



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 04:24 PM EST

PDB ID : 2B4B  
Title : SSAT+COA+BE-3-3-3, K6R mutant  
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Deposited on : 2005-09-23  
Resolution : 2.00 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	:	2.16
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)	:	2.16

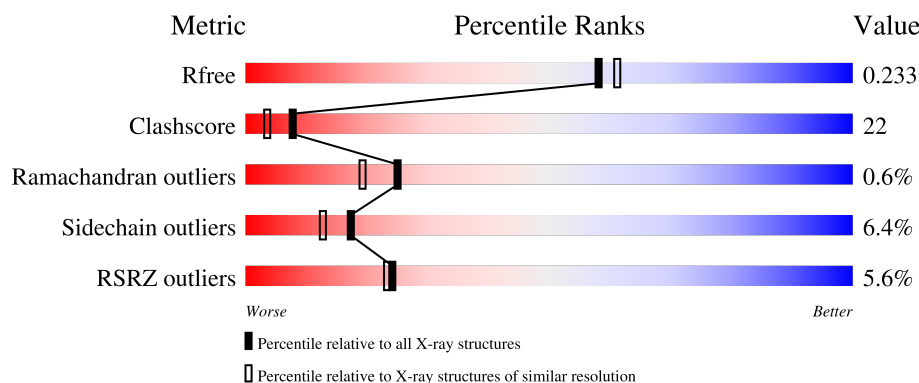
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	171	<div> <div>4%</div> <div>61%</div> <div>29%</div> <div>8%</div> <div>..</div> </div>
1	B	171	<div> <div>6%</div> <div>68%</div> <div>25%</div> <div>5%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	A	200	X	-	-	-
2	COA	B	172	X	-	-	-
3	B33	B	173	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2985 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.

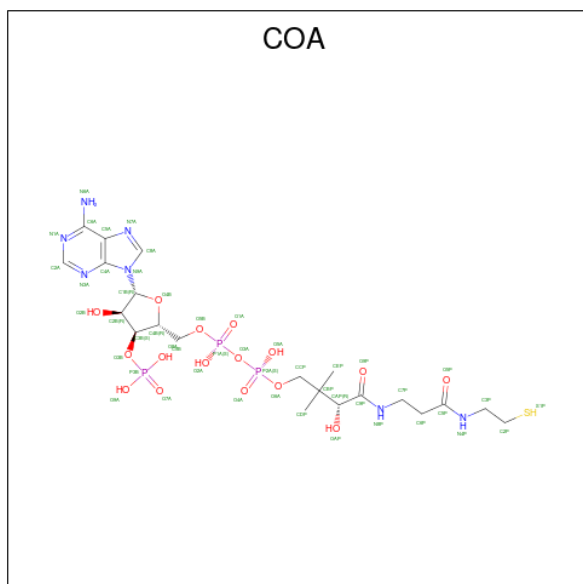
- Molecule 1 is a protein called Diamine acetyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	Se	19	0	0
			1389	901	223	255	4	6			
1	B	170	Total	C	N	O	S	Se	0	0	0
			1403	910	226	257	4	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	LYS	engineered mutation	UNP P21673
B	26	ARG	LYS	engineered mutation	UNP P21673

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



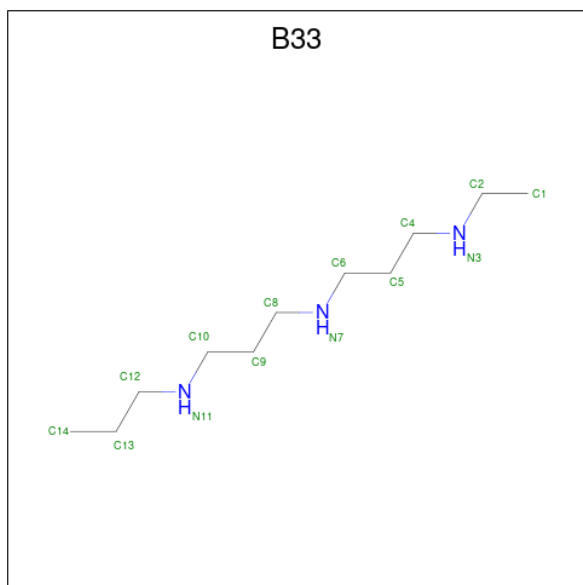
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	9	0
			48	21	7	16	3	1		

