



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:30 am BST

PDB ID : 3NFD  
Title : Chronobacterium ammoniagenes ACPS-CoA complex  
Authors : Gokulan, K.  
Deposited on : 2010-06-10  
Resolution : 1.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 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

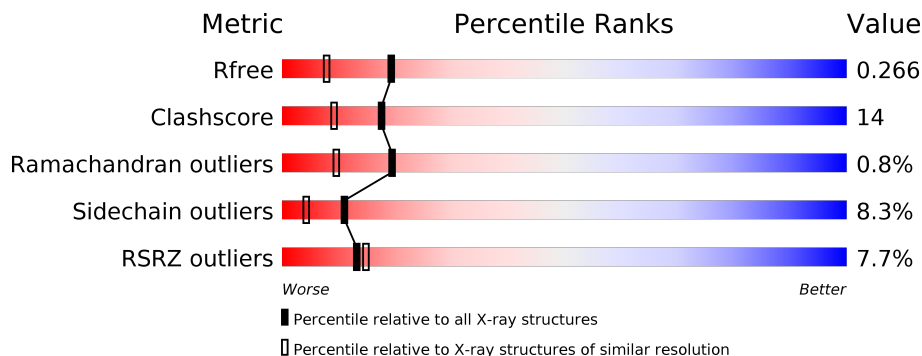
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	
1	C	153	
1	D	153	
1	E	153	
1	F	153	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	COA	A	154	X	-	-	-
2	COA	C	154	X	-	-	-
2	COA	D	154	X	-	-	-
2	COA	E	154	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6824 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.

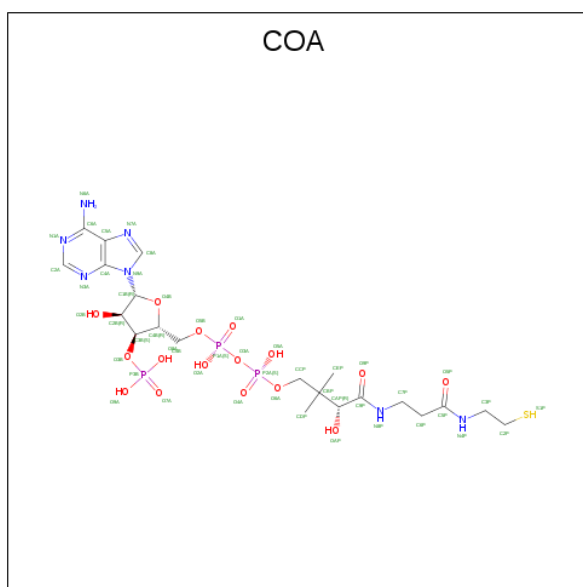
- Molecule 1 is a protein called Phosphopantetheine protein transferase, Ppt1p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	136	1065	676	190	197	1	1	0	0	0
1	B	137	1076	682	194	198	1	1	0	0	0
1	C	137	1076	682	194	198	1	1	0	0	0
1	D	134	1056	671	188	195	1	1	0	0	0
1	E	139	1095	692	200	201	1	1	0	0	0
1	F	136	1065	676	190	197	1	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	SER	ASP	SEE REMARK 999	UNP O31302
A	146	LEU	GLN	SEE REMARK 999	UNP O31302
B	48	SER	ASP	SEE REMARK 999	UNP O31302
B	146	LEU	GLN	SEE REMARK 999	UNP O31302
C	48	SER	ASP	SEE REMARK 999	UNP O31302
C	146	LEU	GLN	SEE REMARK 999	UNP O31302
D	48	SER	ASP	SEE REMARK 999	UNP O31302
D	146	LEU	GLN	SEE REMARK 999	UNP O31302
E	48	SER	ASP	SEE REMARK 999	UNP O31302
E	146	LEU	GLN	SEE REMARK 999	UNP O31302
F	48	SER	ASP	SEE REMARK 999	UNP O31302
F	146	LEU	GLN	SEE REMARK 999	UNP O31302

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0
2	C	1	27	10	5	10	2	0	0
2	D	1	27	10	5	10	2	0	0
2	E	1	27	10	5	10	2	0	0
2	F	1	27	10	5	10	2	0	0

- Molecule 3 is water.

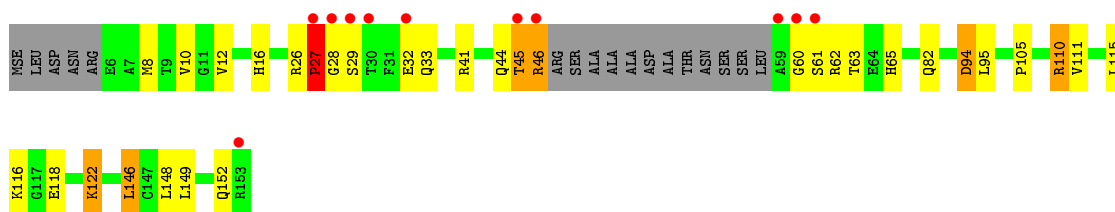
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	46	Total	O	0	0
			46	46		
3	C	44	Total	O	0	0
			44	44		
3	D	29	Total	O	0	0
			29	29		
3	E	41	Total	O	0	0
			41	41		
3	F	22	Total	O	0	0
			22	22		

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

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.

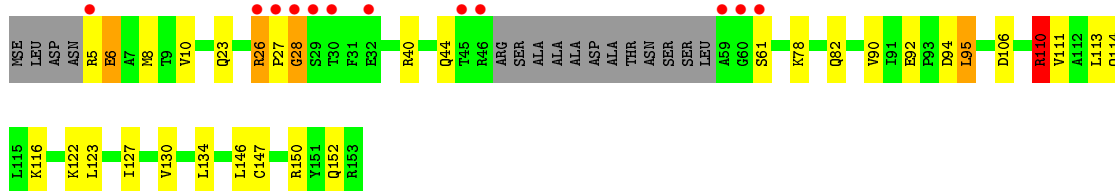
- Molecule 1: Phosphopantetheine protein transferase, Ppt1p

Chain A: 



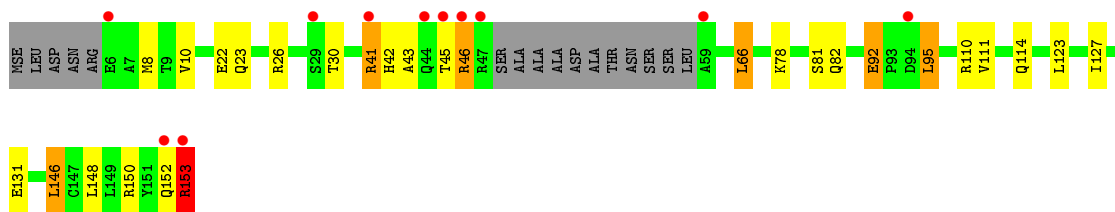
- Molecule 1: Phosphopantetheine protein transferase, Ppt1p

Chain B: 



- Molecule 1: Phosphopantetheine protein transferase, Ppt1p

Chain C: 

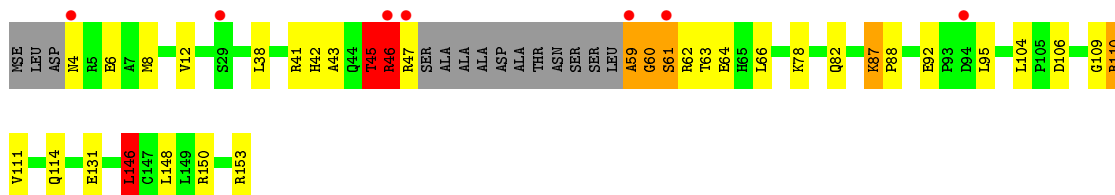


- Molecule 1: Phosphopantetheine protein transferase, Ppt1p

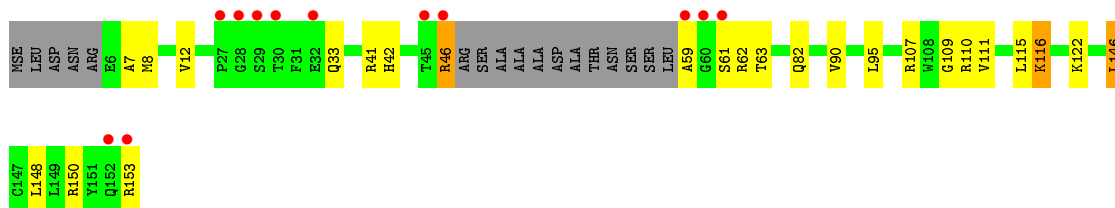
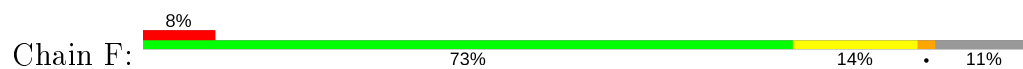
Chain D: 



- Molecule 1: Phosphopantetheine protein transferase, Ppt1p



- Molecule 1: Phosphopantetheine protein transferase, Ppt1p



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.78Å 56.02Å 88.28Å 80.88° 76.23° 60.92°	Depositor
Resolution (Å)	20.00 – 1.89 19.26 – 1.89	Depositor EDS
% Data completeness (in resolution range)	70.3 (20.00-1.89) 73.1 (19.26-1.89)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.47 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0000, CNS	Depositor
R, $R_{free}$	0.212 , 0.259 0.231 , 0.266	Depositor DCC
$R_{free}$ test set	2637 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.023 for -h,-h+k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

