



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:29 PM UTC

PDB ID : 7ZTK / pdb_00007ztk
Title : NME1 in complex with CoA
Authors : Garcia-Saez, I.; Iuso, D.; Khochbin, S.; Petosa, C.
Deposited on : 2022-05-10
Resolution : 2.60 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

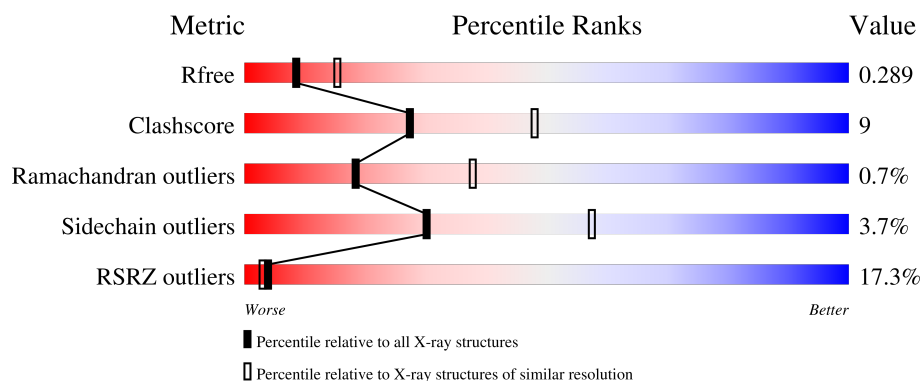
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	156	4% 75% 22% .
1	B	156	15% 79% 17% ...
1	C	156	28% 79% 15% ..
1	D	156	10% 77% 17% ..
1	E	156	17% 76% 21% ..

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Mol	Chain	Length	Quality of chain
1	F	156	28% 77% 20% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7603 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 Nucleoside diphosphate kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	1	0
			1210	775	208	222	5			
1	B	153	Total	C	N	O	S	0	0	0
			1217	778	209	224	6			
1	C	151	Total	C	N	O	S	0	0	0
			1204	770	207	222	5			
1	D	152	Total	C	N	O	S	0	0	0
			1212	775	208	223	6			
1	E	153	Total	C	N	O	S	0	0	0
			1217	778	209	224	6			
1	F	152	Total	C	N	O	S	0	0	0
			1212	775	208	223	6			

There are 24 discrepancies between the modelled and reference sequences:

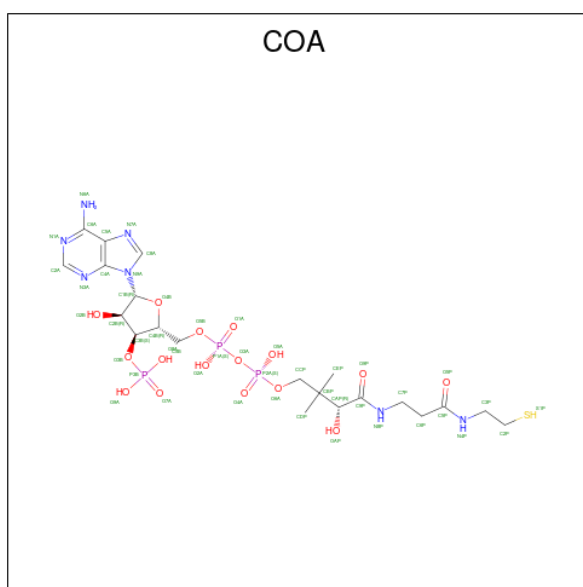
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P15532
A	-2	ALA	-	expression tag	UNP P15532
A	-1	MET	-	expression tag	UNP P15532
A	0	ALA	-	expression tag	UNP P15532
B	-3	GLY	-	expression tag	UNP P15532
B	-2	ALA	-	expression tag	UNP P15532
B	-1	MET	-	expression tag	UNP P15532
B	0	ALA	-	expression tag	UNP P15532
C	-3	GLY	-	expression tag	UNP P15532
C	-2	ALA	-	expression tag	UNP P15532
C	-1	MET	-	expression tag	UNP P15532
C	0	ALA	-	expression tag	UNP P15532
D	-3	GLY	-	expression tag	UNP P15532
D	-2	ALA	-	expression tag	UNP P15532
D	-1	MET	-	expression tag	UNP P15532
D	0	ALA	-	expression tag	UNP P15532
E	-3	GLY	-	expression tag	UNP P15532

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ALA	-	expression tag	UNP P15532
E	-1	MET	-	expression tag	UNP P15532
E	0	ALA	-	expression tag	UNP P15532
F	-3	GLY	-	expression tag	UNP P15532
F	-2	ALA	-	expression tag	UNP P15532
F	-1	MET	-	expression tag	UNP P15532
F	0	ALA	-	expression tag	UNP P15532

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			39	10	5	19	5		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	16	3		
2	E	1	Total	C	N	O	P	0	0
			40	16	6	15	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

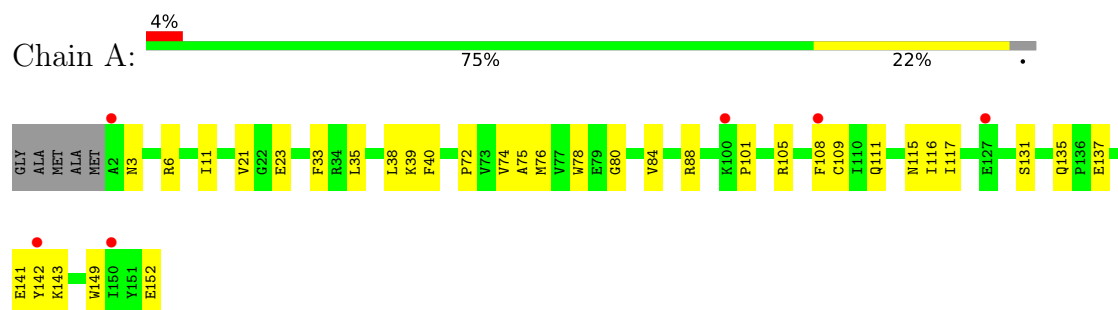
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total 17	O 17	0	0
3	B	14	Total 14	O 14	0	0
3	C	8	Total 8	O 8	0	0
3	D	10	Total 10	O 10	0	0
3	E	17	Total 17	O 17	0	0
3	F	11	Total 11	O 11	0	0

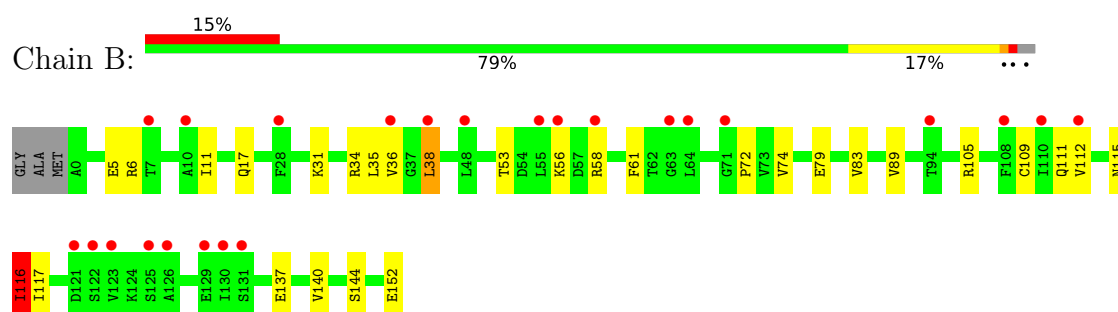
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

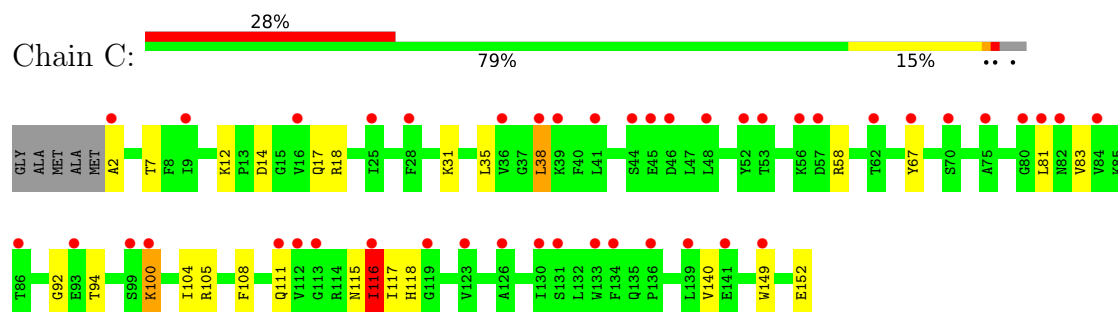
- Molecule 1: Nucleoside diphosphate kinase A



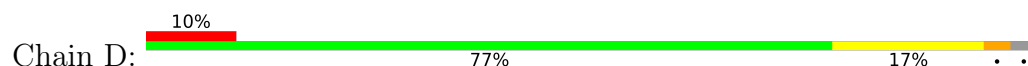
- Molecule 1: Nucleoside diphosphate kinase A

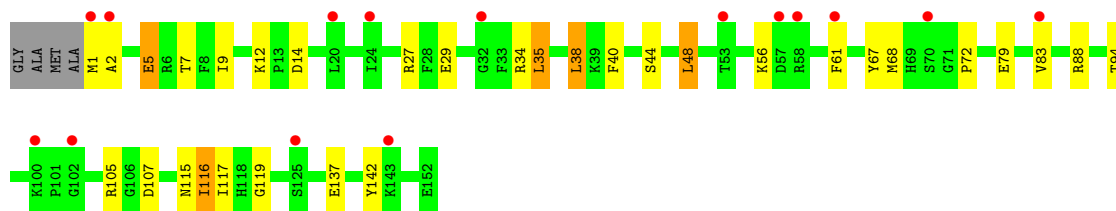


- Molecule 1: Nucleoside diphosphate kinase A

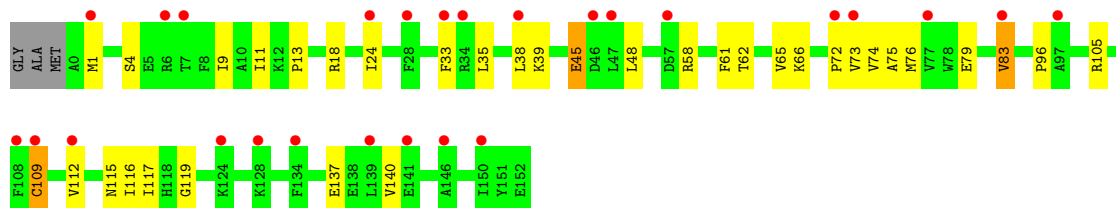
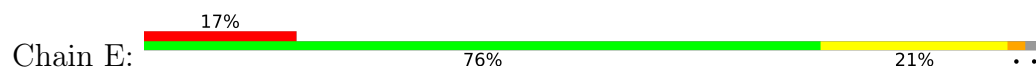


