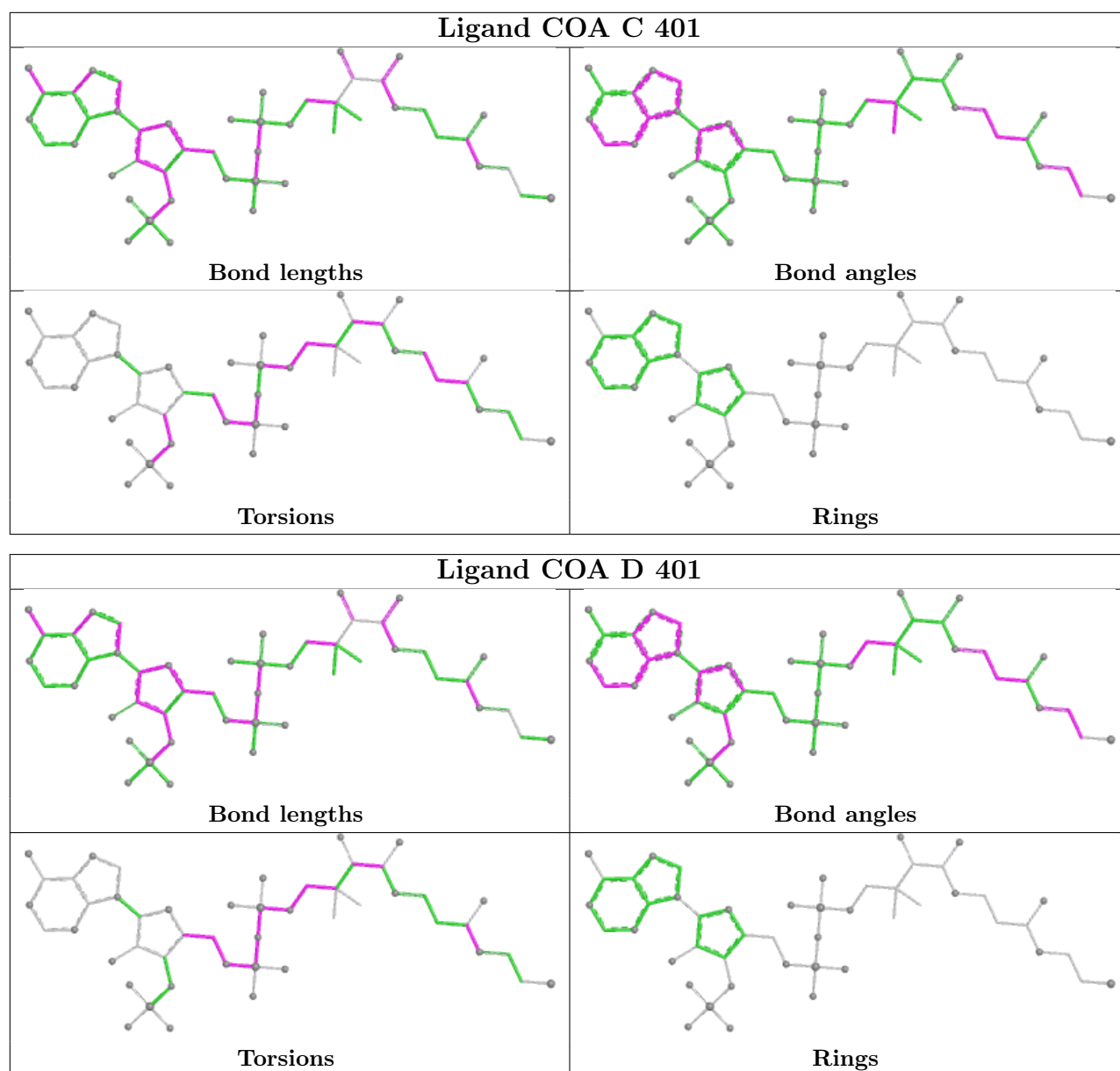
There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	COA	7	0
2	B	401	COA	7	0
2	C	401	COA	10	0
2	D	401	COA	10	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	326/328 (99%)	0.26	4 (1%) 76 79	25, 32, 47, 59	0
1	B	326/328 (99%)	0.46	16 (4%) 35 39	24, 33, 52, 67	0
1	C	326/328 (99%)	0.35	8 (2%) 58 62	25, 32, 47, 60	0
1	D	326/328 (99%)	0.29	12 (3%) 45 49	23, 31, 48, 78	0
All	All	1304/1312 (99%)	0.34	40 (3%) 51 55	23, 32, 49, 78	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	ILE	9.4
1	B	51	GLY	9.2
1	B	204	PHE	7.5
1	D	204	PHE	7.5
1	D	210	ALA	7.1
1	B	207	GLY	6.0
1	C	204	PHE	5.6
1	D	207	GLY	5.3
1	A	204	PHE	5.0
1	B	206	ALA	4.8
1	B	208	MET	4.8
1	D	208	MET	4.4
1	C	207	GLY	4.2
1	B	209	ILE	4.1
1	D	205	SER	3.7
1	D	60	ARG	3.5
1	D	206	ALA	3.5
1	B	210	ALA	3.3
1	D	212	ASP	3.2
1	B	240	HIS	3.0
1	D	2	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	2.6
1	B	28	SER	2.5
1	C	210	ALA	2.5
1	A	207	GLY	2.4
1	B	32	GLU	2.4
1	C	54	LEU	2.4
1	C	33	ALA	2.3
1	A	258	ASN	2.3
1	B	198	GLY	2.3
1	C	29	LEU	2.2
1	D	32	GLU	2.2
1	C	2	GLN	2.2
1	B	175	LYS	2.2
1	C	75	ASP	2.2
1	B	328	VAL	2.2
1	B	151	ALA	2.2
1	D	272	GLU	2.1
1	B	2	GLN	2.1
1	A	260	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	A1ECI	A	115	14/15	0.92	0.11	28,33,39,40	0
1	A1ECI	B	115	14/15	0.92	0.11	29,33,39,39	0
1	A1ECI	D	115	14/15	0.92	0.11	29,35,37,38	0
1	A1ECI	C	115	14/15	0.94	0.09	26,33,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