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

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	0.92	0/1087	0.93	1/1470 (0.1%)
1	B	0.79	1/1098 (0.1%)	0.84	1/1484 (0.1%)
1	C	0.76	0/1098	0.90	4/1484 (0.3%)
1	D	0.74	0/1078	0.81	0/1458
1	E	0.92	1/1117 (0.1%)	0.89	1/1509 (0.1%)
1	F	0.82	0/1087	0.82	0/1470
All	All	0.83	2/6565 (0.0%)	0.87	7/8875 (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	1	0
1	C	0	1
1	D	0	1
1	E	0	4
All	All	1	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	ARG	CG-CD	-5.51	1.38	1.51
1	E	64	GLU	CD-OE2	-5.24	1.19	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	ARG	NE-CZ-NH2	7.39	124.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	LEU	CA-CB-CG	6.94	131.27	115.30
1	C	153	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	B	110	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	146	LEU	CA-CB-CG	5.86	128.79	115.30
1	A	94	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	66	LEU	CB-CG-CD1	5.05	119.58	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	153	ARG	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	152	GLN	Peptide
1	D	61	SER	Peptide
1	E	45	THR	Peptide
1	E	59	ALA	Peptide
1	E	60	GLY	Peptide
1	E	61	SER	Peptide

## 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	1065	0	1055	34	0
1	B	1076	0	1068	20	1
1	C	1076	0	1068	33	1
1	D	1056	0	1047	26	0
1	E	1095	0	1087	49	0
1	F	1065	0	1055	38	0
2	A	27	0	11	2	0
2	B	27	0	11	3	0
2	C	27	0	11	2	0
2	D	27	0	11	3	0
2	E	27	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	27	0	11	10	0
3	A	47	0	0	2	0
3	B	46	0	0	0	0
3	C	44	0	0	4	0
3	D	29	0	0	1	0
3	E	41	0	0	0	0
3	F	22	0	0	0	0
All	All	6824	0	6445	178	1

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 14.

All (178) 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:46:ARG:HH21	1:A:46:ARG:CB	1.44	1.28
1:A:46:ARG:HH21	1:A:46:ARG:HB3	1.06	1.15
1:E:46:ARG:CG	1:E:46:ARG:HH21	1.60	1.12
1:E:8:MSE:HE2	1:E:148:LEU:HD11	1.11	1.07
1:E:12:VAL:HG12	1:E:146:LEU:HD22	1.40	1.03
1:C:42:HIS:O	1:C:45:THR:HG22	1.58	1.03
1:A:146:LEU:HD21	1:C:146:LEU:HG	1.40	1.01
1:A:46:ARG:NH2	1:A:46:ARG:HB3	1.75	1.01
1:E:8:MSE:CE	1:E:148:LEU:HD11	1.91	1.01
2:C:154:COA:H2A	3:C:422:HOH:O	1.60	1.00
1:B:8:MSE:HE2	1:B:150:ARG:HD3	1.41	1.00
1:E:46:ARG:NH2	1:E:46:ARG:HG3	1.46	0.99
1:F:8:MSE:CE	1:F:148:LEU:HD11	1.95	0.96
1:F:153:ARG:HG2	1:F:153:ARG:HH21	1.30	0.96
1:A:46:ARG:NH2	1:A:46:ARG:CB	2.29	0.95
1:E:46:ARG:HH21	1:E:46:ARG:HG3	0.79	0.94
1:B:111:VAL:H	1:C:82:GLN:HE22	1.12	0.93
1:A:8:MSE:CE	1:A:148:LEU:HD11	1.99	0.93
1:E:8:MSE:HE2	1:E:148:LEU:CD1	2.00	0.92
1:F:8:MSE:HE2	1:F:148:LEU:HD11	1.54	0.89
1:E:111:VAL:H	1:F:82:GLN:HE22	1.21	0.88
1:D:78:LYS:HG2	2:F:154:COA:C2A	2.03	0.87
1:D:111:VAL:H	1:E:82:GLN:HE22	1.23	0.85
1:C:153:ARG:HH21	1:C:153:ARG:HG3	1.39	0.85
1:D:78:LYS:HG2	2:F:154:COA:H2A	1.60	0.83
1:A:8:MSE:HE2	1:A:148:LEU:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD23	1:F:146:LEU:HD13	1.63	0.80
1:F:46:ARG:HB2	1:F:46:ARG:NH1	1.96	0.80
2:C:154:COA:C2A	3:C:422:HOH:O	2.23	0.78
1:A:111:VAL:H	1:B:82:GLN:HE22	1.29	0.77
1:A:46:ARG:HB2	1:A:46:ARG:HH21	1.47	0.77
1:A:82:GLN:HE22	1:C:111:VAL:H	1.32	0.76
1:F:153:ARG:HG2	1:F:153:ARG:NH2	1.93	0.76
1:B:8:MSE:HE2	1:B:150:ARG:CD	2.15	0.76
1:A:27:PRO:HB3	1:A:28:GLY:HA3	1.68	0.75
1:D:78:LYS:CG	2:F:154:COA:H2A	2.17	0.75
1:F:46:ARG:NH2	2:F:154:COA:O7A	2.19	0.74
1:A:10:VAL:HG21	1:C:146:LEU:HD12	1.69	0.74
1:C:146:LEU:HD11	1:C:148:LEU:CD2	2.17	0.74
1:D:46:ARG:NH1	2:D:154:COA:O7A	2.18	0.73
1:E:146:LEU:CG	1:F:146:LEU:HD11	2.19	0.73
1:F:46:ARG:NE	2:F:154:COA:O7A	2.22	0.73
2:D:154:COA:O1A	1:E:78:LYS:NZ	2.21	0.72
1:C:42:HIS:O	1:C:45:THR:CG2	2.36	0.72
1:C:146:LEU:CD1	1:C:148:LEU:HD23	2.21	0.71
1:A:44:GLN:HG2	3:A:365:HOH:O	1.92	0.70
1:A:27:PRO:CB	1:A:28:GLY:HA3	2.22	0.70
1:D:82:GLN:HE22	1:F:111:VAL:H	1.38	0.70
1:E:106:ASP:OD2	1:E:110:ARG:HG2	1.92	0.69
1:D:146:LEU:CD2	1:F:146:LEU:HD13	2.21	0.69
1:E:46:ARG:HG2	1:E:61:SER:OG	1.92	0.68
1:E:146:LEU:HG	1:F:146:LEU:HD11	1.74	0.68
1:A:46:ARG:CG	1:A:46:ARG:HH21	2.07	0.67
1:A:118:GLU:HG3	1:A:122:LYS:HE3	1.75	0.66
1:E:4:ASN:O	1:E:153:ARG:NH1	2.30	0.65
1:E:59:ALA:HB3	1:E:63:THR:HB	1.78	0.63
1:C:123:LEU:HD11	1:C:127:ILE:HD11	1.80	0.63
1:F:46:ARG:HB2	1:F:46:ARG:HH11	1.63	0.62
1:B:8:MSE:CE	1:B:150:ARG:HD3	2.23	0.62
1:D:80:TRP:CZ2	1:D:90:VAL:HG11	2.34	0.62
1:D:6:GLU:OE2	1:D:8:MSE:HE3	1.99	0.62
1:C:146:LEU:CD1	1:C:148:LEU:CD2	2.79	0.61
1:E:60:GLY:O	1:E:61:SER:OG	2.18	0.61
1:E:46:ARG:NH2	1:E:46:ARG:CG	2.30	0.59
1:E:8:MSE:HE1	1:E:148:LEU:HD21	1.85	0.59
1:D:78:LYS:CB	2:F:154:COA:H2A	2.32	0.59
2:A:154:COA:C2A	1:B:78:LYS:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:NE2	3:C:414:HOH:O	2.35	0.59
1:E:146:LEU:HD11	1:F:146:LEU:HD11	1.84	0.59
1:F:59:ALA:HB3	1:F:63:THR:HG21	1.84	0.59
1:A:27:PRO:CB	1:A:28:GLY:CA	2.80	0.59
1:C:41:ARG:NH1	1:C:41:ARG:O	2.36	0.58
1:D:146:LEU:HB2	1:E:12:VAL:HG11	1.85	0.58
1:C:41:ARG:HH11	1:C:42:HIS:HA	1.69	0.58
1:E:146:LEU:CD1	1:F:146:LEU:HD11	2.33	0.58
1:C:41:ARG:C	1:C:41:ARG:CZ	2.73	0.57
1:C:153:ARG:HH21	1:C:153:ARG:CG	2.14	0.57
1:F:46:ARG:CZ	2:F:154:COA:O7A	2.53	0.57
1:C:41:ARG:NH2	1:C:41:ARG:HB2	2.20	0.56
1:B:123:LEU:HD21	1:B:130:VAL:HG21	1.88	0.56
1:D:146:LEU:HD21	1:F:146:LEU:HD22	1.88	0.56
1:D:80:TRP:HZ2	1:D:90:VAL:HG11	1.71	0.55
1:D:90:VAL:HG12	1:D:91:ILE:HG13	1.89	0.55
1:F:42:HIS:O	1:F:46:ARG:HB3	2.07	0.55
1:B:146:LEU:HG	1:C:146:LEU:HD21	1.88	0.55
1:C:146:LEU:HD11	1:C:148:LEU:HD21	1.89	0.54
1:F:46:ARG:HH11	1:F:46:ARG:CB	2.19	0.54
1:B:26:ARG:O	1:B:28:GLY:N	2.39	0.54
1:A:61:SER:HB3	1:A:65:HIS:HB2	1.90	0.54
1:E:43:ALA:O	1:E:46:ARG:HA	2.08	0.53
1:F:59:ALA:HB3	1:F:63:THR:CB	2.38	0.53
2:D:154:COA:H8A	2:D:154:COA:H3B	1.91	0.53
1:E:104:LEU:HD22	1:E:114:GLN:HG3	1.89	0.53
1:E:12:VAL:HG12	1:E:146:LEU:CD2	2.25	0.53
1:E:146:LEU:HG	1:F:12:VAL:HG11	1.90	0.52
1:F:109:GLY:HA3	2:F:154:COA:H8A	1.92	0.52
1:B:123:LEU:HD11	1:B:127:ILE:HD11	1.92	0.51
1:A:41:ARG:NH2	3:A:363:HOH:O	2.42	0.51
1:B:40:ARG:O	1:B:44:GLN:HG3	2.11	0.51
1:E:146:LEU:HG	1:F:12:VAL:CG1	2.41	0.50
1:F:109:GLY:O	2:F:154:COA:C8A	2.59	0.50
1:E:8:MSE:CE	1:E:148:LEU:HD21	2.42	0.50
1:C:153:ARG:NH2	1:C:153:ARG:HG3	2.16	0.50
1:E:46:ARG:O	1:E:47:ARG:C	2.50	0.50
1:F:116:LYS:NZ	1:F:116:LYS:HB3	2.27	0.50
1:F:59:ALA:HB3	1:F:63:THR:CG2	2.41	0.49
1:B:10:VAL:CG2	1:B:146:LEU:HD21	2.42	0.49
1:C:153:ARG:NH2	1:C:153:ARG:CG	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:C	1:D:62:ARG:HE	2.15	0.49
1:E:110:ARG:CG	1:E:110:ARG:HH11	2.26	0.49
1:E:46:ARG:O	1:E:47:ARG:O	2.30	0.49
1:A:61:SER:HA	1:A:62:ARG:C	2.33	0.48
1:B:6:GLU:OE1	1:B:8:MSE:CE	2.62	0.48
1:B:110:ARG:CD	1:C:81:SER:HB3	2.44	0.47
1:B:90:VAL:HG11	1:B:122:LYS:HB3	1.96	0.47
1:F:109:GLY:C	2:F:154:COA:C8A	2.83	0.47
1:A:16:HIS:HD2	3:C:203:HOH:O	1.98	0.47
1:D:46:ARG:C	1:D:62:ARG:HG2	2.35	0.47
1:E:87:LYS:HB3	1:E:88:PRO:HD2	1.97	0.47
1:C:10:VAL:HG12	1:C:148:LEU:HD13	1.95	0.47
1:E:12:VAL:CG1	1:E:146:LEU:HD22	2.28	0.47
1:A:29:SER:O	1:A:32:GLU:HG2	2.15	0.47
1:E:42:HIS:CE1	1:E:47:ARG:HG3	2.50	0.47
1:A:95:LEU:HD12	1:A:95:LEU:N	2.31	0.46
1:A:61:SER:HB3	1:A:65:HIS:CB	2.46	0.46
1:E:46:ARG:CB	1:E:46:ARG:HH21	2.23	0.46
1:D:40:ARG:O	1:D:44:GLN:HG2	2.16	0.46
1:A:26:ARG:HB3	1:A:27:PRO:HD2	1.97	0.46
1:F:8:MSE:HG2	1:F:150:ARG:HG2	1.99	0.45
1:C:92:GLU:HG3	1:C:95:LEU:HD22	1.99	0.45
1:D:123:LEU:HD11	1:D:127:ILE:HD11	1.98	0.45
1:A:46:ARG:CG	1:A:46:ARG:NH2	2.70	0.45
1:D:105:PRO:HA	1:D:110:ARG:O	2.16	0.45
1:A:105:PRO:HA	1:A:110:ARG:O	2.16	0.45
1:F:59:ALA:HB3	1:F:63:THR:HB	1.99	0.45
1:A:8:MSE:HG2	1:C:150:ARG:NH2	2.32	0.45
1:E:38:LEU:HA	1:E:41:ARG:CZ	2.47	0.44
2:B:154:COA:N1A	1:C:78:LYS:HA	2.32	0.44
1:D:93:PRO:O	1:D:96:VAL:HG22	2.18	0.44
1:A:8:MSE:HE3	1:A:148:LEU:HD11	1.93	0.44
1:A:149:LEU:C	1:A:149:LEU:HD23	2.38	0.44
1:D:128:GLY:O	3:D:431:HOH:O	2.21	0.44
1:A:12:VAL:HG23	1:A:146:LEU:HD12	2.00	0.43
2:B:154:COA:O2A	1:C:78:LYS:NZ	2.52	0.43
2:A:154:COA:H2A	1:B:78:LYS:HA	2.00	0.43
1:D:7:ALA:HA	1:F:150:ARG:HH22	1.83	0.43
1:E:131:GLU:OE1	1:F:153:ARG:NH1	2.52	0.43
1:D:104:LEU:HD22	1:D:114:GLN:NE2	2.34	0.42
1:E:61:SER:O	1:E:63:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLY:O	1:A:63:THR:N	2.52	0.42
1:B:113:LEU:HG	1:B:134:LEU:HD22	2.00	0.42
1:C:22:GLU:O	1:C:26:ARG:HB3	2.20	0.42
1:E:110:ARG:HG2	1:E:110:ARG:HH11	1.83	0.42
1:E:8:MSE:HG2	1:E:150:ARG:HG2	2.01	0.42
1:E:47:ARG:HH12	1:E:109:GLY:N	2.18	0.42
1:A:27:PRO:HB2	1:A:28:GLY:C	2.40	0.42
1:E:146:LEU:CD2	1:F:146:LEU:HD11	2.49	0.42
1:A:94:ASP:C	1:A:95:LEU:HD12	2.39	0.42
2:B:154:COA:N1A	1:C:81:SER:HB2	2.35	0.42
1:E:60:GLY:O	1:E:61:SER:CB	2.68	0.42
1:E:43:ALA:O	1:E:46:ARG:CA	2.68	0.42
1:E:61:SER:C	1:E:63:THR:N	2.73	0.42
1:C:41:ARG:HB2	1:C:41:ARG:CZ	2.50	0.41
1:D:96:VAL:CG2	1:D:98:PHE:CE2	3.02	0.41
1:E:46:ARG:O	1:E:61:SER:HB2	2.20	0.41
1:C:43:ALA:O	1:C:46:ARG:HB2	2.19	0.41
1:F:46:ARG:HB2	1:F:46:ARG:CZ	2.51	0.41
1:F:90:VAL:HG11	1:F:122:LYS:HB3	2.03	0.41
1:C:8:MSE:HE2	1:C:8:MSE:HB3	1.96	0.41
1:E:45:THR:O	1:E:46:ARG:CB	2.69	0.41
1:F:7:ALA:HB2	1:F:153:ARG:HG3	2.01	0.41
1:B:92:GLU:HB2	1:B:95:LEU:HD22	2.02	0.41
1:D:97:ASN:HB3	1:D:100:GLU:HG3	2.03	0.41
1:E:146:LEU:HD21	1:F:146:LEU:HD11	2.02	0.41
1:E:8:MSE:CE	1:E:148:LEU:CD1	2.76	0.40
1:B:146:LEU:HD13	1:B:147:CYS:N	2.36	0.40
1:B:106:ASP:OD2	1:B:110:ARG:HG3	2.22	0.40
1:C:131:GLU:HB3	1:C:150:ARG:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASP:O	1:C:41:ARG:NE[1_455]	1.59	0.61