- Molecule 1: Nucleoside diphosphate kinase A

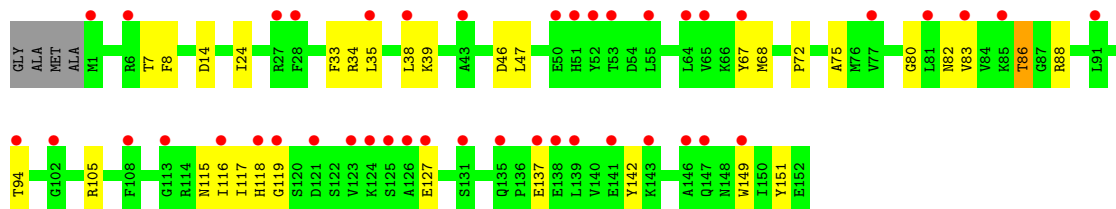
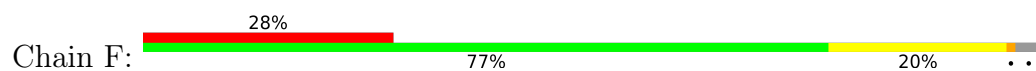




● Molecule 1: Nucleoside diphosphate kinase A



● Molecule 1: Nucleoside diphosphate kinase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.17Å 69.45Å 116.30Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	49.13 – 2.60 49.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.13-2.60) 99.3 (49.13-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.273 , 0.289 0.272 , 0.289	Depositor DCC
R_{free} test set	1332 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	1.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7603	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.53% 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

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	0.12	0/1239	0.33	0/1668
1	B	0.11	0/1243	0.32	0/1673
1	C	0.13	0/1230	0.33	0/1656
1	D	0.15	0/1238	0.35	0/1666
1	E	0.22	0/1243	0.39	0/1673
1	F	0.12	0/1238	0.34	0/1666
All	All	0.15	0/7431	0.34	0/10002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1210	0	1217	29	0
1	B	1217	0	1221	25	0
1	C	1204	0	1204	25	0
1	D	1212	0	1216	25	0
1	E	1217	0	1221	21	0
1	F	1212	0	1216	20	0
2	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	32	4	0
2	C	48	0	32	6	0
2	D	48	0	32	4	0
2	E	40	0	21	2	0
2	F	31	0	11	2	0
3	A	17	0	0	4	0
3	B	14	0	0	5	0
3	C	8	0	0	1	0
3	D	10	0	0	2	0
3	E	17	0	0	5	0
3	F	11	0	0	5	0
All	All	7603	0	7423	136	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 9.

All (136) 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)
2:D:201:COA:O4B	2:D:201:COA:C1B	1.63	1.29
2:C:201:COA:C1B	2:C:201:COA:O4B	1.63	1.25
2:E:201:COA:O4B	2:E:201:COA:C1B	1.63	1.24
2:B:201:COA:C1B	2:B:201:COA:O4B	1.63	1.23
1:F:34:ARG:NH1	1:F:142:TYR:O	2.21	0.72
1:C:12:LYS:HE3	1:C:118:HIS:HB2	1.73	0.71
1:D:44:SER:O	3:D:301:HOH:O	2.09	0.70
1:E:115:ASN:O	1:E:117:ILE:N	2.22	0.70
1:B:34:ARG:O	3:B:301:HOH:O	2.09	0.70
1:E:105:ARG:NH2	1:E:117:ILE:O	2.24	0.69
1:D:5:GLU:HG2	1:D:83:VAL:HG12	1.75	0.69
1:A:6:ARG:NH2	1:A:141:GLU:OE1	2.25	0.69
1:D:105:ARG:NH2	1:D:117:ILE:O	2.25	0.69
1:A:38:LEU:HB3	1:D:40:PHE:HB2	1.73	0.68
1:C:118:HIS:ND1	2:C:201:COA:O7A	2.29	0.66
1:B:112:VAL:O	3:B:302:HOH:O	2.15	0.65
1:D:34:ARG:NH1	1:D:142:TYR:O	2.31	0.64
1:F:115:ASN:O	1:F:117:ILE:N	2.28	0.63
1:E:39:LYS:HG2	1:E:75:ALA:HB3	1.80	0.63
1:E:58:ARG:NH2	3:E:303:HOH:O	2.33	0.61
1:F:8:PHE:O	3:F:301:HOH:O	2.16	0.61
1:A:111:GLN:OE1	1:B:152:GLU:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:N	3:D:301:HOH:O	2.16	0.60
1:C:18:ARG:NH2	1:C:108:PHE:O	2.33	0.60
1:A:23:GLU:OE1	3:A:301:HOH:O	2.17	0.60
1:A:115:ASN:O	1:A:117:ILE:N	2.30	0.59
1:D:34:ARG:NH2	1:D:79:GLU:OE2	2.35	0.58
1:B:11:ILE:HB	1:B:74:VAL:HB	1.84	0.58
1:B:140:VAL:HG11	1:E:72:PRO:HB3	1.84	0.57
1:D:88:ARG:NH2	2:D:201:COA:O1A	2.36	0.57
1:E:24:ILE:HD13	1:E:117:ILE:HD12	1.87	0.57
1:F:33:PHE:HD1	1:F:80:GLY:HA3	1.69	0.56
1:F:7:THR:HB	1:F:83:VAL:HG13	1.88	0.55
1:A:38:LEU:HD13	1:A:76:MET:HG2	1.88	0.55
1:A:3:ASN:ND2	3:A:307:HOH:O	2.34	0.55
1:C:115:ASN:O	1:C:117:ILE:N	2.37	0.55
1:E:45:GLU:HG3	1:E:65:VAL:HG12	1.90	0.54
1:E:109:CYS:SG	1:E:115:ASN:HA	2.48	0.54
1:C:58:ARG:NH2	2:C:201:COA:O9P	2.41	0.54
1:D:115:ASN:O	1:D:117:ILE:N	2.30	0.54
1:C:140:VAL:HG11	1:F:72:PRO:HB3	1.90	0.54
1:F:33:PHE:CD1	1:F:80:GLY:HA3	2.44	0.53
1:B:105:ARG:NH2	1:B:117:ILE:O	2.35	0.53
1:A:35:LEU:HD21	1:A:38:LEU:HD22	1.90	0.53
1:D:12:LYS:HG2	1:D:68:MET:SD	2.49	0.53
1:F:68:MET:O	3:F:302:HOH:O	2.19	0.53
1:E:11:ILE:HB	1:E:74:VAL:HB	1.91	0.53
1:F:14:ASP:OD1	1:F:67:TYR:OH	2.22	0.53
1:B:117:ILE:O	3:B:303:HOH:O	2.18	0.52
1:C:94:THR:HG21	2:C:201:COA:H3B	1.91	0.52
2:E:201:COA:H8A	2:E:201:COA:H52A	1.91	0.52
1:C:14:ASP:OD1	1:C:67:TYR:OH	2.27	0.51
2:B:201:COA:O2A	2:B:201:COA:H10	2.11	0.51
1:D:12:LYS:N	1:D:116:ILE:O	2.38	0.51
1:D:27:ARG:NH2	1:D:107:ASP:OD2	2.43	0.50
1:D:105:ARG:HE	1:D:115:ASN:HB2	1.77	0.50
1:B:5:GLU:HG2	1:B:83:VAL:HG12	1.93	0.50
1:D:94:THR:HG21	2:D:201:COA:H52A	1.93	0.50
1:A:109:CYS:O	1:B:31:LYS:NZ	2.43	0.50
1:B:115:ASN:O	1:B:117:ILE:N	2.41	0.50
1:C:94:THR:CG2	2:C:201:COA:H3B	2.42	0.50
1:E:58:ARG:O	3:E:301:HOH:O	2.19	0.49
1:C:118:HIS:HD1	2:C:201:COA:P3B	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:HD3	1:B:144:SER:HB2	1.94	0.49
1:B:109:CYS:O	1:C:31:LYS:NZ	2.38	0.48
1:A:35:LEU:HD13	1:A:78:TRP:CE2	2.49	0.48
1:D:7:THR:HB	1:D:83:VAL:HG13	1.95	0.48
1:B:35:LEU:HD11	1:B:38:LEU:HD12	1.94	0.48
1:F:88:ARG:NH1	1:F:119:GLY:O	2.47	0.48
1:B:115:ASN:O	1:B:116:ILE:HG12	2.13	0.47
1:B:111:GLN:HE22	1:C:152:GLU:H	1.62	0.47
1:A:131:SER:O	3:A:302:HOH:O	2.20	0.47
1:F:82:ASN:O	1:F:86:THR:HG23	2.14	0.47
1:D:35:LEU:HD11	1:D:38:LEU:HD12	1.96	0.47
1:E:61:PHE:HB3	3:E:301:HOH:O	2.15	0.47
1:A:105:ARG:NH2	1:A:117:ILE:O	2.47	0.46
1:F:149:TRP:O	3:F:303:HOH:O	2.21	0.46
1:A:152:GLU:HG2	1:C:111:GLN:OE1	2.15	0.46
1:C:115:ASN:O	1:C:116:ILE:HG12	2.14	0.46
1:C:92:GLY:O	3:C:301:HOH:O	2.21	0.46
2:B:201:COA:O8A	2:B:201:COA:O2B	2.32	0.46
1:E:96:PRO:HB3	1:E:109:CYS:HB3	1.98	0.45
1:B:111:GLN:NE2	1:C:152:GLU:H	2.14	0.45
1:A:72:PRO:HG2	1:D:142:TYR:CD1	2.51	0.45
1:D:14:ASP:OD1	1:D:67:TYR:OH	2.28	0.45
1:A:11:ILE:HD13	1:A:21:VAL:HA	1.99	0.45
1:B:58:ARG:HH12	2:B:201:COA:H121	1.81	0.45
1:B:117:ILE:N	3:B:303:HOH:O	2.48	0.45
1:F:14:ASP:OD1	1:F:14:ASP:N	2.50	0.45
1:A:11:ILE:HB	1:A:74:VAL:HB	1.98	0.45
1:F:39:LYS:HG2	1:F:75:ALA:HB3	1.99	0.45
1:A:23:GLU:HG2	1:A:108:PHE:CZ	2.52	0.44
1:C:35:LEU:HD21	1:C:38:LEU:HD12	1.98	0.44
1:B:79:GLU:HB3	3:B:301:HOH:O	2.16	0.44
1:E:48:LEU:HB2	1:E:65:VAL:HG13	1.98	0.44
1:C:7:THR:HB	1:C:83:VAL:HG13	1.99	0.44
1:A:33:PHE:HD1	1:A:80:GLY:HA3	1.82	0.44
1:C:104:ILE:HG22	1:C:116:ILE:HD11	2.00	0.44
1:E:9:ILE:HD13	1:E:119:GLY:HA2	2.00	0.44
1:A:39:LYS:HG2	1:A:75:ALA:HB3	2.00	0.43
1:F:118:HIS:HD1	2:F:201:COA:P3B	2.41	0.43
1:F:137:GLU:HG3	3:F:309:HOH:O	2.18	0.43
1:A:84:VAL:O	1:A:88:ARG:HG2	2.18	0.43
1:E:13:PRO:HD3	1:E:73:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:NH2	1:F:117:ILE:O	2.47	0.43
1:D:12:LYS:HD3	1:D:67:TYR:OH	2.19	0.43
1:E:45:GLU:OE1	1:E:66:LYS:HG2	2.19	0.43
2:D:201:COA:H131	2:D:201:COA:HN8	1.84	0.43
1:D:9:ILE:HD13	1:D:119:GLY:HA2	2.01	0.42
1:E:76:MET:HB3	3:E:305:HOH:O	2.19	0.42
1:E:18:ARG:NH1	3:E:310:HOH:O	2.52	0.42
1:A:101:PRO:HD3	1:B:89:VAL:HG12	2.01	0.42
1:A:135:GLN:N	1:A:135:GLN:OE1	2.53	0.42
1:B:53:THR:HA	1:B:56:LYS:HE3	2.00	0.42
1:C:105:ARG:HE	1:C:115:ASN:HB2	1.84	0.42
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.52	0.42
1:B:6:ARG:HG2	1:B:79:GLU:HB2	2.02	0.42
1:F:94:THR:HA	1:F:105:ARG:NH1	2.35	0.42
1:B:56:LYS:HG2	1:B:61:PHE:CZ	2.55	0.41
2:F:201:COA:O5A	2:F:201:COA:H8A	2.20	0.41
1:B:17:GLN:HG3	1:C:149:TRP:CE2	2.55	0.41
1:E:4:SER:HA	1:E:79:GLU:HG3	2.01	0.41
1:A:21:VAL:HB	1:D:29:GLU:OE1	2.21	0.41
1:A:40:PHE:HB2	1:D:38:LEU:CB	2.51	0.41
1:A:149:TRP:CZ2	1:C:17:GLN:HG3	2.55	0.41
1:B:72:PRO:HB3	1:E:140:VAL:HG11	2.02	0.41
1:A:3:ASN:O	3:A:303:HOH:O	2.21	0.41
1:F:151:TYR:HB3	3:F:307:HOH:O	2.21	0.41
1:D:1:MET:HG2	1:D:2:ALA:H	1.86	0.41
1:A:33:PHE:CD1	1:A:80:GLY:HA3	2.56	0.41
1:F:24:ILE:HD13	1:F:117:ILE:HD12	2.03	0.41
1:A:142:TYR:CD1	1:D:72:PRO:HG2	2.56	0.40
1:A:149:TRP:CE2	1:C:17:GLN:HG3	2.57	0.40
1:E:33:PHE:CE1	1:E:83:VAL:HB	2.57	0.40
1:C:2:ALA:O	1:C:81:LEU:HD13	2.21	0.40
1:D:56:LYS:HG2	1:D:61:PHE:CZ	2.56	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	150/156 (96%)	147 (98%)	2 (1%)	1 (1%)	18	38
1	B	151/156 (97%)	148 (98%)	2 (1%)	1 (1%)	18	38
1	C	149/156 (96%)	146 (98%)	2 (1%)	1 (1%)	18	38
1	D	150/156 (96%)	147 (98%)	2 (1%)	1 (1%)	18	38
1	E	151/156 (97%)	144 (95%)	6 (4%)	1 (1%)	18	38
1	F	150/156 (96%)	144 (96%)	5 (3%)	1 (1%)	18	38
All	All	901/936 (96%)	876 (97%)	19 (2%)	6 (1%)	18	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	B	116	ILE
1	C	116	ILE
1	D	116	ILE
1	E	116	ILE
1	F	116	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/132 (99%)	129 (98%)	2 (2%)	57	80
1	B	131/132 (99%)	127 (97%)	4 (3%)	35	63
1	C	130/132 (98%)	127 (98%)	3 (2%)	44	71
1	D	131/132 (99%)	126 (96%)	5 (4%)	29	56
1	E	131/132 (99%)	122 (93%)	9 (7%)	14	32
1	F	131/132 (99%)	125 (95%)	6 (5%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	785/792 (99%)	756 (96%)	29 (4%)	30 57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	143	LYS
1	B	36	VAL
1	B	38	LEU
1	B	116	ILE
1	B	137	GLU
1	C	38	LEU
1	C	100	LYS
1	C	116	ILE
1	D	5	GLU
1	D	35	LEU
1	D	38	LEU
1	D	48	LEU
1	D	137	GLU
1	E	1	MET
1	E	35	LEU
1	E	38	LEU
1	E	45	GLU
1	E	62	THR
1	E	83	VAL
1	E	109	CYS
1	E	112	VAL
1	E	137	GLU
1	F	35	LEU
1	F	38	LEU
1	F	46	ASP
1	F	47	LEU
1	F	86	THR
1	F	127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	D	201	-	47,50,50	3.05	19 (40%)	69,75,75	1.62	13 (18%)
2	COA	B	201	-	47,50,50	3.01	19 (40%)	69,75,75	1.62	13 (18%)
2	COA	C	201	-	47,50,50	2.94	20 (42%)	69,75,75	1.64	12 (17%)
2	COA	A	201[A]	-	32,33,50	2.94	10 (31%)	50,52,75	1.84	15 (30%)
2	COA	A	201[B]	-	32,33,50	3.01	12 (37%)	50,52,75	1.85	15 (30%)
2	COA	F	201	-	32,33,50	3.07	14 (43%)	50,52,75	1.76	11 (22%)
2	COA	E	201	-	40,42,50	3.06	16 (40%)	62,66,75	1.66	12 (19%)