- Molecule 3 is N-ETHYL-N-[3-(PROPYLAMINO)PROPYL]PROPANE-1,3-DIAMINE (three-letter code: B33) (formula:  $C_{11}H_{27}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	7	0
			14	11	3		

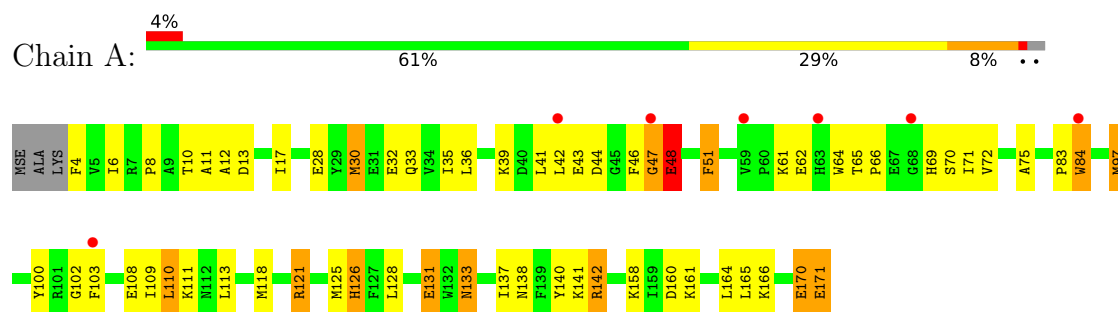
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	38	Total	O	0	0
			38	38		

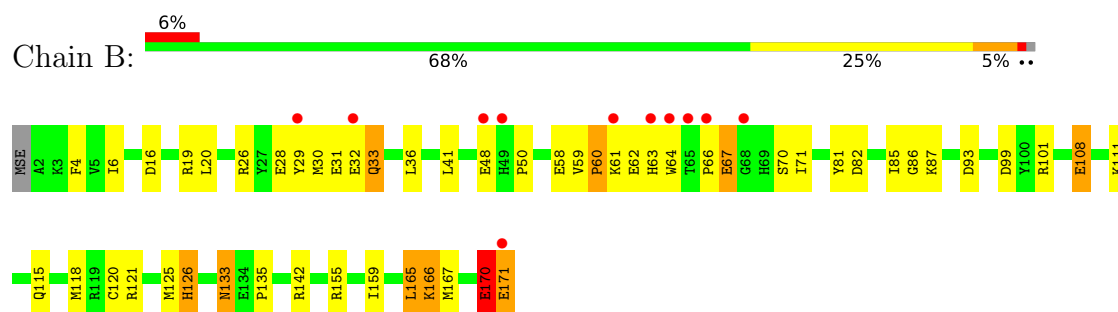
### 3 Residue-property plots [i](#)

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: Diamine acetyltransferase 1



#### • Molecule 1: Diamine acetyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.81Å 73.81Å 64.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.6 (29.34-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.98 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.265 0.230 , 0.233	Depositor DCC
$R_{free}$ test set	1110 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, B33

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	0.70	2/1422 (0.1%)	1.05	8/1910 (0.4%)
1	B	1.04	1/1436 (0.1%)	0.74	2/1928 (0.1%)
All	All	0.89	3/2858 (0.1%)	0.91	10/3838 (0.3%)

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	3
1	B	0	1
All	All	1	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	PRO	N-CD	-34.80	0.99	1.47
1	A	46	PHE	CA-C	-13.66	1.17	1.52
1	A	8	PRO	N-CD	-10.39	1.33	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	MSE	CG-SE-CE	18.77	140.20	98.90
1	A	170	GLU	CA-CB-CG	-16.29	77.56	113.40
1	A	48	GLU	O-C-N	-10.94	105.20	122.70
1	B	60	PRO	N-CD-CG	9.13	116.90	103.20
1	A	97	MSE	CG-SE-CE	8.95	118.59	98.90
1	B	170	GLU	C-N-CA	8.15	142.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLU	CB-CA-C	8.00	126.41	110.40
1	A	47	GLY	C-N-CA	7.79	141.19	121.70
1	A	46	PHE	CB-CA-C	6.66	123.73	110.40
1	A	48	GLU	CA-C-N	6.43	131.35	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	48	GLU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	GLY	Peptide
1	A	48	GLU	Mainchain,Peptide
1	B	170	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1389	0	1336	68	0
1	B	1403	0	1354	66	1
2	A	48	0	29	2	0
2	B	48	0	28	3	0
3	B	14	0	25	5	1
4	A	45	0	0	6	0
4	B	38	0	0	7	0
All	All	2985	0	2772	121	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 22.