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/153 (86%)	125 (95%)	5 (4%)	2 (2%)	10	3
1	B	133/153 (87%)	125 (94%)	6 (4%)	2 (2%)	10	3
1	C	133/153 (87%)	130 (98%)	3 (2%)	0	100	100
1	D	130/153 (85%)	127 (98%)	3 (2%)	0	100	100
1	E	135/153 (88%)	129 (96%)	4 (3%)	2 (2%)	10	3
1	F	132/153 (86%)	129 (98%)	3 (2%)	0	100	100
All	All	795/918 (87%)	765 (96%)	24 (3%)	6 (1%)	19	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	PRO
1	A	45	THR
1	E	46	ARG
1	E	62	ARG
1	B	27	PRO
1	B	28	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/120 (91%)	99 (91%)	10 (9%)	9	3
1	B	110/120 (92%)	100 (91%)	10 (9%)	9	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	110/120 (92%)	101 (92%)	9 (8%)	11	4
1	D	109/120 (91%)	103 (94%)	6 (6%)	21	12
1	E	112/120 (93%)	103 (92%)	9 (8%)	12	5
1	F	109/120 (91%)	98 (90%)	11 (10%)	7	2
All	All	659/720 (92%)	604 (92%)	55 (8%)	11	4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PRO
1	A	33	GLN
1	A	45	THR
1	A	46	ARG
1	A	110	ARG
1	A	115	LEU
1	A	116	LYS
1	A	122	LYS
1	A	146	LEU
1	A	152	GLN
1	B	5	ARG
1	B	6	GLU
1	B	23	GLN
1	B	26	ARG
1	B	61	SER
1	B	95	LEU
1	B	110	ARG
1	B	114	GLN
1	B	116	LYS
1	B	152	GLN
1	C	30	THR
1	C	41	ARG
1	C	46	ARG
1	C	66	LEU
1	C	92	GLU
1	C	95	LEU
1	C	110	ARG
1	C	114	GLN
1	C	153	ARG
1	D	6	GLU
1	D	22	GLU
1	D	26	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	61	SER
1	D	107	ARG
1	D	110	ARG
1	E	6	GLU
1	E	45	THR
1	E	46	ARG
1	E	66	LEU
1	E	87	LYS
1	E	92	GLU
1	E	95	LEU
1	E	110	ARG
1	E	146	LEU
1	F	33	GLN
1	F	41	ARG
1	F	46	ARG
1	F	61	SER
1	F	62	ARG
1	F	95	LEU
1	F	107	ARG
1	F	110	ARG
1	F	115	LEU
1	F	116	LYS
1	F	146	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	16	HIS
1	A	33	GLN
1	A	82	GLN
1	A	124	GLN
1	A	152	GLN
1	B	44	GLN
1	B	82	GLN
1	B	124	GLN
1	B	152	GLN
1	C	16	HIS
1	C	82	GLN
1	C	124	GLN
1	D	16	HIS
1	D	23	GLN
1	D	82	GLN