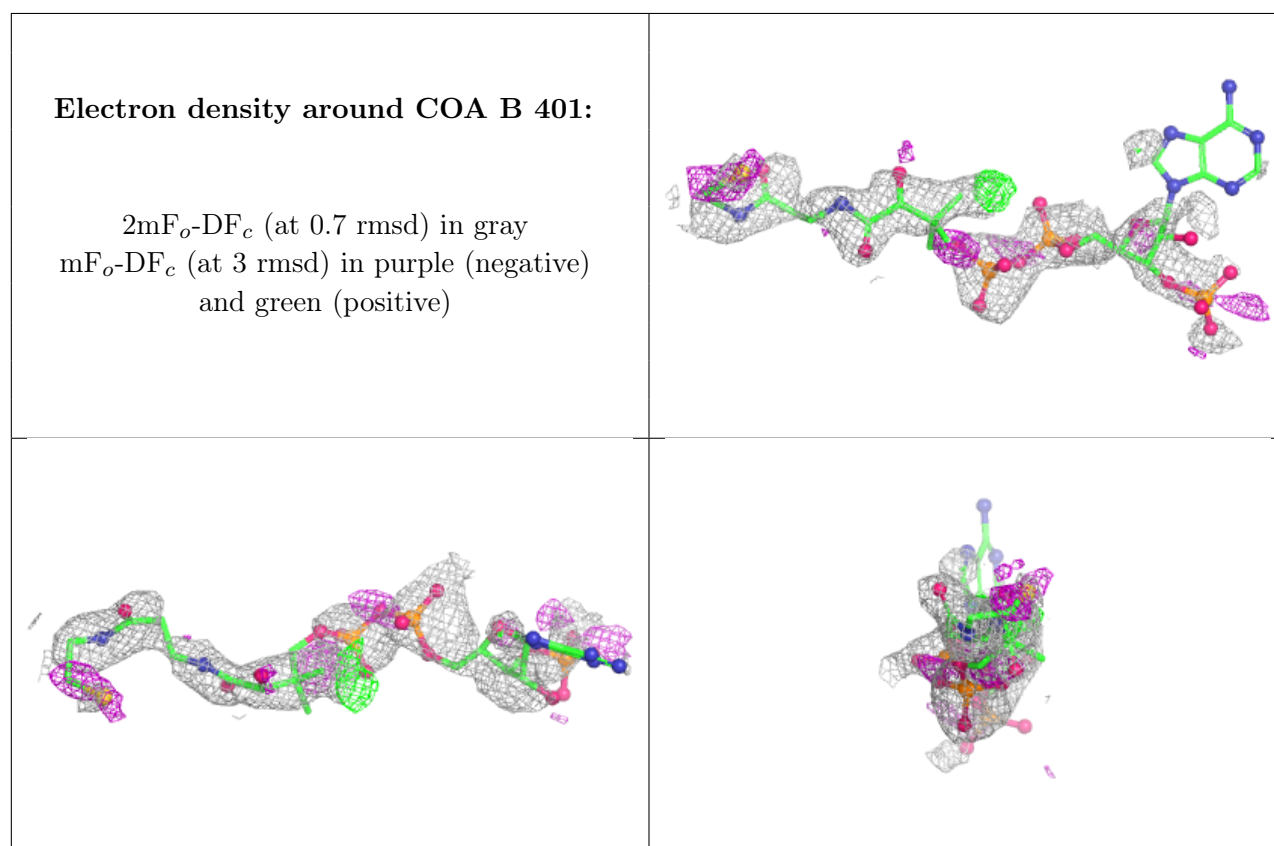
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