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	D	201	-	-	24/48/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	201	-	-	16/48/64/64	0/3/3/3
2	COA	C	201	-	-	16/48/64/64	0/3/3/3
2	COA	A	201[A]	-	-	2/21/37/64	0/3/3/3
2	COA	A	201[B]	-	-	2/21/37/64	0/3/3/3
2	COA	F	201	-	-	2/21/37/64	0/3/3/3
2	COA	E	201	-	-	10/37/54/64	0/3/3/3

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	COA	O4B-C1B	9.43	1.63	1.42
2	E	201	COA	O4B-C1B	9.39	1.63	1.42
2	D	201	COA	O4B-C1B	9.35	1.63	1.42
2	C	201	COA	O4B-C1B	9.31	1.63	1.42
2	F	201	COA	O4B-C1B	9.20	1.63	1.42
2	A	201[A]	COA	O4B-C1B	8.99	1.62	1.42
2	A	201[B]	COA	O4B-C1B	8.99	1.62	1.42
2	D	201	COA	P2A-O3A	6.62	1.66	1.59
2	B	201	COA	P2A-O3A	6.57	1.66	1.59
2	F	201	COA	C2B-C1B	-6.37	1.33	1.53
2	E	201	COA	C2B-C1B	-6.29	1.33	1.53
2	A	201[A]	COA	C2B-C1B	-6.26	1.33	1.53
2	A	201[B]	COA	C2B-C1B	-6.26	1.33	1.53
2	D	201	COA	C2B-C1B	-6.26	1.33	1.53
2	C	201	COA	C2B-C1B	-6.21	1.34	1.53
2	E	201	COA	P2A-O3A	6.16	1.66	1.59
2	B	201	COA	O4B-C4B	-6.06	1.31	1.45
2	D	201	COA	C5P-N4P	6.03	1.47	1.33
2	E	201	COA	O4B-C4B	-6.02	1.31	1.45
2	C	201	COA	O4B-C4B	-6.00	1.31	1.45
2	B	201	COA	C2B-C1B	-5.91	1.34	1.53
2	D	201	COA	O4B-C4B	-5.88	1.31	1.45
2	A	201[A]	COA	O4B-C4B	-5.88	1.31	1.45
2	A	201[B]	COA	O4B-C4B	-5.88	1.31	1.45
2	B	201	COA	C5P-N4P	5.84	1.47	1.33
2	F	201	COA	O4B-C4B	-5.79	1.32	1.45
2	C	201	COA	C5P-N4P	5.78	1.47	1.33
2	E	201	COA	C9P-N8P	5.65	1.46	1.32
2	A	201[A]	COA	C6A-N6A	5.64	1.48	1.34
2	A	201[B]	COA	C6A-N6A	5.64	1.48	1.34
2	B	201	COA	C6A-N6A	5.62	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	COA	C6A-N6A	5.61	1.48	1.34
2	C	201	COA	C6A-N6A	5.60	1.48	1.34
2	E	201	COA	C6A-N6A	5.56	1.48	1.34
2	F	201	COA	C6A-N6A	5.56	1.48	1.34
2	D	201	COA	C9P-N8P	5.42	1.46	1.33
2	C	201	COA	P2A-O3A	5.42	1.65	1.59
2	C	201	COA	C9P-N8P	5.27	1.46	1.33
2	B	201	COA	C9P-N8P	5.17	1.45	1.33
2	D	201	COA	P1A-O3A	4.84	1.64	1.59
2	B	201	COA	P1A-O3A	4.34	1.64	1.59
2	B	201	COA	P3B-O3B	4.19	1.66	1.59
2	E	201	COA	P1A-O3A	4.16	1.64	1.59
2	F	201	COA	P1A-O3A	4.04	1.63	1.59
2	A	201[B]	COA	P2A-O6A	3.96	1.69	1.54
2	A	201[A]	COA	P2A-O6A	3.91	1.69	1.54
2	F	201	COA	P3B-O3B	3.85	1.66	1.59
2	E	201	COA	P3B-O3B	3.78	1.66	1.59
2	D	201	COA	P3B-O3B	3.77	1.66	1.59
2	F	201	COA	P2A-O6A	3.71	1.68	1.54
2	A	201[B]	COA	P1A-O3A	3.64	1.63	1.59
2	C	201	COA	P3B-O3B	3.59	1.65	1.59
2	A	201[A]	COA	C2A-N3A	3.42	1.40	1.33
2	A	201[B]	COA	C2A-N3A	3.42	1.40	1.33
2	F	201	COA	C2A-N3A	3.41	1.40	1.33
2	C	201	COA	P1A-O3A	3.40	1.63	1.59
2	C	201	COA	C2A-N3A	3.39	1.40	1.33
2	D	201	COA	C2A-N3A	3.36	1.39	1.33
2	E	201	COA	C2A-N3A	3.36	1.39	1.33
2	A	201[A]	COA	P3B-O3B	3.35	1.65	1.59
2	A	201[B]	COA	P3B-O3B	3.35	1.65	1.59
2	B	201	COA	C2A-N3A	3.31	1.39	1.33
2	B	201	COA	O5P-C5P	-2.93	1.17	1.23
2	D	201	COA	O5P-C5P	-2.91	1.17	1.23
2	E	201	COA	O9P-C9P	-2.88	1.18	1.23
2	A	201[B]	COA	P1A-O5B	2.84	1.70	1.59
2	A	201[A]	COA	O3B-C3B	-2.82	1.34	1.44
2	A	201[B]	COA	O3B-C3B	-2.82	1.34	1.44
2	C	201	COA	O5P-C5P	-2.79	1.17	1.23
2	C	201	COA	C5A-C4A	-2.75	1.34	1.39
2	D	201	COA	P1A-O5B	2.75	1.70	1.59
2	D	201	COA	C5A-C4A	-2.70	1.34	1.39
2	C	201	COA	P1A-O5B	2.70	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	COA	P1A-O5B	2.70	1.69	1.59
2	F	201	COA	C5A-N7A	-2.69	1.34	1.39
2	B	201	COA	C5A-N7A	-2.68	1.34	1.39
2	E	201	COA	C5A-N7A	-2.67	1.34	1.39
2	E	201	COA	C5A-C4A	-2.67	1.34	1.39
2	A	201[A]	COA	C5A-N7A	-2.67	1.34	1.39
2	A	201[B]	COA	C5A-N7A	-2.67	1.34	1.39
2	C	201	COA	C5A-N7A	-2.66	1.34	1.39
2	B	201	COA	C5A-C4A	-2.65	1.34	1.39
2	D	201	COA	C5A-N7A	-2.65	1.34	1.39
2	F	201	COA	C5A-C4A	-2.63	1.34	1.39
2	E	201	COA	O3B-C3B	-2.62	1.35	1.44
2	D	201	COA	C6P-C5P	2.60	1.56	1.51
2	C	201	COA	O9P-C9P	-2.60	1.18	1.23
2	E	201	COA	P1A-O5B	2.59	1.69	1.59
2	C	201	COA	C6P-C5P	2.58	1.56	1.51
2	C	201	COA	O3B-C3B	-2.56	1.35	1.44
2	D	201	COA	O3B-C3B	-2.55	1.35	1.44
2	B	201	COA	P1A-O5B	2.53	1.69	1.59
2	D	201	COA	O9P-C9P	-2.50	1.18	1.23
2	F	201	COA	O3B-C3B	-2.48	1.35	1.44
2	B	201	COA	O9P-C9P	-2.47	1.18	1.23
2	A	201[A]	COA	C5A-C4A	-2.47	1.34	1.39
2	A	201[B]	COA	C5A-C4A	-2.47	1.34	1.39
2	D	201	COA	P2A-O6A	2.42	1.68	1.59
2	B	201	COA	P2A-O6A	2.42	1.68	1.59
2	E	201	COA	P2A-O6A	2.36	1.68	1.59
2	C	201	COA	C4A-N9A	-2.26	1.33	1.37
2	B	201	COA	C6P-C5P	2.24	1.55	1.51
2	F	201	COA	C3B-C4B	2.21	1.58	1.52
2	B	201	COA	C4A-N9A	-2.21	1.33	1.37
2	C	201	COA	P2A-O6A	2.16	1.67	1.59
2	E	201	COA	C4A-N9A	-2.09	1.33	1.37
2	C	201	COA	C3B-C4B	2.05	1.58	1.52
2	D	201	COA	C4A-N9A	-2.05	1.33	1.37
2	F	201	COA	C4A-N9A	-2.02	1.33	1.37
2	B	201	COA	O3B-C3B	-2.01	1.37	1.44