All (121) 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:121:ARG:HH21	1:A:121:ARG:HG3	1.12	1.06
1:A:30:MSE:HE3	1:A:33:GLN:OE1	1.59	1.02
1:A:166:LYS:O	1:A:170:GLU:HG3	1.60	1.00
1:A:65:THR:HG21	1:A:97:MSE:HE1	1.52	0.92
1:A:102:GLY:HA2	2:A:200:COA:H52A	1.53	0.88
1:A:171:GLU:HB3	1:B:111:LYS:HZ1	1.43	0.84
1:B:166:LYS:O	1:B:170:GLU:HG2	1.80	0.82
1:B:6:ILE:HG13	1:B:108:GLU:HG2	1.62	0.79
1:B:61:LYS:HE3	1:B:64:TRP:CZ3	2.19	0.78
1:B:20:LEU:HD11	1:B:71:ILE:HG22	1.65	0.77
1:A:171:GLU:HB3	1:B:111:LYS:NZ	1.97	0.77
1:A:170:GLU:O	1:A:171:GLU:HG3	1.86	0.76
1:A:30:MSE:HE2	1:A:33:GLN:CD	2.07	0.75
1:B:126:HIS:HE1	4:B:174:HOH:O	1.70	0.75
1:A:125:MSE:HE2	1:B:159:ILE:HD12	1.67	0.74
1:A:83:PRO:HG2	1:A:84:TRP:CE3	2.21	0.74
1:A:30:MSE:CE	1:A:33:GLN:CD	2.56	0.74
1:A:131:GLU:HG3	1:B:155:ARG:CZ	2.19	0.73
1:A:72:VAL:HG12	1:A:97:MSE:HE3	1.70	0.72
1:B:120:CYS:SG	4:B:190:HOH:O	2.48	0.72
1:A:121:ARG:CG	1:A:121:ARG:HH21	1.95	0.72
1:B:6:ILE:CG1	1:B:108:GLU:HG2	2.21	0.71
1:A:39:LYS:O	1:A:43:GLU:HG3	1.90	0.71
1:A:110:LEU:HD21	1:A:125:MSE:HE1	1.73	0.70
1:B:166:LYS:HE2	1:B:167:MSE:HG3	1.72	0.70
1:A:121:ARG:NH2	1:A:121:ARG:HG3	1.92	0.70
1:A:126:HIS:HD2	4:B:180:HOH:O	1.76	0.69
1:A:11:ALA:HB1	1:A:42:LEU:HD11	1.77	0.67
1:B:26:ARG:HB2	1:B:31:GLU:OE2	1.94	0.67
1:A:62:GLU:CD	1:A:62:GLU:H	1.98	0.66
1:B:166:LYS:HE2	1:B:167:MSE:CG	2.26	0.66
1:A:128:LEU:O	3:B:173:B33:H12	1.96	0.65
1:B:32:GLU:CD	1:B:32:GLU:H	1.99	0.65
1:A:36:LEU:HD13	1:B:81:TYR:OH	1.98	0.64
1:A:6:ILE:HG13	1:A:108:GLU:HB3	1.78	0.63
1:A:4:PHE:HE1	1:A:108:GLU:HG3	1.63	0.62
1:A:140:TYR:OH	2:A:200:COA:H22	2.00	0.61
1:B:142:ARG:NE	2:B:172:COA:O8A	2.32	0.61
1:A:164:LEU:HD22	1:B:125:MSE:HE3	1.82	0.60
1:B:59:VAL:HB	1:B:60:PRO:HD2	1.84	0.59
1:A:170:GLU:C	1:A:171:GLU:HG3	2.22	0.59
1:B:61:LYS:HD3	1:B:61:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:O	1:B:29:TYR:CD2	2.55	0.59
1:A:138:ASN:O	1:A:142:ARG:HD3	2.02	0.58
1:A:118:MSE:SE	1:B:165:LEU:HD12	2.53	0.58
1:A:121:ARG:NH2	1:A:121:ARG:CG	2.61	0.57
1:B:142:ARG:NH2	2:B:172:COA:O8A	2.38	0.57
4:A:244:HOH:O	3:B:173:B33:H42	2.04	0.57
1:A:103:PHE:HB2	4:A:218:HOH:O	2.04	0.56
1:B:167:MSE:HA	1:B:170:GLU:HG2	1.88	0.56
1:B:101:ARG:HD3	2:B:172:COA:OAP	2.05	0.55
1:B:36:LEU:HD21	1:B:41:LEU:HD21	1.87	0.55
1:A:10:THR:N	1:A:13:ASP:OD2	2.40	0.55
1:A:69:HIS:HD2	4:A:211:HOH:O	1.89	0.55
1:B:170:GLU:HG3	4:B:179:HOH:O	2.07	0.55
1:A:35:ILE:HD11	1:B:86:GLY:CA	2.37	0.55
1:B:66:PRO:HG2	1:B:67:GLU:OE2	2.06	0.54
1:A:65:THR:HG23	1:A:69:HIS:O	2.08	0.54
1:B:166:LYS:HG2	1:B:167:MSE:N	2.20	0.54
1:B:29:TYR:CZ	1:B:30:MSE:HE3	2.43	0.54
1:A:110:LEU:HD23	1:A:113:LEU:HD12	1.91	0.53