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Mol	Chain	Res	Type
1	D	114	GLN
1	D	152	GLN
1	E	16	HIS
1	E	33	GLN
1	E	42	HIS
1	E	82	GLN
1	E	124	GLN
1	F	16	HIS
1	F	82	GLN
1	F	114	GLN
1	F	124	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	154	-	26,29,50	2.07	8 (30%)	31,45,75	1.96	9 (29%)
2	COA	B	154	-	26,29,50	2.20	10 (38%)	31,45,75	1.83	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	COA	C	154	-	26,29,50	2.13	7 (26%)	31,45,75	2.17	11 (35%)
2	COA	D	154	-	26,29,50	1.96	5 (19%)	31,45,75	2.38	10 (32%)
2	COA	E	154	-	26,29,50	2.23	9 (34%)	31,45,75	2.49	11 (35%)
2	COA	F	154	-	26,29,50	1.59	7 (26%)	31,45,75	1.75	6 (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	A	154	-	1/1/6/13	6/11/31/64	0/3/3/3
2	COA	B	154	-	-	7/11/31/64	0/3/3/3
2	COA	C	154	-	1/1/6/13	6/11/31/64	0/3/3/3
2	COA	D	154	-	1/1/6/13	4/11/31/64	0/3/3/3
2	COA	E	154	-	2/2/6/13	4/11/31/64	0/3/3/3
2	COA	F	154	-	-	7/11/31/64	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	COA	P3B-O3B	7.20	1.72	1.59
2	C	154	COA	O2B-C2B	7.04	1.59	1.43
2	E	154	COA	O2B-C2B	6.52	1.58	1.43
2	B	154	COA	P1A-O5B	-5.45	1.42	1.60
2	D	154	COA	P1A-O5B	-5.10	1.43	1.60
2	D	154	COA	P1A-O3A	-4.94	1.35	1.54
2	B	154	COA	P3B-O3B	-4.15	1.51	1.59
2	E	154	COA	C2B-C1B	4.06	1.59	1.53
2	A	154	COA	P1A-O5B	-3.60	1.48	1.60
2	E	154	COA	P1A-O3A	-3.58	1.41	1.54
2	B	154	COA	P1A-O3A	-3.42	1.41	1.54
2	D	154	COA	P1A-O1A	-3.38	1.39	1.50
2	F	154	COA	P3B-O3B	3.19	1.65	1.59
2	C	154	COA	P1A-O3A	-3.00	1.43	1.54
2	C	154	COA	C5B-C4B	2.99	1.60	1.51
2	E	154	COA	C5B-C4B	2.97	1.60	1.51
2	A	154	COA	P1A-O3A	-2.88	1.43	1.54
2	A	154	COA	O4B-C1B	2.75	1.44	1.41
2	C	154	COA	C2B-C1B	2.75	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	154	COA	P1A-O3A	-2.73	1.44	1.54
2	B	154	COA	P3B-O9A	-2.72	1.44	1.54
2	B	154	COA	P1A-O2A	-2.68	1.44	1.54
2	E	154	COA	P1A-O1A	-2.62	1.42	1.50
2	D	154	COA	P3B-O7A	-2.60	1.42	1.50
2	B	154	COA	C4A-N3A	-2.58	1.32	1.35
2	F	154	COA	O4B-C1B	2.53	1.44	1.41
2	C	154	COA	C4A-N3A	-2.52	1.32	1.35
2	F	154	COA	C2B-C1B	2.51	1.57	1.53
2	E	154	COA	P3B-O3B	2.48	1.64	1.59
2	F	154	COA	C4A-N3A	-2.44	1.32	1.35
2	A	154	COA	P3B-O7A	-2.38	1.42	1.50
2	B	154	COA	P3B-O7A	-2.30	1.43	1.50
2	B	154	COA	C5A-N7A	-2.28	1.31	1.39
2	E	154	COA	C2A-N1A	-2.27	1.29	1.33
2	E	154	COA	O5B-C5B	2.24	1.53	1.44
2	B	154	COA	O4B-C1B	2.19	1.44	1.41
2	F	154	COA	C5A-N7A	-2.16	1.31	1.39
2	E	154	COA	P3B-O9A	-2.16	1.46	1.54
2	F	154	COA	P1A-O1A	-2.14	1.43	1.50
2	C	154	COA	O4B-C1B	2.10	1.44	1.41
2	C	154	COA	P3B-O3B	2.09	1.63	1.59
2	A	154	COA	C4A-N3A	-2.08	1.32	1.35
2	A	154	COA	P1A-O1A	-2.07	1.43	1.50
2	D	154	COA	C5A-N7A	-2.05	1.32	1.39
2	B	154	COA	C5A-C4A	-2.03	1.35	1.40
2	A	154	COA	C5A-N7A	-2.00	1.32	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	154	COA	O4B-C1B-C2B	-8.16	95.01	106.93
2	E	154	COA	C5B-C4B-C3B	5.73	133.38	114.40
2	E	154	COA	O5B-P1A-O1A	5.66	122.36	106.47
2	B	154	COA	N3A-C2A-N1A	-5.31	120.38	128.68
2	F	154	COA	O5B-P1A-O1A	5.18	121.00	106.47
2	D	154	COA	C2B-C3B-C4B	-5.13	94.13	103.22
2	C	154	COA	N3A-C2A-N1A	-5.05	120.78	128.68
2	E	154	COA	O2B-C2B-C3B	4.97	125.28	111.17
2	C	154	COA	O2B-C2B-C3B	4.90	125.08	111.17
2	A	154	COA	O5B-P1A-O1A	4.84	120.04	106.47
2	A	154	COA	C2B-C3B-C4B	-4.57	95.12	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	COA	O4B-C4B-C5B	4.37	123.75	109.37
2	D	154	COA	O4B-C4B-C5B	3.85	122.05	109.37
2	E	154	COA	C4A-C5A-N7A	-3.75	105.49	109.40
2	C	154	COA	C4A-C5A-N7A	-3.73	105.52	109.40
2	C	154	COA	C5A-C6A-N6A	3.70	125.97	120.35
2	B	154	COA	C3B-C2B-C1B	3.59	107.84	99.89
2	C	154	COA	O5B-P1A-O1A	3.54	116.40	106.47
2	D	154	COA	N3A-C2A-N1A	-3.46	123.27	128.68
2	E	154	COA	N3A-C2A-N1A	-3.41	123.35	128.68
2	A	154	COA	N3A-C2A-N1A	-3.32	123.49	128.68
2	E	154	COA	O2B-C2B-C1B	3.30	123.05	110.85
2	A	154	COA	O3A-P1A-O5B	-3.14	98.38	106.73
2	F	154	COA	O2A-P1A-O5B	-3.03	98.67	106.73
2	B	154	COA	O3A-P1A-O5B	-2.98	98.82	106.73
2	A	154	COA	O9A-P3B-O3B	2.97	119.29	105.99
2	E	154	COA	O3B-C3B-C2B	2.96	122.41	111.68
2	E	154	COA	O3A-P1A-O5B	-2.95	98.88	106.73
2	E	154	COA	C5A-C6A-N6A	2.95	124.84	120.35
2	D	154	COA	C4A-C5A-N7A	-2.93	106.35	109.40
2	E	154	COA	O4B-C1B-C2B	-2.88	102.71	106.93
2	F	154	COA	O3B-C3B-C4B	2.79	120.18	110.08
2	C	154	COA	O5B-C5B-C4B	2.76	118.48	108.99
2	E	154	COA	O3A-P1A-O2A	2.69	117.91	107.64
2	D	154	COA	O2A-P1A-O1A	2.68	121.17	110.68
2	F	154	COA	O2B-C2B-C1B	2.58	120.38	110.85
2	C	154	COA	C2A-N1A-C6A	2.52	123.06	118.75
2	F	154	COA	N3A-C2A-N1A	-2.49	124.78	128.68
2	C	154	COA	O3B-C3B-C2B	2.46	120.59	111.68
2	B	154	COA	P1A-O5B-C5B	2.46	125.06	118.30
2	F	154	COA	C4A-C5A-N7A	-2.40	106.90	109.40
2	D	154	COA	O3A-P1A-O2A	-2.39	98.51	107.64
2	A	154	COA	C4A-C5A-N7A	-2.37	106.93	109.40
2	C	154	COA	O4B-C4B-C5B	2.35	117.09	109.37
2	A	154	COA	O4B-C1B-C2B	-2.32	103.54	106.93
2	A	154	COA	C5B-C4B-C3B	2.29	121.97	114.40
2	C	154	COA	O2A-P1A-O5B	-2.21	100.85	106.73
2	B	154	COA	O4B-C1B-C2B	-2.12	103.82	106.93
2	C	154	COA	O2B-C2B-C1B	2.12	118.67	110.85
2	D	154	COA	C5A-C6A-N6A	2.10	123.54	120.35
2	A	154	COA	O8A-P3B-O3B	-2.08	96.69	105.99
2	D	154	COA	O2B-C2B-C1B	2.07	118.50	110.85
2	D	154	COA	C2A-N1A-C6A	2.06	122.28	118.75

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	154	COA	C2B
2	C	154	COA	C2B
2	D	154	COA	C2B
2	E	154	COA	C4B
2	E	154	COA	C2B