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	COA	N3A-C2A-N1A	-5.66	120.01	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	COA	N3A-C2A-N1A	-5.64	120.05	128.58
2	C	201	COA	N3A-C2A-N1A	-5.58	120.13	128.58
2	F	201	COA	N3A-C2A-N1A	-5.54	120.20	128.58
2	E	201	COA	N3A-C2A-N1A	-5.53	120.21	128.58
2	A	201[A]	COA	C5A-C4A-N3A	-5.36	119.34	126.72
2	A	201[B]	COA	C5A-C4A-N3A	-5.36	119.34	126.72
2	A	201[A]	COA	N3A-C2A-N1A	-5.02	120.98	128.58
2	A	201[B]	COA	N3A-C2A-N1A	-5.02	120.98	128.58
2	F	201	COA	C5A-C4A-N3A	-4.79	120.13	126.72
2	D	201	COA	C5A-C4A-N3A	-4.67	120.29	126.72
2	E	201	COA	C5A-C4A-N3A	-4.65	120.31	126.72
2	B	201	COA	C5A-C4A-N3A	-4.63	120.34	126.72
2	C	201	COA	C5A-C4A-N3A	-4.53	120.48	126.72
2	E	201	COA	N9A-C8A-N7A	-4.39	107.71	113.94
2	C	201	COA	N9A-C8A-N7A	-4.37	107.73	113.94
2	D	201	COA	N9A-C8A-N7A	-4.33	107.80	113.94
2	B	201	COA	N9A-C8A-N7A	-4.28	107.86	113.94
2	F	201	COA	N9A-C8A-N7A	-4.23	107.93	113.94
2	A	201[A]	COA	N9A-C8A-N7A	-4.17	108.01	113.94
2	A	201[B]	COA	N9A-C8A-N7A	-4.17	108.01	113.94
2	B	201	COA	C2A-N3A-C4A	3.32	119.93	111.83
2	D	201	COA	C2A-N3A-C4A	3.31	119.91	111.83
2	A	201[A]	COA	C2A-N3A-C4A	3.29	119.88	111.83
2	A	201[B]	COA	C2A-N3A-C4A	3.29	119.88	111.83
2	F	201	COA	C2A-N3A-C4A	3.29	119.88	111.83
2	E	201	COA	C2A-N3A-C4A	3.24	119.75	111.83
2	C	201	COA	C2A-N3A-C4A	3.22	119.70	111.83
2	B	201	COA	C7P-C6P-C5P	-3.21	107.05	112.39
2	A	201[A]	COA	N3A-C4A-N9A	3.12	132.47	127.17
2	A	201[B]	COA	N3A-C4A-N9A	3.12	132.47	127.17
2	A	201[A]	COA	C5A-N7A-C8A	3.10	108.32	103.45
2	A	201[B]	COA	C5A-N7A-C8A	3.10	108.32	103.45
2	A	201[A]	COA	O4B-C1B-N9A	2.96	113.77	108.09
2	A	201[B]	COA	O4B-C1B-N9A	2.96	113.77	108.09
2	F	201	COA	O4B-C1B-N9A	2.96	113.77	108.09
2	E	201	COA	O9P-C9P-CAP	2.95	122.05	119.11
2	C	201	COA	C2B-C1B-N9A	-2.87	106.18	113.30
2	D	201	COA	P3B-O3B-C3B	-2.85	115.82	123.43
2	F	201	COA	N3A-C4A-N9A	2.84	132.00	127.17
2	E	201	COA	C5A-N7A-C8A	2.83	107.90	103.45
2	D	201	COA	C5A-N7A-C8A	2.83	107.89	103.45
2	C	201	COA	CEP-CBP-CAP	2.81	113.56	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	COA	N3A-C4A-N9A	2.79	131.92	127.17
2	B	201	COA	C5A-N7A-C8A	2.77	107.81	103.45
2	F	201	COA	C5A-N7A-C8A	2.76	107.79	103.45
2	C	201	COA	C5A-N7A-C8A	2.74	107.76	103.45
2	D	201	COA	N3A-C4A-N9A	2.68	131.72	127.17
2	C	201	COA	N3A-C4A-N9A	2.67	131.71	127.17
2	A	201[A]	COA	P3B-O3B-C3B	-2.64	116.37	123.43
2	A	201[B]	COA	P3B-O3B-C3B	-2.64	116.37	123.43
2	C	201	COA	C4A-N9A-C8A	2.64	108.51	105.74
2	C	201	COA	C3B-C2B-C1B	2.62	105.66	99.89
2	E	201	COA	C4A-N9A-C8A	2.57	108.44	105.74
2	B	201	COA	N3A-C4A-N9A	2.55	131.50	127.17
2	F	201	COA	C4B-O4B-C1B	-2.49	103.96	109.47
2	A	201[A]	COA	C4A-C5A-N7A	-2.49	107.74	110.58
2	A	201[B]	COA	C4A-C5A-N7A	-2.49	107.74	110.58
2	C	201	COA	C3P-N4P-C5P	-2.44	118.28	122.82
2	B	201	COA	C3B-C2B-C1B	2.44	105.25	99.89
2	D	201	COA	C4A-N9A-C8A	2.38	108.24	105.74
2	D	201	COA	C2B-C1B-N9A	-2.37	107.41	113.30
2	D	201	COA	C5B-C4B-C3B	-2.37	106.49	114.38
2	F	201	COA	C4A-N9A-C8A	2.36	108.22	105.74
2	D	201	COA	C3B-C2B-C1B	2.34	105.03	99.89
2	B	201	COA	C7P-N8P-C9P	-2.34	118.34	122.55
2	A	201[A]	COA	C6A-C5A-C4A	2.31	120.33	117.18
2	A	201[B]	COA	C6A-C5A-C4A	2.31	120.33	117.18
2	B	201	COA	C4A-N9A-C8A	2.28	108.13	105.74
2	B	201	COA	C5B-C4B-C3B	-2.27	106.82	114.38
2	E	201	COA	O9P-C9P-N8P	-2.27	119.04	123.04
2	A	201[A]	COA	O5B-C5B-C4B	-2.24	101.37	108.99
2	A	201[B]	COA	O5B-C5B-C4B	-2.24	101.37	108.99
2	B	201	COA	C4A-C5A-N7A	-2.22	108.04	110.58
2	D	201	COA	C4A-C5A-N7A	-2.19	108.08	110.58
2	A	201[A]	COA	C5A-C4A-N9A	2.19	108.19	105.81
2	A	201[B]	COA	C5A-C4A-N9A	2.19	108.19	105.81
2	E	201	COA	CAP-C9P-N8P	2.16	118.91	117.16
2	A	201[A]	COA	O2A-P1A-O3A	2.16	113.10	107.27
2	B	201	COA	C5A-C4A-N9A	2.15	108.16	105.81
2	A	201[A]	COA	C5B-C4B-C3B	-2.11	107.33	114.38
2	A	201[B]	COA	C5B-C4B-C3B	-2.11	107.33	114.38
2	E	201	COA	C2B-C1B-N9A	-2.10	108.09	113.30
2	E	201	COA	C4A-C5A-N7A	-2.10	108.18	110.58
2	F	201	COA	C4A-C5A-N7A	-2.10	108.19	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	C4A-C5A-N7A	-2.09	108.19	110.58
2	A	201[A]	COA	C3B-C2B-C1B	2.08	104.47	99.89
2	A	201[B]	COA	C3B-C2B-C1B	2.08	104.47	99.89
2	F	201	COA	O4B-C1B-C2B	-2.08	102.16	106.62
2	D	201	COA	C6P-C7P-N8P	-2.08	107.58	112.00
2	A	201[B]	COA	O5A-P2A-O3A	2.02	111.40	104.64

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201[B]	COA	P2A-O3A-P1A-O5B
2	B	201	COA	C5B-O5B-P1A-O3A
2	B	201	COA	CDP-CBP-CCP-O6A
2	B	201	COA	CEP-CBP-CCP-O6A
2	B	201	COA	CAP-CBP-CCP-O6A
2	B	201	COA	C5P-C6P-C7P-N8P
2	C	201	COA	C5B-O5B-P1A-O1A
2	C	201	COA	CCP-O6A-P2A-O3A
2	C	201	COA	CCP-O6A-P2A-O4A
2	C	201	COA	CCP-O6A-P2A-O5A
2	C	201	COA	OAP-CAP-CBP-CCP
2	C	201	COA	C9P-CAP-CBP-CCP
2	C	201	COA	OAP-CAP-CBP-CDP
2	C	201	COA	C9P-CAP-CBP-CDP
2	C	201	COA	OAP-CAP-CBP-CEP
2	C	201	COA	C9P-CAP-CBP-CEP
2	D	201	COA	C5B-O5B-P1A-O1A
2	D	201	COA	CCP-O6A-P2A-O3A
2	D	201	COA	CCP-O6A-P2A-O4A
2	D	201	COA	CDP-CBP-CCP-O6A
2	D	201	COA	CEP-CBP-CCP-O6A
2	D	201	COA	CAP-CBP-CCP-O6A
2	D	201	COA	C9P-CAP-CBP-CCP
2	D	201	COA	O9P-C9P-CAP-CBP
2	D	201	COA	N8P-C9P-CAP-CBP
2	D	201	COA	N8P-C9P-CAP-OAP
2	D	201	COA	C5P-C6P-C7P-N8P
2	E	201	COA	C5B-O5B-P1A-O1A
2	E	201	COA	C5B-O5B-P1A-O2A
2	E	201	COA	CCP-O6A-P2A-O3A
2	E	201	COA	CCP-O6A-P2A-O4A