1:A:30:MSE:HE1	1:A:33:GLN:OE1	1.98	0.53
1:B:133:ASN:HD22	1:B:133:ASN:C	2.11	0.53
1:B:126:HIS:HD2	4:B:175:HOH:O	1.91	0.53
1:B:133:ASN:HD22	1:B:135:PRO:HD2	1.74	0.53
1:B:167:MSE:HA	1:B:170:GLU:CG	2.39	0.52
1:A:111:LYS:HG3	1:B:167:MSE:O	2.08	0.52
1:B:62:GLU:HG2	1:B:63:HIS:ND1	2.25	0.52
1:A:110:LEU:HB3	1:B:167:MSE:HE1	1.92	0.52
1:A:165:LEU:HD13	1:B:118:MSE:SE	2.59	0.52
1:A:118:MSE:HA	1:A:118:MSE:HE2	1.91	0.51
1:A:110:LEU:CD2	1:A:125:MSE:HE1	2.41	0.51
1:A:100:TYR:HA	1:A:103:PHE:CE2	2.46	0.51
1:A:10:THR:HG22	1:A:12:ALA:H	1.76	0.50
4:A:237:HOH:O	3:B:173:B33:C2	2.60	0.50
1:B:28:GLU:O	1:B:30:MSE:HG2	2.12	0.49
1:A:133:ASN:O	1:A:137:ILE:HG13	2.12	0.49
1:A:4:PHE:CE1	1:A:108:GLU:HG3	2.47	0.49
1:B:82:ASP:HB3	1:B:85:ILE:HB	1.93	0.49
1:B:58:GLU:HA	1:B:70:SER:O	2.13	0.49
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.78	0.48
1:B:108:GLU:HA	4:B:183:HOH:O	2.13	0.48
1:A:75:ALA:HB2	1:A:109:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:TYR:CD1	1:B:29:TYR:O	2.67	0.47
1:A:118:MSE:N	1:A:118:MSE:HE2	2.30	0.47
1:B:118:MSE:HE2	1:B:118:MSE:HA	1.97	0.47
1:A:64:TRP:CE2	1:A:70:SER:HB3	2.50	0.46
1:B:16:ASP:OD2	1:B:19:ARG:NH2	2.31	0.46
1:B:4:PHE:CD1	1:B:4:PHE:C	2.88	0.46
1:A:164:LEU:CD2	1:B:125:MSE:HE3	2.44	0.46
1:A:118:MSE:HE2	1:A:118:MSE:CA	2.45	0.46
1:A:161:LYS:HE3	4:B:200:HOH:O	2.15	0.46
1:B:60:PRO:HB2	1:B:62:GLU:CD	2.36	0.46
1:A:83:PRO:HG3	1:B:93:ASP:OD2	2.16	0.46
4:A:202:HOH:O	3:B:173:B33:H11	2.16	0.45
1:B:61:LYS:HG2	1:B:64:TRP:CZ2	2.52	0.45
1:A:35:ILE:HD11	1:B:86:GLY:HA2	2.00	0.44
1:B:133:ASN:ND2	1:B:135:PRO:HD2	2.33	0.44
1:A:6:ILE:CG1	1:A:108:GLU:HB3	2.47	0.44
4:A:237:HOH:O	3:B:173:B33:H22	2.18	0.43
1:A:17:ILE:CG2	1:A:41:LEU:HD21	2.48	0.43
1:B:61:LYS:HE3	1:B:64:TRP:CE3	2.53	0.43
1:A:51:PHE:CE1	1:B:87:LYS:HG3	2.54	0.43
1:A:51:PHE:CE1	1:B:81:TYR:HB2	2.54	0.43
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.76	0.42
1:A:30:MSE:HE2	1:A:33:GLN:NE2	2.34	0.42
1:B:48:GLU:O	1:B:50:PRO:HD3	2.18	0.42
1:B:61:LYS:HA	1:B:64:TRP:CD1	2.54	0.42
1:A:65:THR:O	1:A:66:PRO:C	2.57	0.42
1:B:32:GLU:CD	1:B:32:GLU:N	2.71	0.42
1:A:61:LYS:H	1:A:61:LYS:CD	2.31	0.42
1:A:158:LYS:HE3	1:A:160:ASP:OD2	2.19	0.42
1:B:171:GLU:O	1:B:171:GLU:HG2	2.18	0.42
1:B:36:LEU:HD21	1:B:41:LEU:CD2	2.49	0.41
1:A:137:ILE:O	1:A:141:LYS:HG3	2.20	0.41
1:A:125:MSE:CE	1:B:159:ILE:HD12	2.45	0.41
1:A:13:ASP:OD1	1:A:71:ILE:HD11	2.21	0.41
1:B:29:TYR:O	1:B:30:MSE:HE2	2.21	0.40
1:A:28:GLU:O	1:A:30:MSE:HG2	2.22	0.40
1:B:111:LYS:O	1:B:115:GLN:HG3	2.21	0.40
1:B:61:LYS:HA	1:B:64:TRP:NE1	2.36	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:121:ARG:NH2	3:B:173:B33:C14[4_565]	2.11	0.09