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	154	COA	C3B-C4B-C5B-O5B
2	A	154	COA	O4B-C4B-C5B-O5B
2	A	154	COA	C5B-O5B-P1A-O1A
2	A	154	COA	C5B-O5B-P1A-O2A
2	A	154	COA	C5B-O5B-P1A-O3A
2	B	154	COA	C3B-C4B-C5B-O5B
2	B	154	COA	O4B-C4B-C5B-O5B
2	B	154	COA	C5B-O5B-P1A-O2A
2	B	154	COA	C5B-O5B-P1A-O3A
2	C	154	COA	C5B-O5B-P1A-O2A
2	C	154	COA	C5B-O5B-P1A-O3A
2	E	154	COA	C3B-C4B-C5B-O5B
2	E	154	COA	C5B-O5B-P1A-O2A
2	E	154	COA	C5B-O5B-P1A-O3A
2	F	154	COA	C3B-C4B-C5B-O5B
2	F	154	COA	O4B-C4B-C5B-O5B
2	F	154	COA	C5B-O5B-P1A-O1A
2	F	154	COA	C5B-O5B-P1A-O2A
2	F	154	COA	C5B-O5B-P1A-O3A
2	C	154	COA	C3B-C4B-C5B-O5B
2	C	154	COA	O4B-C4B-C5B-O5B
2	D	154	COA	O4B-C4B-C5B-O5B
2	B	154	COA	C5B-O5B-P1A-O1A
2	C	154	COA	C5B-O5B-P1A-O1A
2	E	154	COA	C5B-O5B-P1A-O1A
2	F	154	COA	C3B-O3B-P3B-O7A
2	C	154	COA	C3B-O3B-P3B-O8A
2	B	154	COA	C3B-O3B-P3B-O7A
2	D	154	COA	C3B-O3B-P3B-O7A
2	A	154	COA	C3B-O3B-P3B-O8A
2	B	154	COA	C3B-O3B-P3B-O8A
2	D	154	COA	C3B-O3B-P3B-O8A
2	F	154	COA	C3B-O3B-P3B-O9A

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Mol	Chain	Res	Type	Atoms
2	D	154	COA	C3B-C4B-C5B-O5B

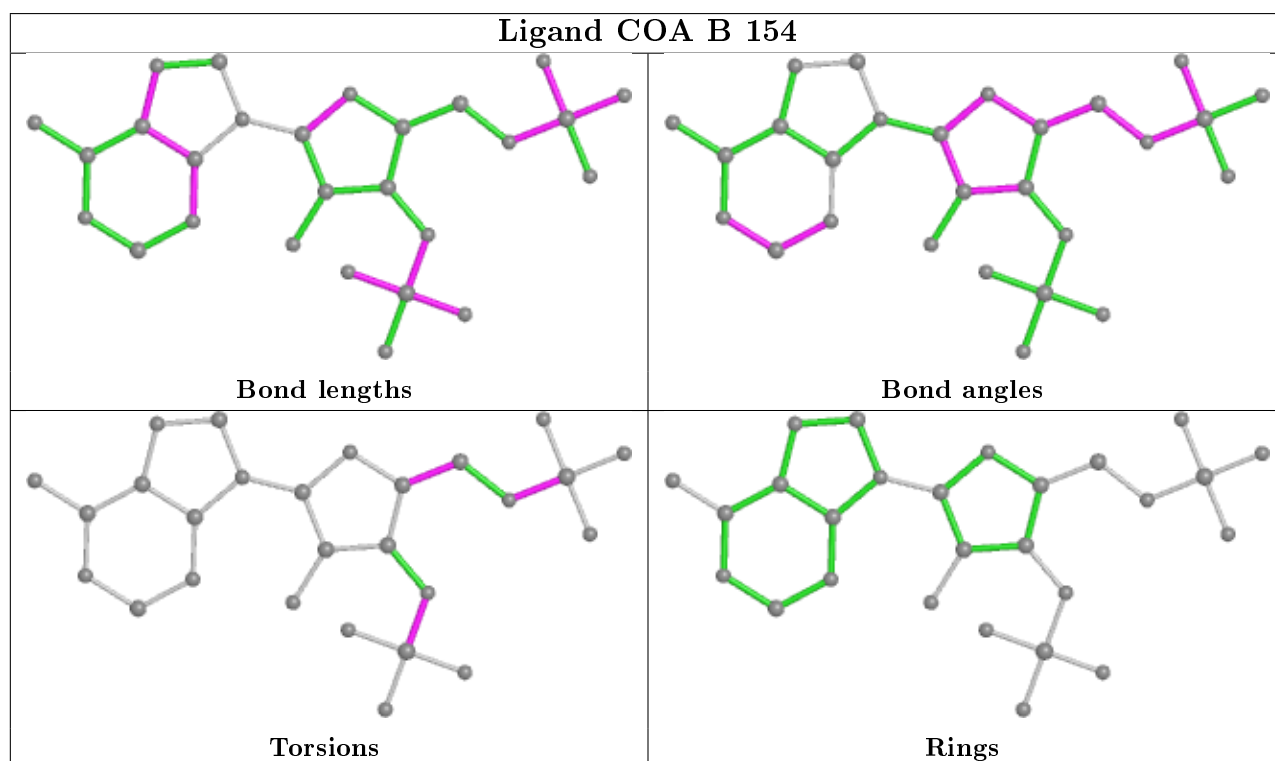
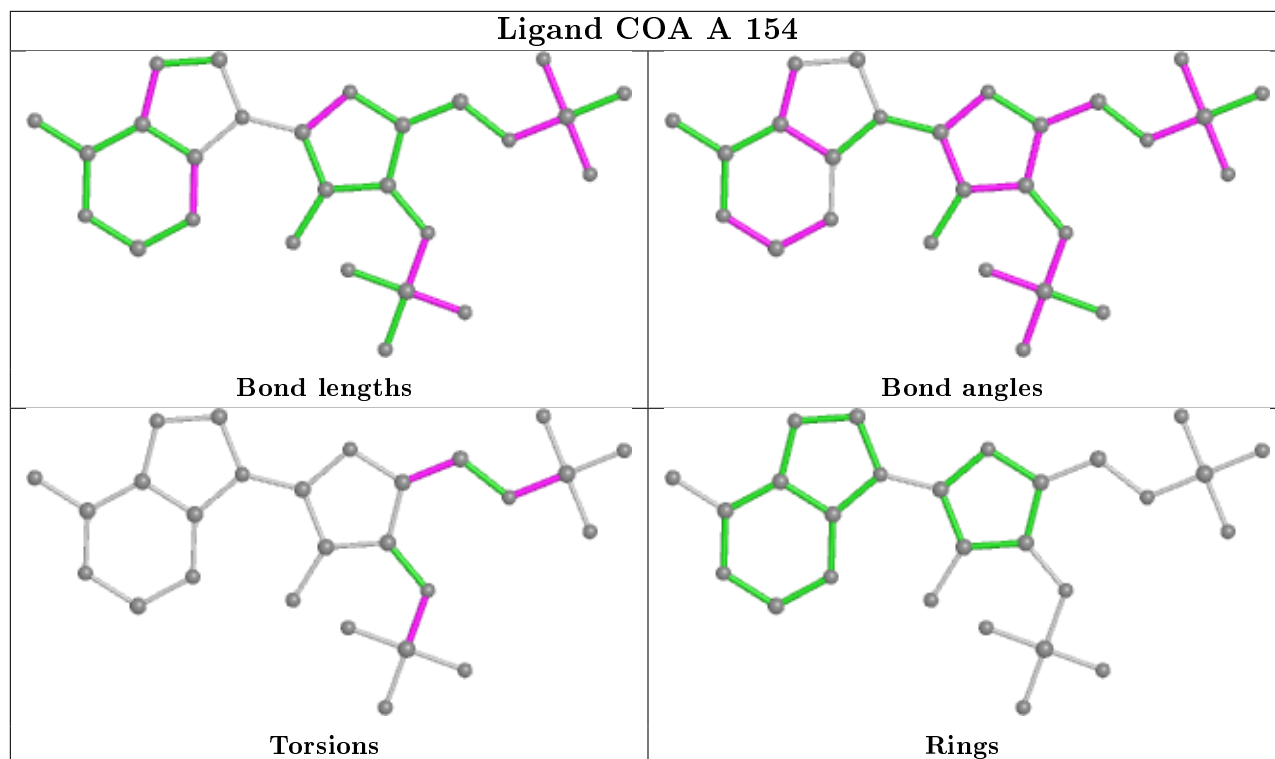
There are no ring outliers.