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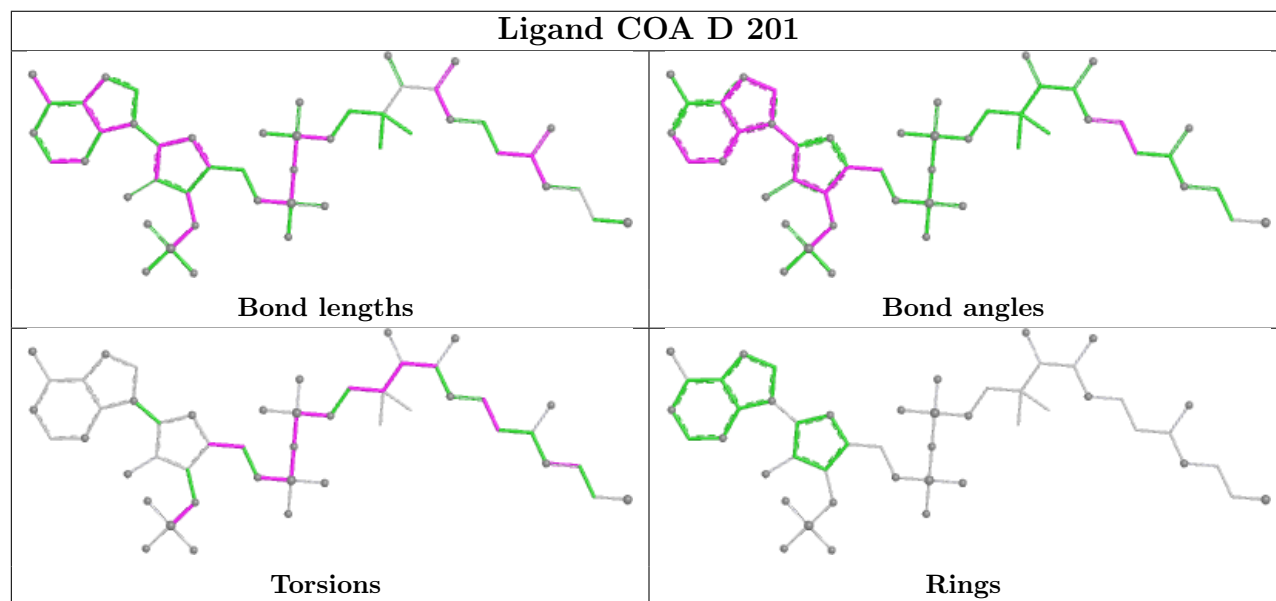
Mol	Chain	Res	Type	Atoms
2	F	201	COA	O4B-C4B-C5B-O5B
2	C	201	COA	O4B-C4B-C5B-O5B
2	D	201	COA	C3B-C4B-C5B-O5B
2	B	201	COA	C4B-C3B-O3B-P3B
2	D	201	COA	O4B-C4B-C5B-O5B
2	F	201	COA	C3B-C4B-C5B-O5B
2	C	201	COA	C4B-C3B-O3B-P3B
2	C	201	COA	C3B-C4B-C5B-O5B
2	E	201	COA	O4B-C4B-C5B-O5B
2	D	201	COA	O9P-C9P-CAP-OAP
2	D	201	COA	P2A-O3A-P1A-O5B
2	D	201	COA	P1A-O3A-P2A-O6A
2	D	201	COA	C9P-CAP-CBP-CEP
2	B	201	COA	P2A-O3A-P1A-O2A
2	B	201	COA	C9P-CAP-CBP-CCP
2	A	201[A]	COA	C5B-O5B-P1A-O3A
2	A	201[B]	COA	C5B-O5B-P1A-O1A
2	B	201	COA	C5B-O5B-P1A-O1A
2	B	201	COA	CCP-O6A-P2A-O3A
2	B	201	COA	CCP-O6A-P2A-O4A
2	B	201	COA	CCP-O6A-P2A-O5A
2	D	201	COA	CCP-O6A-P2A-O5A
2	D	201	COA	OAP-CAP-CBP-CCP
2	E	201	COA	C5B-O5B-P1A-O3A
2	E	201	COA	CCP-O6A-P2A-O5A
2	B	201	COA	OAP-CAP-CBP-CDP
2	D	201	COA	OAP-CAP-CBP-CDP
2	D	201	COA	P1A-O3A-P2A-O4A
2	D	201	COA	C2P-C3P-N4P-C5P
2	D	201	COA	C3B-O3B-P3B-O7A
2	E	201	COA	O9P-C9P-CAP-CBP
2	A	201[A]	COA	P1A-O3A-P2A-O6A
2	E	201	COA	C3B-C4B-C5B-O5B
2	B	201	COA	C9P-CAP-CBP-CEP
2	D	201	COA	C9P-CAP-CBP-CDP
2	C	201	COA	C2B-C3B-O3B-P3B
2	B	201	COA	OAP-CAP-CBP-CEP
2	C	201	COA	P1A-O3A-P2A-O5A
2	C	201	COA	CBP-CCP-O6A-P2A
2	B	201	COA	C2B-C3B-O3B-P3B
2	E	201	COA	P2A-O3A-P1A-O2A

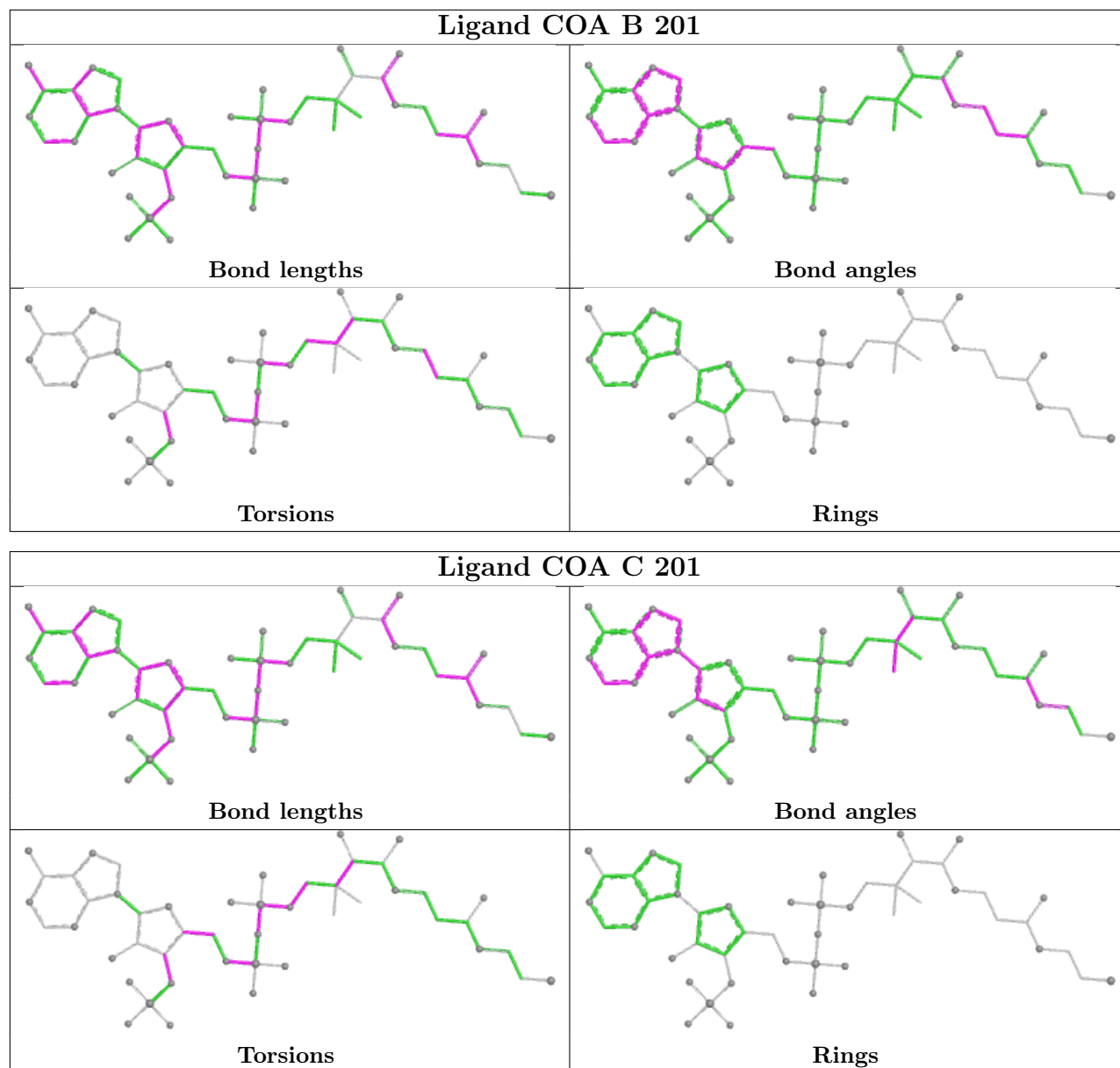
There are no ring outliers.

5 monomers are involved in 18 short contacts:

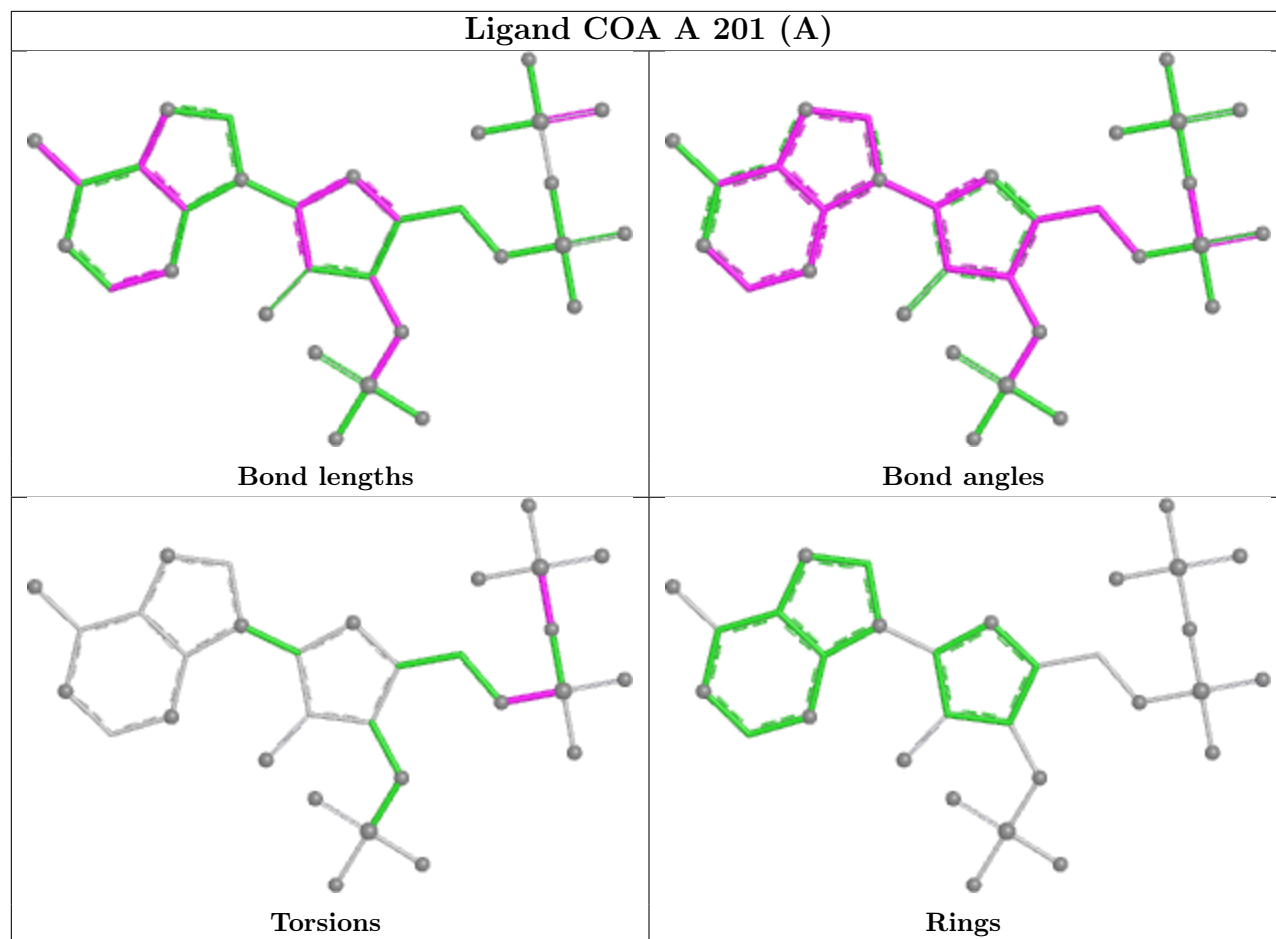
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	COA	4	0
2	B	201	COA	4	0
2	C	201	COA	6	0
2	F	201	COA	2	0
2	E	201	COA	2	0