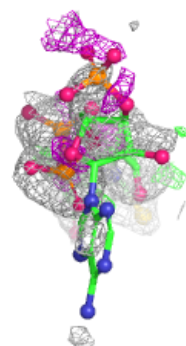
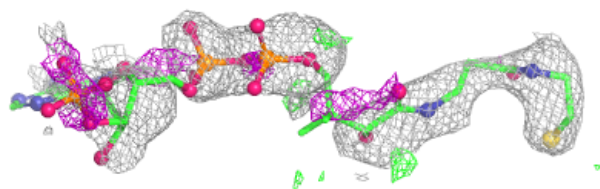
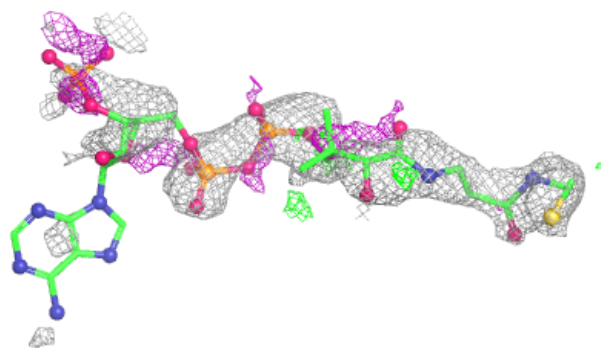
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	B	401	48/48	0.58	0.19	39,93,123,127	0
2	COA	C	401	48/48	0.60	0.19	39,90,104,122	0
2	COA	D	401	48/48	0.63	0.19	39,89,118,127	0
2	COA	A	401	48/48	0.67	0.18	39,87,105,129	0

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.

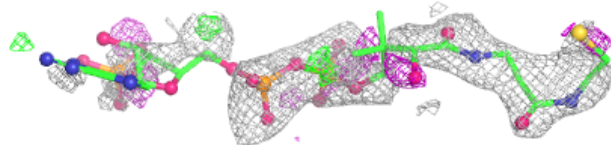
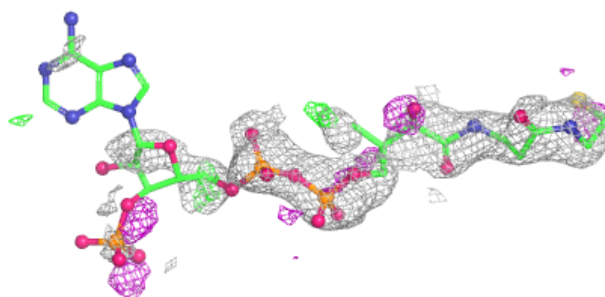


Electron density around COA C 401:

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

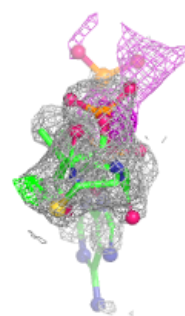
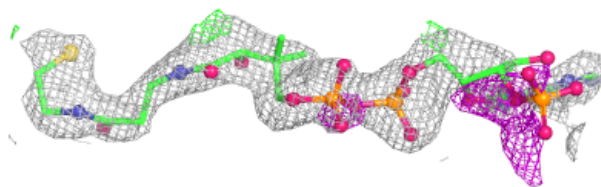
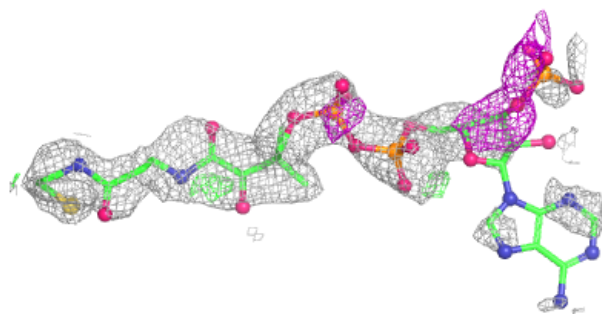
**Electron density around COA D 401:**

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



Electron density around COA 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 [i](#)

There are no such residues in this entry.