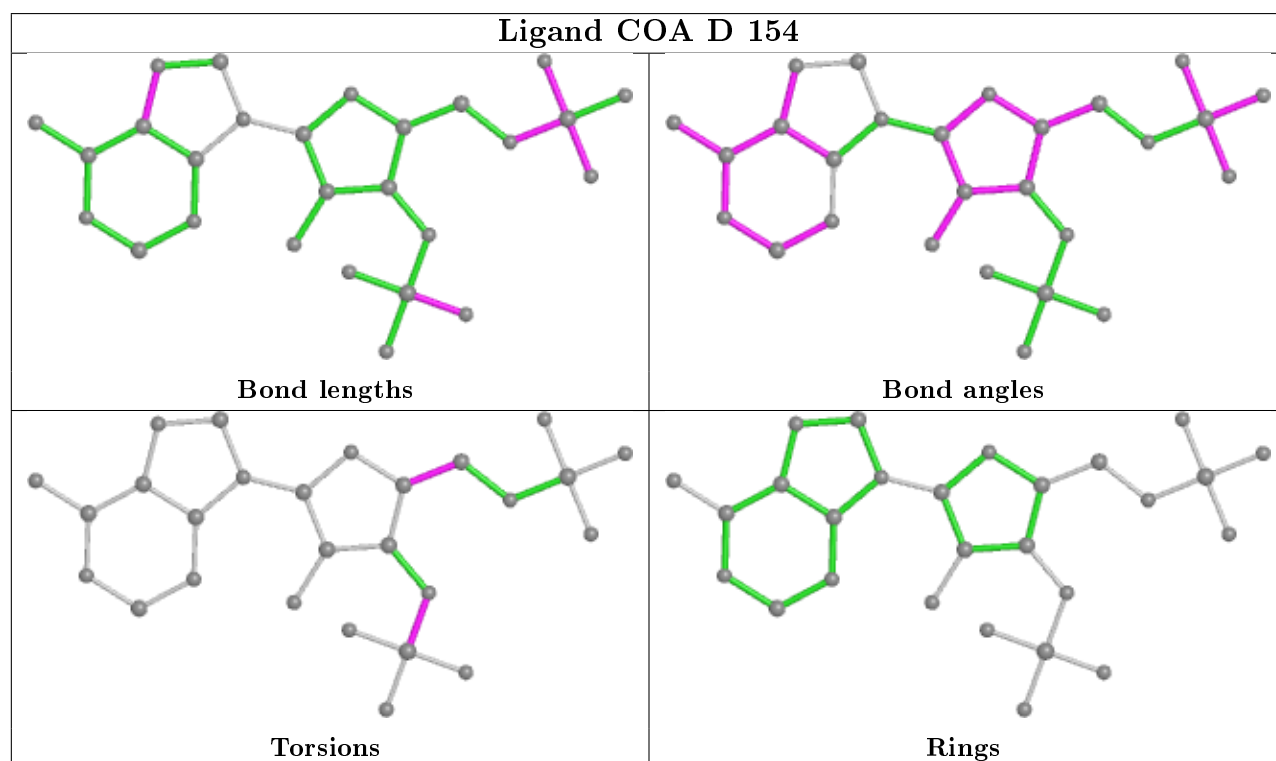
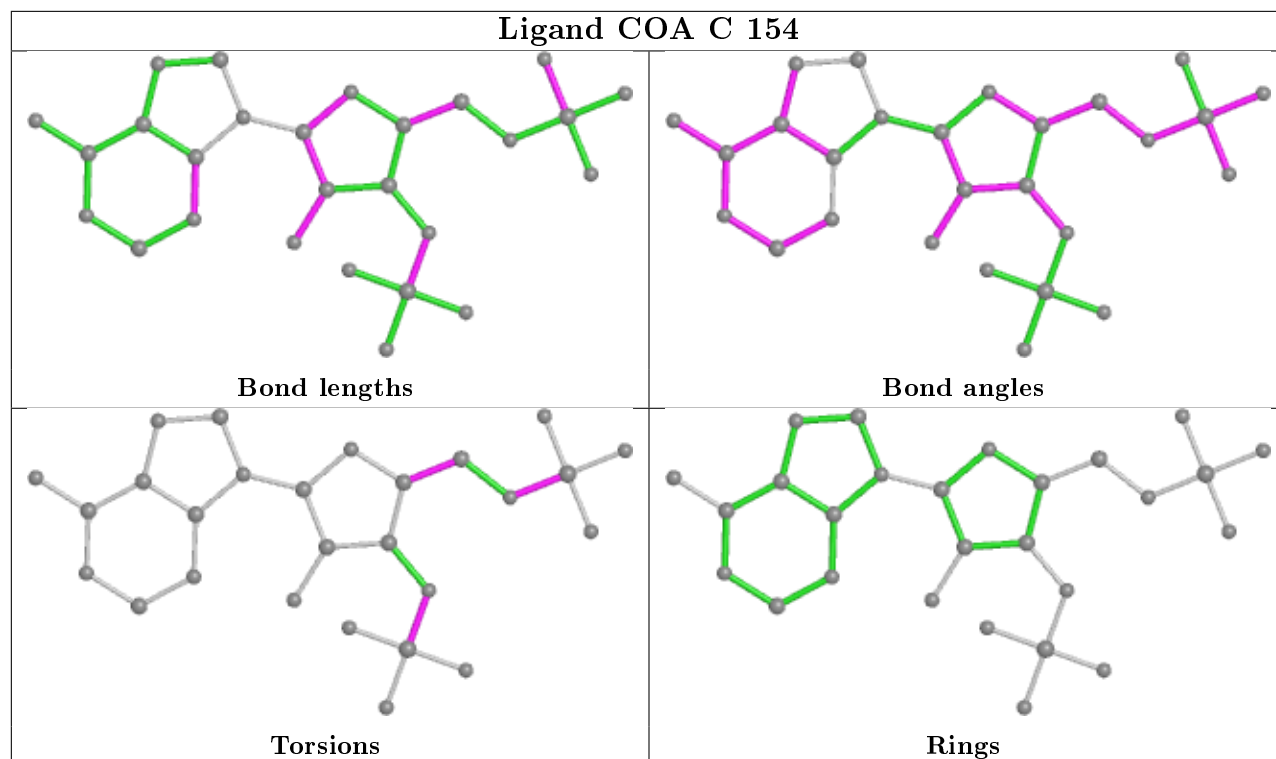
5 monomers are involved in 20 short contacts:

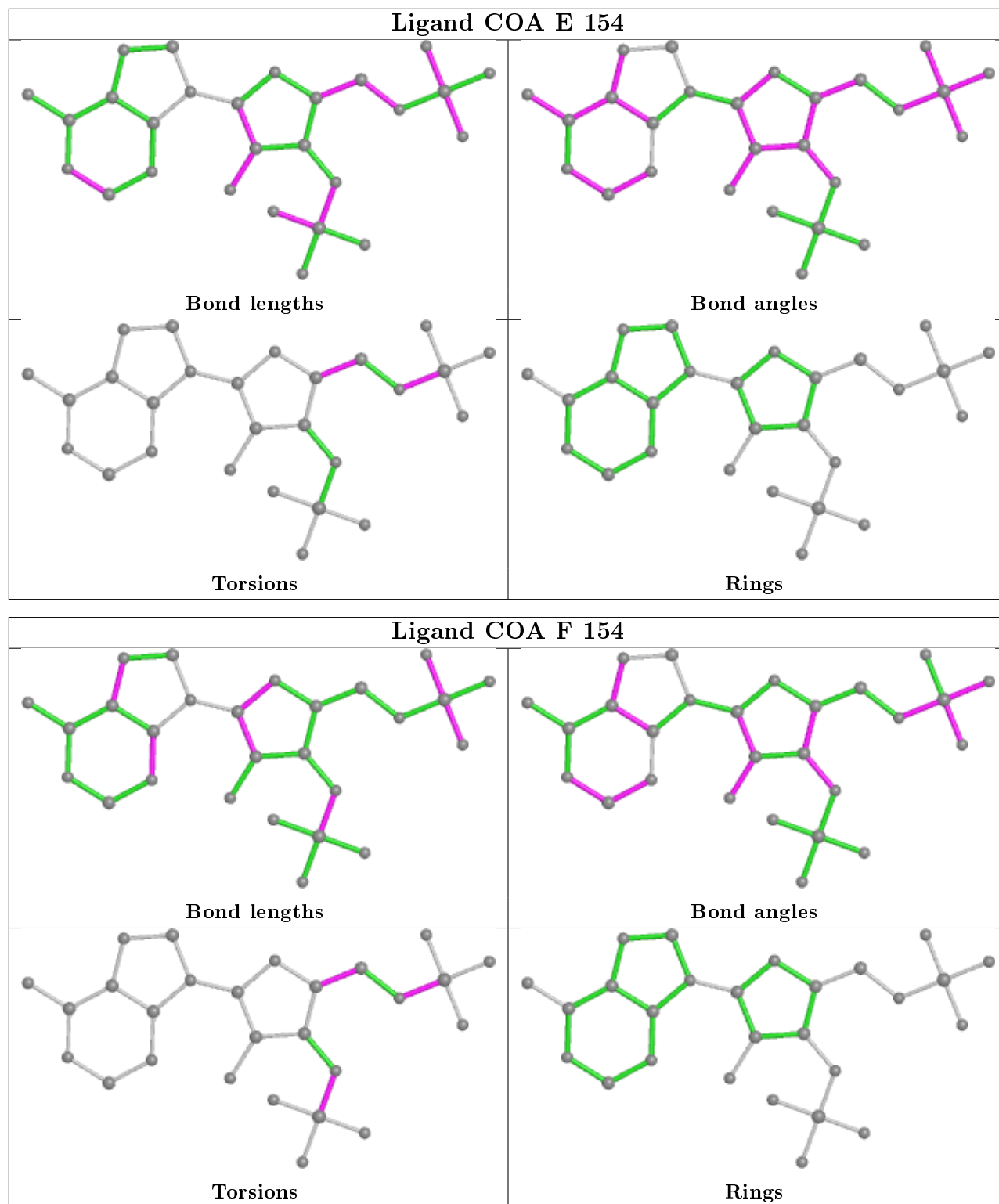
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	COA	2	0
2	B	154	COA	3	0
2	C	154	COA	2	0
2	D	154	COA	3	0
2	F	154	COA	10	0

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

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	135/153 (88%)	0.62	11 (8%) 12 13	12, 23, 44, 53	0
1	B	136/153 (88%)	0.65	12 (8%) 10 11	14, 25, 45, 51	0
1	C	136/153 (88%)	0.47	11 (8%) 12 13	13, 23, 40, 52	0
1	D	133/153 (86%)	0.69	10 (7%) 14 15	14, 27, 47, 52	0
1	E	138/153 (90%)	0.38	7 (5%) 28 31	13, 23, 39, 54	0
1	F	135/153 (88%)	0.48	12 (8%) 9 11	11, 22, 41, 53	0
All	All	813/918 (88%)	0.55	63 (7%) 13 15	11, 24, 44, 54	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	PRO	6.7
1	B	59	ALA	6.5
1	B	27	PRO	5.9
1	A	59	ALA	5.6
1	D	27	PRO	5.4
1	A	46	ARG	5.1
1	E	4	ASN	5.0
1	D	153	ARG	4.9
1	A	45	THR	4.8
1	A	61	SER	4.7
1	F	45	THR	4.6
1	D	28	GLY	4.5
1	B	46	ARG	4.4
1	D	46	ARG	4.3
1	A	28	GLY	4.3
1	D	32	GLU	4.2
1	A	30	THR	4.2
1	E	61	SER	4.1
1	D	45	THR	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	30	THR	3.9
1	E	46	ARG	3.9
1	B	26	ARG	3.8
1	C	47	ARG	3.8
1	E	47	ARG	3.8
1	C	153	ARG	3.7
1	B	28	GLY	3.7
1	F	28	GLY	3.6
1	A	60	GLY	3.6
1	A	153	ARG	3.6
1	D	26	ARG	3.4
1	B	30	THR	3.3
1	A	32	GLU	3.2
1	C	44	GLN	3.2
1	D	152	GLN	3.2
1	F	30	THR	3.2
1	F	32	GLU	3.1
1	C	59	ALA	3.1
1	F	60	GLY	3.1
1	F	59	ALA	3.0
1	C	41	ARG	3.0
1	B	60	GLY	3.0
1	B	45	THR	2.9
1	F	61	SER	2.9
1	B	29	SER	2.8
1	D	29	SER	2.8
1	F	46	ARG	2.8
1	B	32	GLU	2.8
1	F	27	PRO	2.6
1	A	29	SER	2.6
1	C	29	SER	2.5
1	C	45	THR	2.5
1	E	29	SER	2.5
1	E	94	ASP	2.5
1	C	46	ARG	2.5
1	F	29	SER	2.3
1	E	59	ALA	2.3
1	F	153	ARG	2.3
1	F	152	GLN	2.2
1	C	152	GLN	2.2
1	B	61	SER	2.1
1	B	5	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	94	ASP	2.0
1	C	6	GLU	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](#)