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

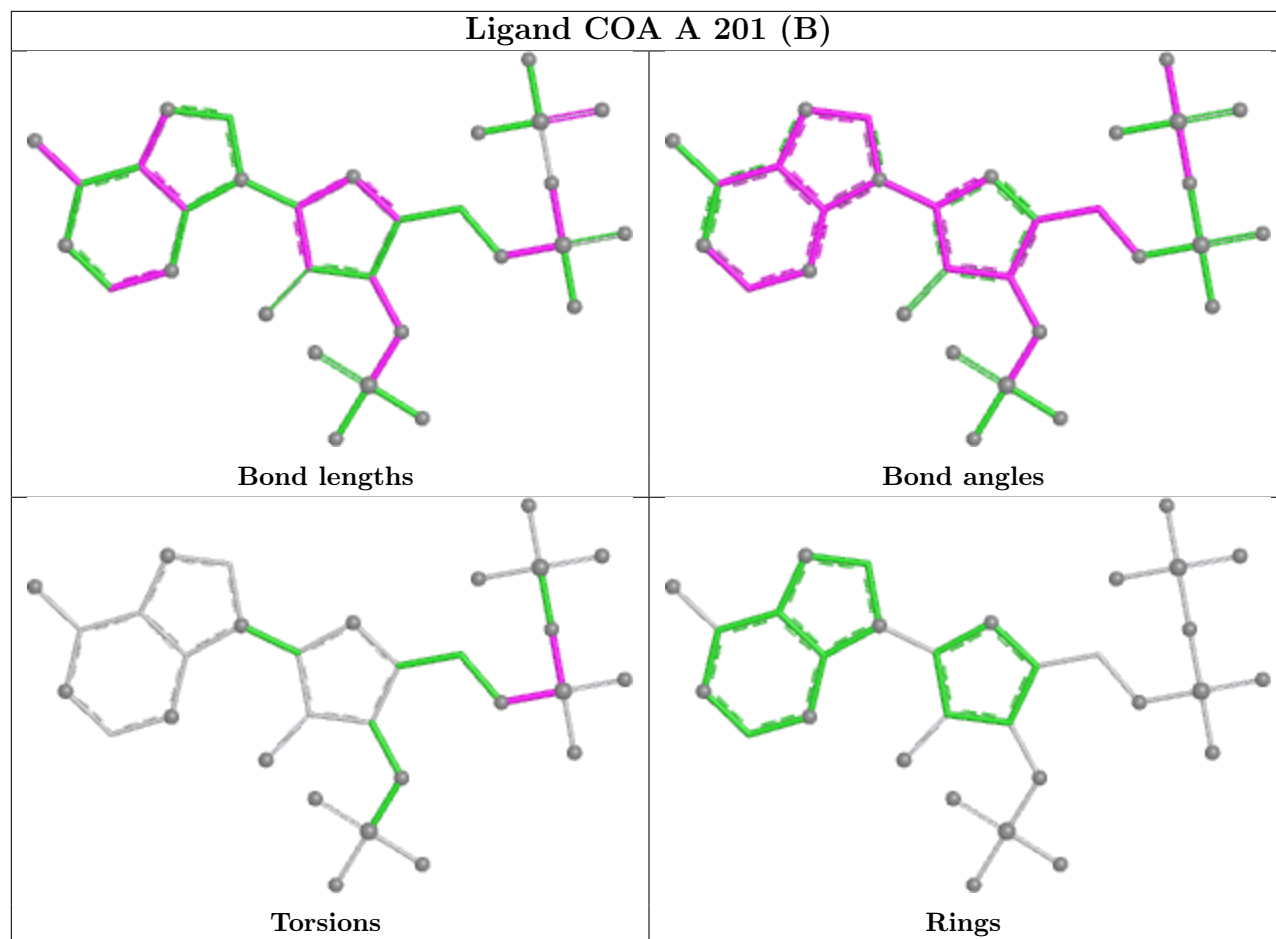




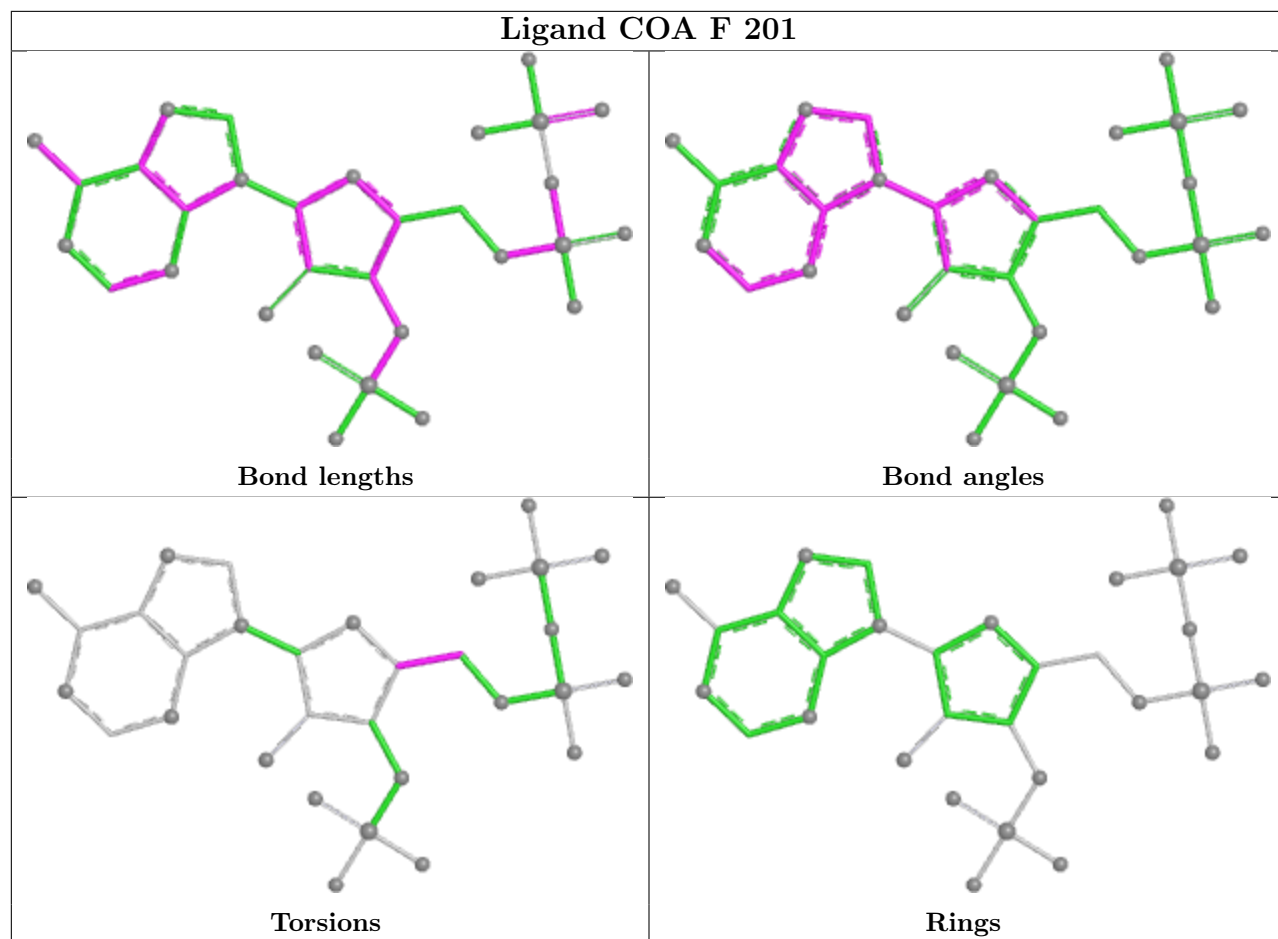
Ligand COA A 201 (A)



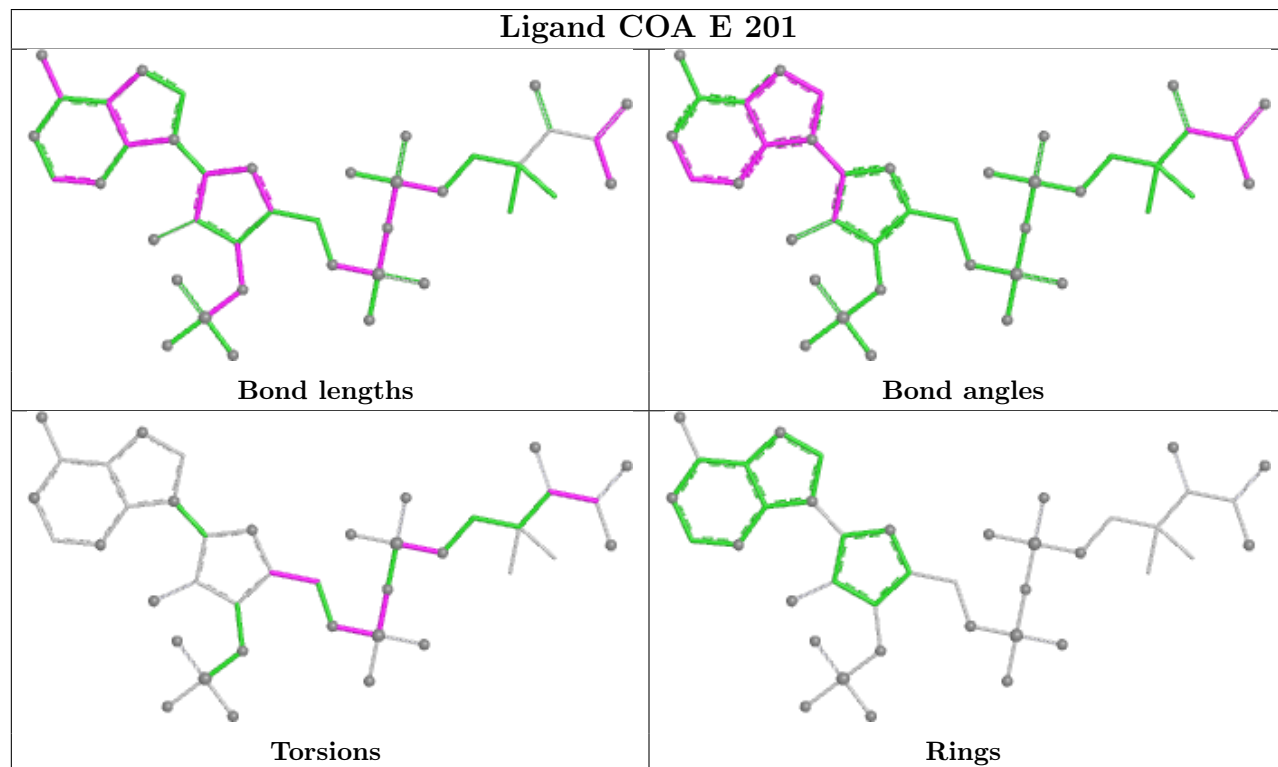
Ligand COA A 201 (B)