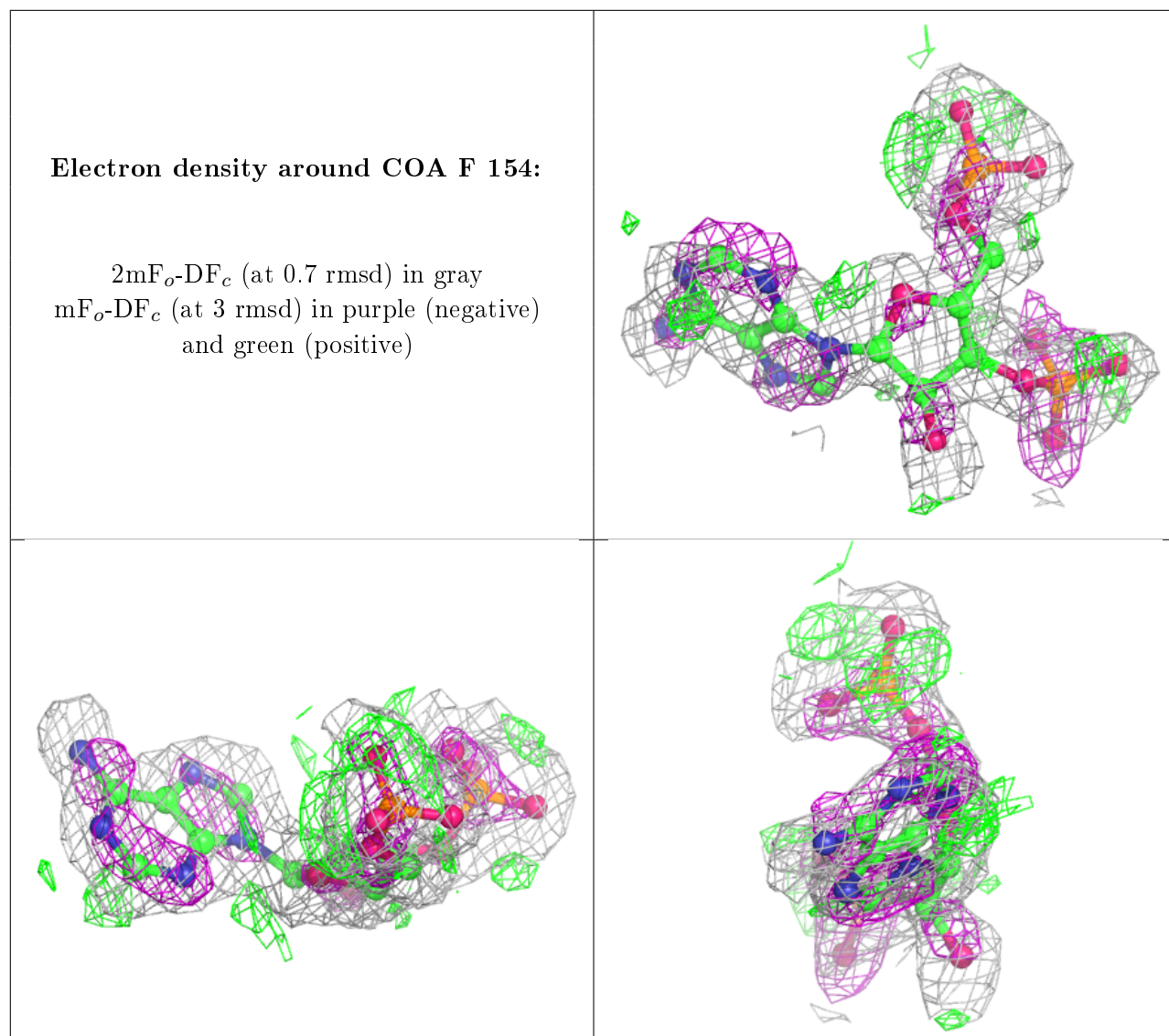
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

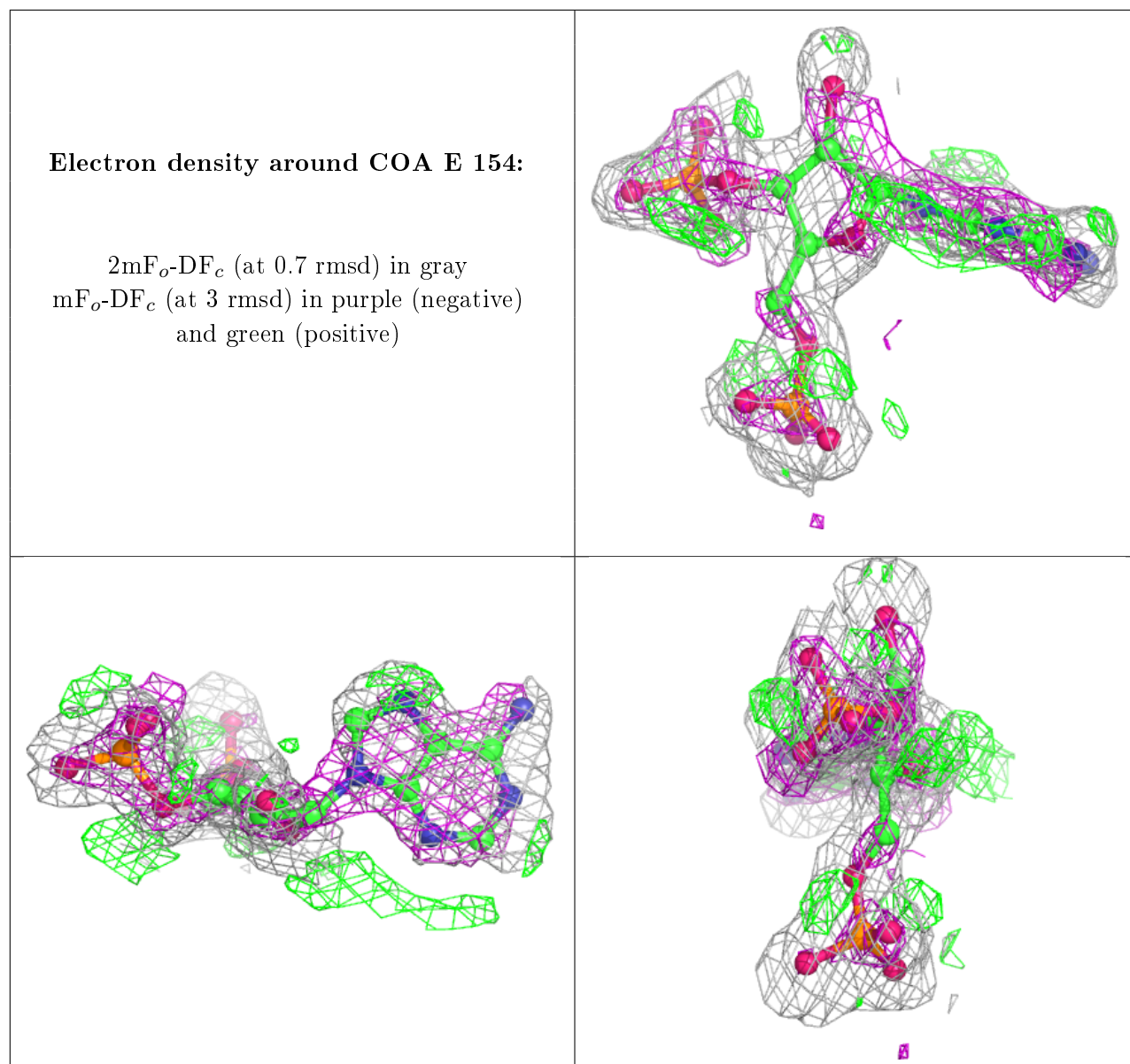
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	COA	F	154	27/48	0.87	0.24	14,19,20,21	0
2	COA	E	154	27/48	0.89	0.28	14,19,20,21	0
2	COA	C	154	27/48	0.89	0.26	14,19,20,21	0
2	COA	A	154	27/48	0.92	0.20	14,19,20,21	0
2	COA	D	154	27/48	0.92	0.20	14,19,20,21	0
2	COA	B	154	27/48	0.93	0.22	14,19,20,21	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.

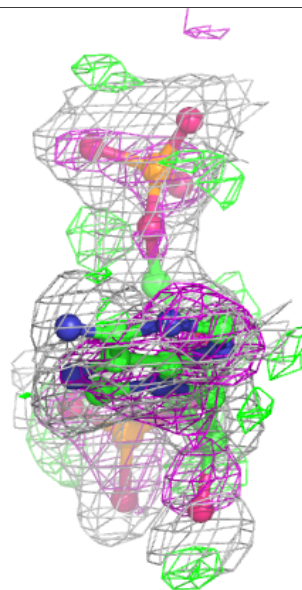
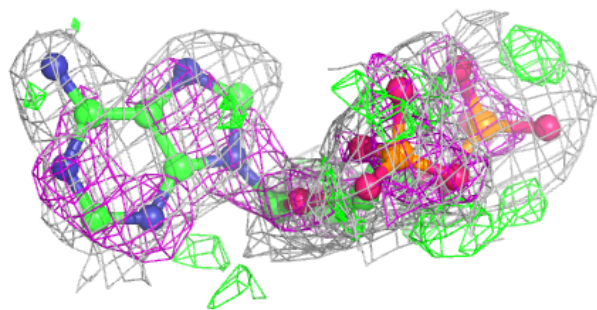
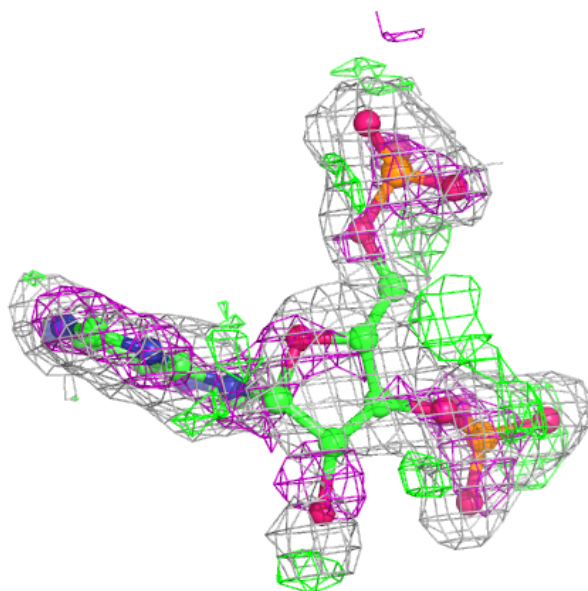






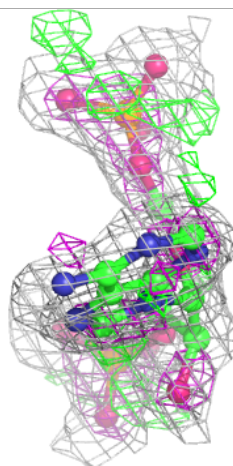
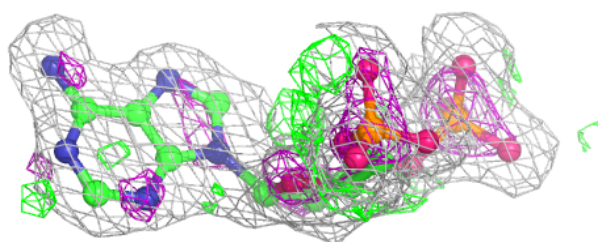
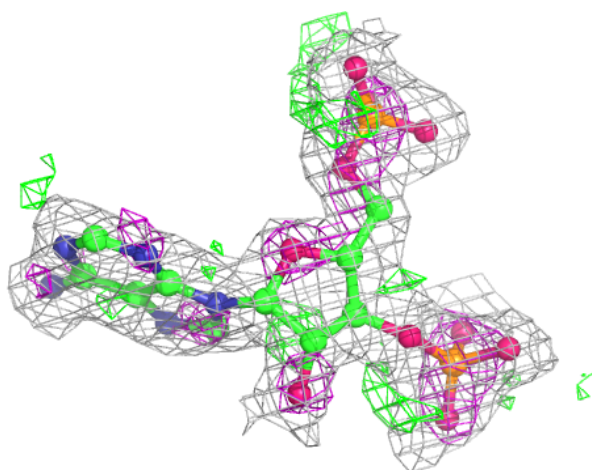
**Electron density around COA C 154:**

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



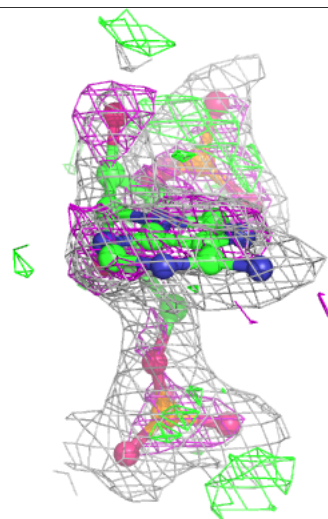
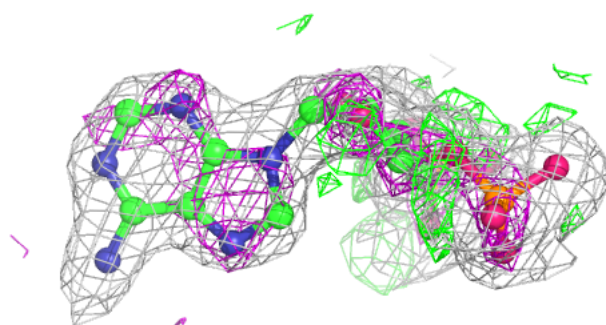
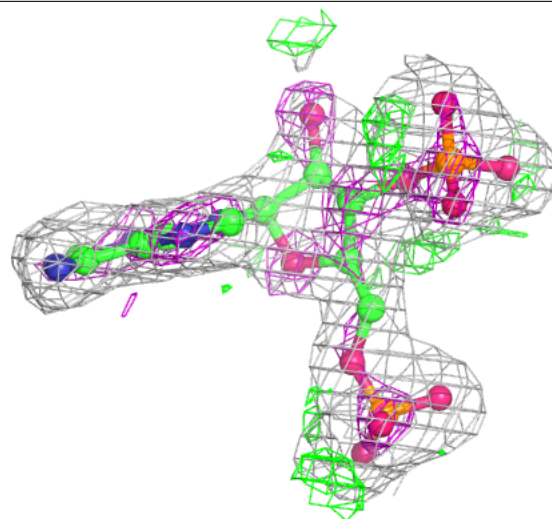
**Electron density around COA A 154:**

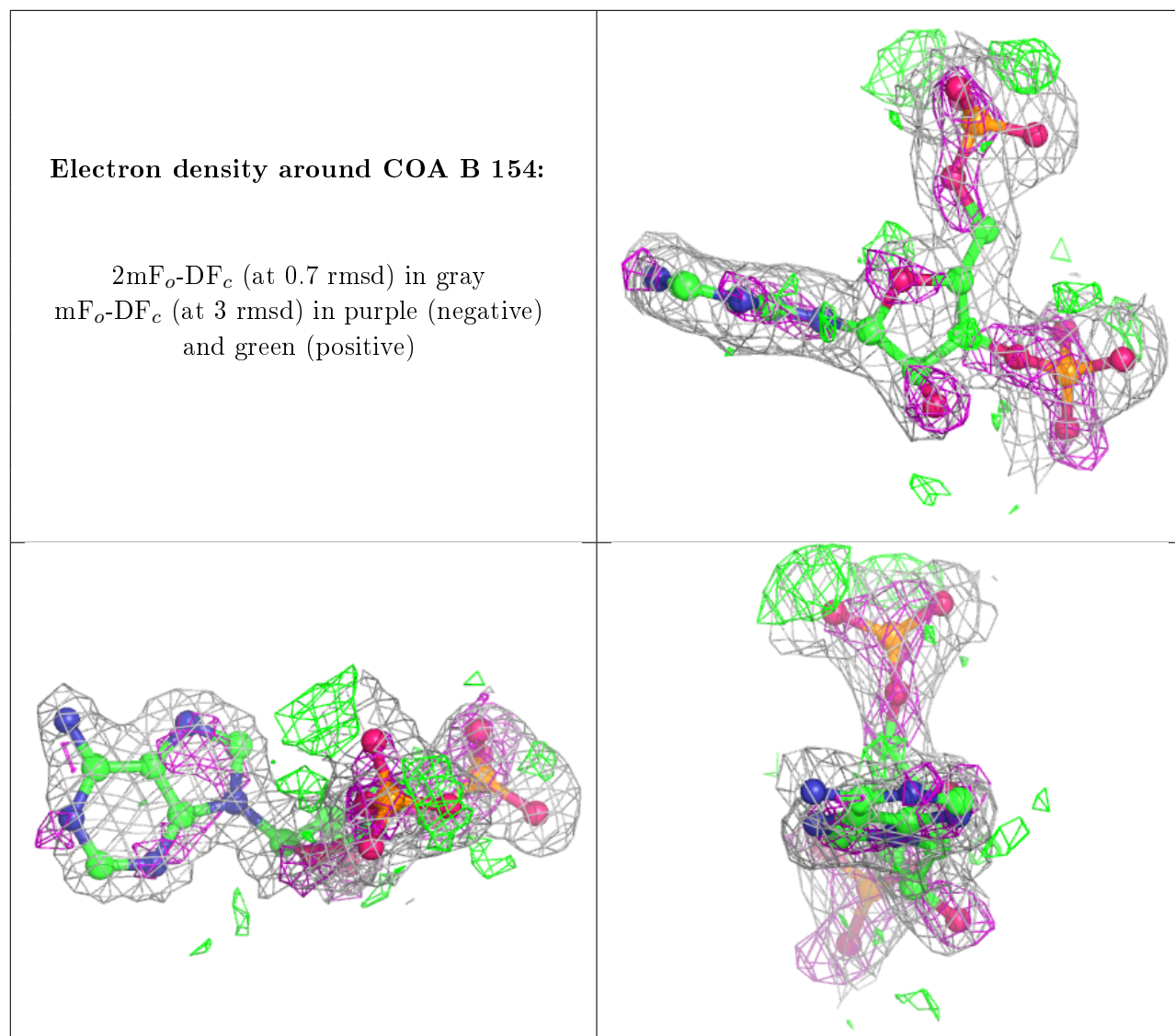
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around COA D 154:**

$2mF_o-DF_c$  (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.