Ligand COA F 201



Ligand COA E 201



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	151/156 (96%)	0.88	6 (3%)	42	37	24, 36, 51, 63	1 (0%)
1	B	153/156 (98%)	1.23	24 (15%)	5	4	24, 43, 64, 79	0
1	C	151/156 (96%)	1.60	44 (29%)	1	1	40, 60, 78, 89	0
1	D	152/156 (97%)	0.97	15 (9%)	13	10	23, 37, 54, 71	0
1	E	153/156 (98%)	1.30	26 (16%)	4	3	30, 42, 59, 71	0
1	F	152/156 (97%)	1.65	43 (28%)	1	1	30, 53, 72, 78	0
All	All	912/936 (97%)	1.27	158 (17%)	4	3	23, 44, 70, 89	1 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	4.3
1	C	2	ALA	3.9
1	E	1	MET	3.9
1	B	131	SER	3.8
1	F	6	ARG	3.7
1	D	1	MET	3.7
1	E	24	ILE	3.5
1	E	28	PHE	3.5
1	C	133	TRP	3.4
1	B	71	GLY	3.4
1	C	134	PHE	3.4
1	D	2	ALA	3.3
1	F	1	MET	3.2
1	D	32	GLY	3.2
1	B	130	ILE	3.2
1	F	119	GLY	3.2
1	C	38	LEU	3.1
1	C	113	GLY	3.1
1	A	2	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	28	PHE	3.0
1	B	56	LYS	3.0
1	F	81	LEU	3.0
1	C	44	SER	3.0
1	F	118	HIS	3.0
1	F	135	GLN	2.9
1	F	137	GLU	2.9
1	C	139	LEU	2.9
1	E	139	LEU	2.9
1	F	138	GLU	2.9
1	B	121	ASP	2.9
1	B	112	VAL	2.9
1	B	10	ALA	2.9
1	F	125	SER	2.8
1	F	116	ILE	2.8
1	D	102	GLY	2.8
1	F	139	LEU	2.8
1	E	141	GLU	2.8
1	E	150	ILE	2.8
1	F	83	VAL	2.8
1	D	57	ASP	2.8
1	B	36	VAL	2.8
1	C	67	TYR	2.8
1	C	82	ASN	2.7
1	F	50	GLU	2.7
1	B	58	ARG	2.7
1	F	108	PHE	2.7
1	C	45	GLU	2.7
1	C	141	GLU	2.7
1	B	55	LEU	2.7
1	B	108	PHE	2.7
1	C	100	LYS	2.7
1	C	41	LEU	2.6
1	C	93	GLU	2.6
1	F	113	GLY	2.6
1	C	86	THR	2.6
1	D	53	THR	2.6
1	E	33	PHE	2.6
1	C	99	SER	2.6
1	C	116	ILE	2.6
1	B	123	VAL	2.6
1	E	108	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	9	ILE	2.5
1	C	130	ILE	2.5
1	A	100[A]	LYS	2.5
1	E	124	LYS	2.5
1	F	143	LYS	2.5
1	A	127	GLU	2.5
1	D	61	PHE	2.5
1	F	121	ASP	2.5
1	F	102	GLY	2.5
1	C	70	SER	2.5
1	E	6	ARG	2.5
1	F	64	LEU	2.5
1	A	108	PHE	2.5
1	F	43	ALA	2.5
1	B	7	THR	2.5
1	D	100	LYS	2.5
1	B	122	SER	2.5
1	F	55	LEU	2.5
1	F	65	VAL	2.5
1	F	123	VAL	2.5
1	D	20	LEU	2.4
1	E	38	LEU	2.4
1	F	91	LEU	2.4
1	B	64	LEU	2.4
1	B	110	ILE	2.4
1	D	70	SER	2.4
1	C	39	LYS	2.4
1	C	36	VAL	2.4
1	E	112	VAL	2.4
1	B	126	ALA	2.4
1	F	126	ALA	2.4
1	C	53	THR	2.4
1	E	7	THR	2.4
1	B	129	GLU	2.4
1	D	58	ARG	2.4
1	C	81	LEU	2.4
1	F	35	LEU	2.4
1	F	51	HIS	2.4
1	F	85	LYS	2.4
1	B	28	PHE	2.4
1	B	48	LEU	2.3
1	E	57	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	GLY	2.3
1	C	75	ALA	2.3
1	F	53	THR	2.3
1	F	94	THR	2.3
1	F	124	LYS	2.3
1	F	149	TRP	2.3
1	E	97	ALA	2.3
1	C	112	VAL	2.3
1	C	48	LEU	2.3
1	E	128	LYS	2.3
1	F	131	SER	2.3
1	C	80	GLY	2.3
1	D	83	VAL	2.2
1	F	77	VAL	2.2
1	D	143	LYS	2.2
1	F	141	GLU	2.2
1	F	52	TYR	2.2
1	C	111	GLN	2.2
1	F	147	GLN	2.2
1	B	125	SER	2.2
1	E	46	ASP	2.2
1	C	123	VAL	2.2
1	D	24	ILE	2.2
1	C	126	ALA	2.2
1	E	146	ALA	2.2
1	F	146	ALA	2.2
1	E	109	CYS	2.2
1	F	67	TYR	2.2
1	C	62	THR	2.2
1	C	119	GLY	2.2
1	C	46	ASP	2.2
1	D	125	SER	2.2
1	E	73	VAL	2.2
1	E	134	PHE	2.2
1	A	142	TYR	2.1
1	A	150	ILE	2.1
1	C	25	ILE	2.1
1	C	56	LYS	2.1
1	F	38	LEU	2.1
1	E	77	VAL	2.1
1	C	28	PHE	2.1
1	B	94	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	136	PRO	2.1
1	B	38	LEU	2.1
1	E	47	LEU	2.1
1	F	127	GLU	2.0
1	C	149	TRP	2.0
1	E	72	PRO	2.0
1	C	16	VAL	2.0
1	C	52	TYR	2.0
1	C	57	ASP	2.0
1	C	131	SER	2.0
1	C	84	VAL	2.0
1	E	34	ARG	2.0
1	F	27	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

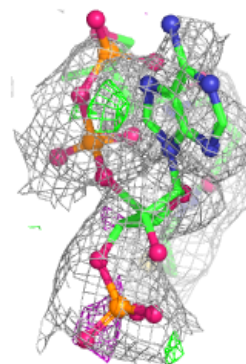
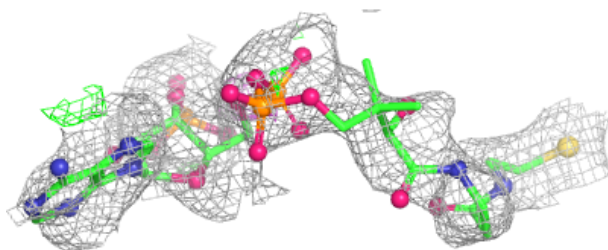
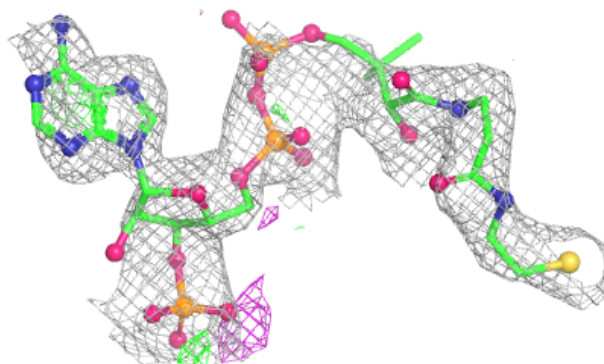
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	B	201	48/48	0.72	0.20	34,77,112,131	0
2	COA	C	201	48/48	0.74	0.19	58,72,100,110	0
2	COA	F	201	31/48	0.78	0.15	34,60,74,87	0
2	COA	E	201	40/48	0.79	0.19	50,77,112,121	0
2	COA	D	201	48/48	0.80	0.18	34,78,95,109	0
2	COA	A	201[B]	31/48	0.88	0.14	34,47,71,92	8
2	COA	A	201[A]	31/48	0.88	0.14	34,47,71,92	8

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.

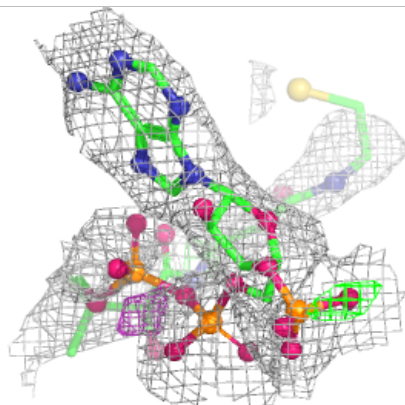
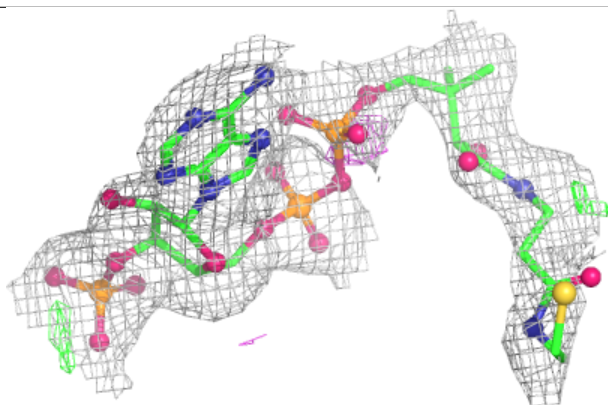
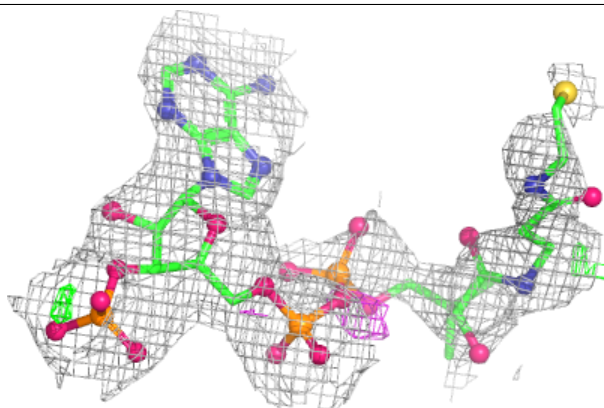
Electron density around COA B 201:

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



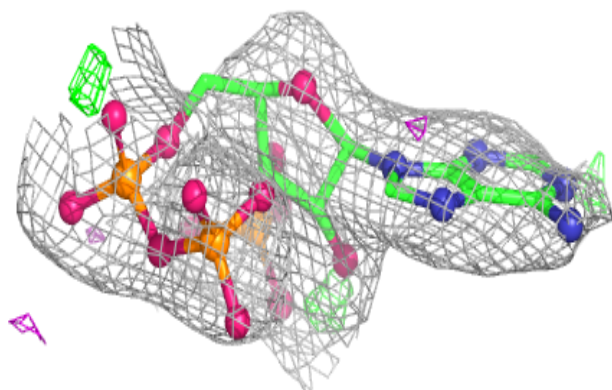
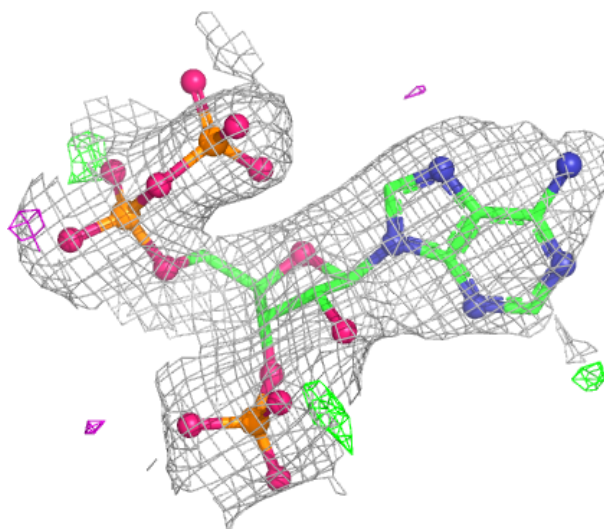
Electron density around COA C 201:

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



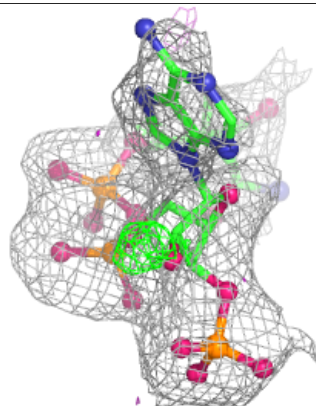
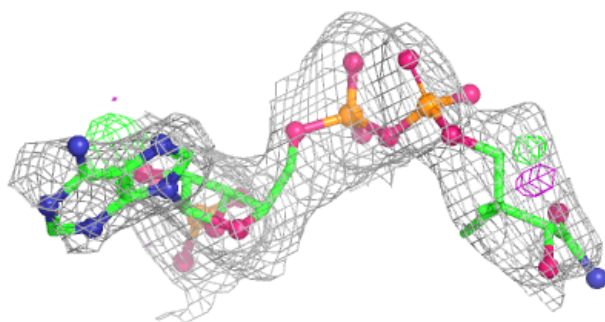
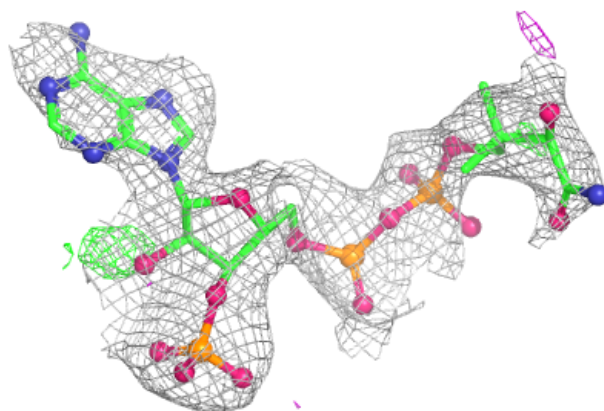
Electron density around COA F 201:

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

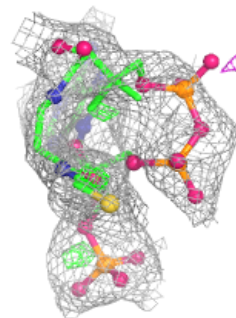
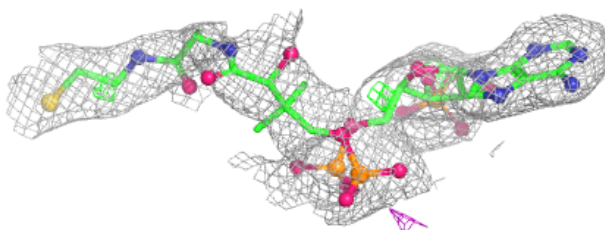
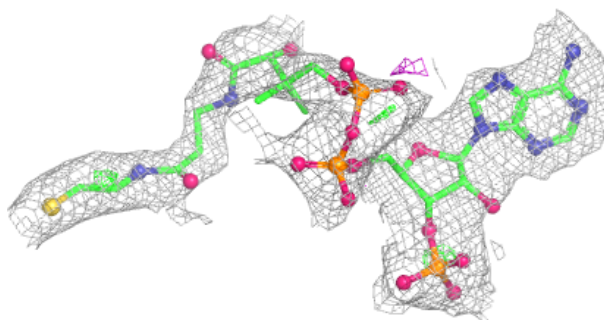


Electron density around COA E 201:

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

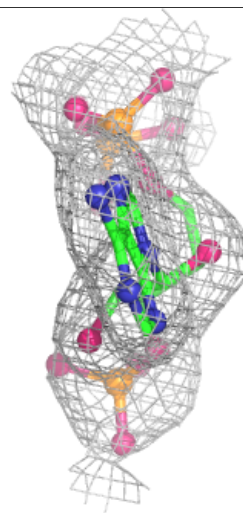
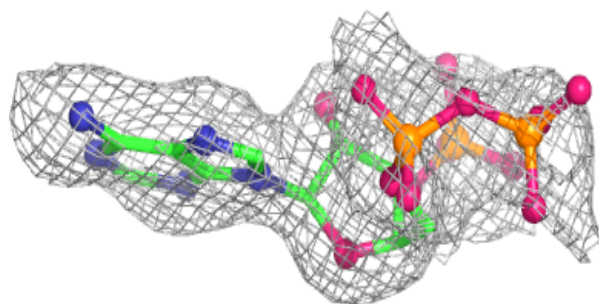
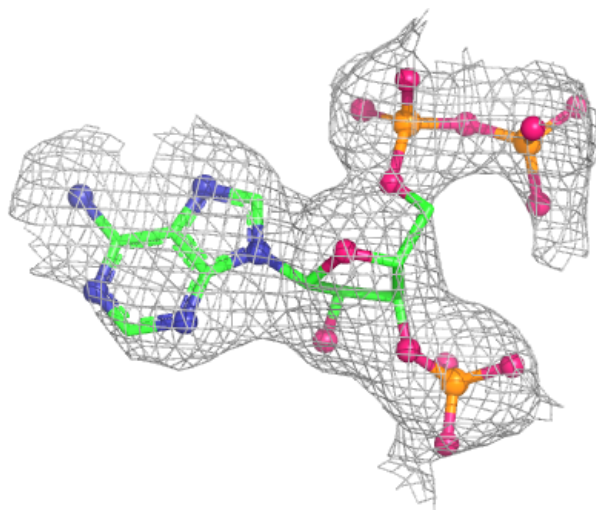
**Electron density around COA D 201:**

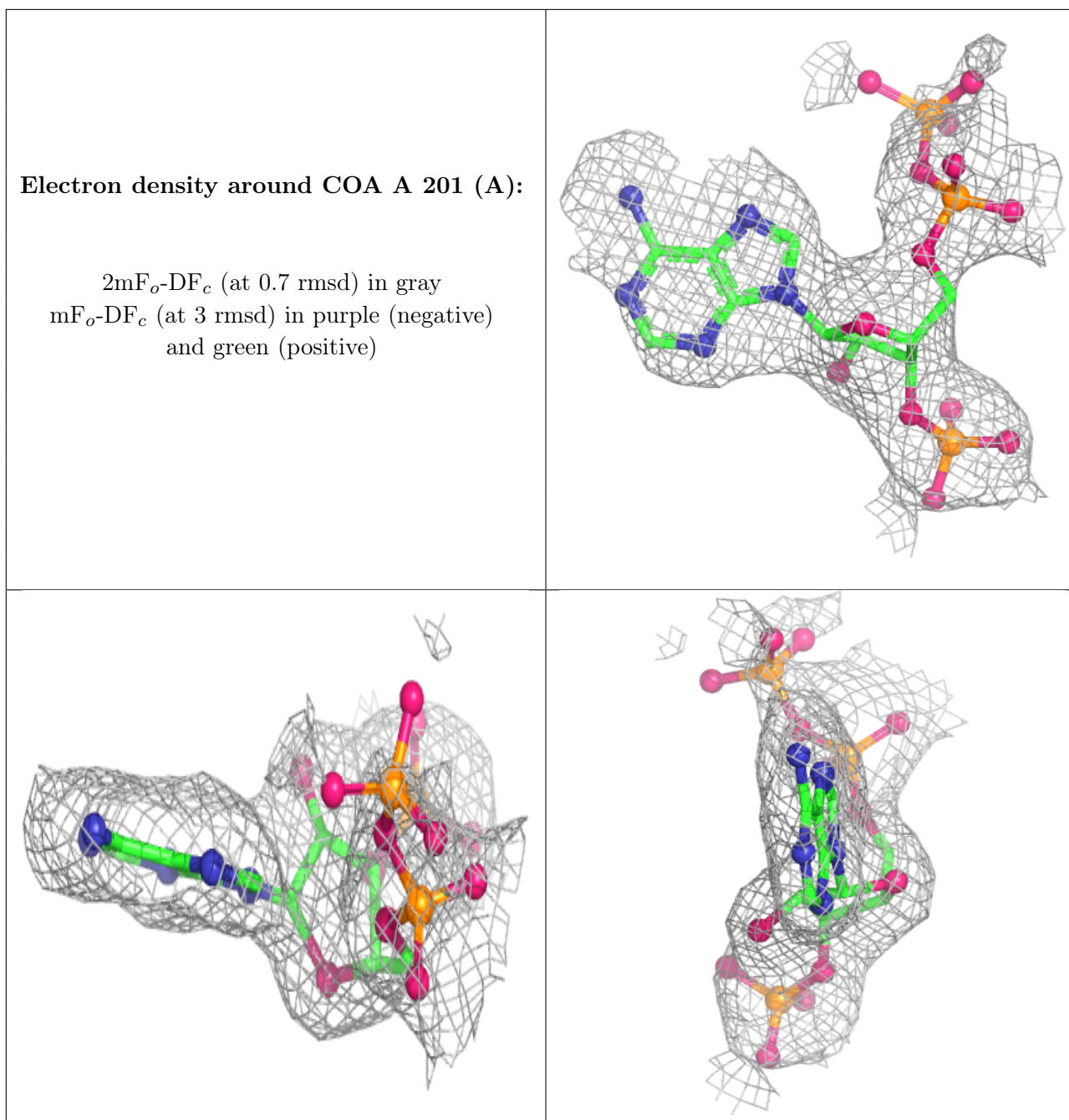
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA A 201 (B):

$2mF_o-DF_c$ (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.