## 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	166/171 (97%)	160 (96%)	5 (3%)	1 (1%)	25	19
1	B	168/171 (98%)	163 (97%)	4 (2%)	1 (1%)	25	19
All	All	334/342 (98%)	323 (97%)	9 (3%)	2 (1%)	25	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	B	99	ASP

### 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	148/143 (104%)	137 (93%)	11 (7%)	13	9
1	B	149/143 (104%)	141 (95%)	8 (5%)	22	18
All	All	297/286 (104%)	278 (94%)	19 (6%)	17	13

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	44	ASP
1	A	51	PHE
1	A	84	TRP
1	A	110	LEU
1	A	121	ARG
1	A	126	HIS
1	A	131	GLU
1	A	133	ASN
1	A	142	ARG
1	A	171	GLU
1	B	33	GLN
1	B	67	GLU
1	B	108	GLU
1	B	126	HIS
1	B	133	ASN
1	B	165	LEU
1	B	166	LYS
1	B	171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	133	ASN
1	B	33	GLN
1	B	126	HIS
1	B	133	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	COA	B	172	-	41,50,50	2.31	9 (21%)	52,75,75	6.64	23 (44%)
3	B33	B	173	1	13,13,13	2.29	3 (23%)	11,12,12	9.42	8 (72%)
2	COA	A	200	-	41,50,50	2.00	9 (21%)	52,75,75	3.57	17 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	172	-	2/2/11/13	17/44/64/64	0/3/3/3
3	B33	B	173	1	-	8/11/11/11	-
2	COA	A	200	-	1/1/11/13	14/44/64/64	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	COA	O9P-C9P	6.92	1.37	1.23
3	B	173	B33	C8-N7	5.91	1.66	1.46
2	B	172	COA	O5P-C5P	5.66	1.34	1.23
2	A	200	COA	O4B-C1B	5.47	1.48	1.41
2	B	172	COA	O4B-C1B	5.43	1.48	1.41
2	A	200	COA	C3P-N4P	-5.08	1.34	1.46
2	B	172	COA	C9P-N8P	4.53	1.43	1.33
3	B	173	B33	C10-N11	4.47	1.61	1.46
2	A	200	COA	O5P-C5P	4.38	1.32	1.23
2	A	200	COA	C7P-N8P	-4.15	1.36	1.46
2	B	172	COA	C7P-N8P	-4.15	1.36	1.46
2	B	172	COA	C3P-N4P	-4.01	1.37	1.46
2	A	200	COA	O9P-C9P	3.65	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	200	COA	O4B-C4B	-3.46	1.37	1.45
2	B	172	COA	O4B-C4B	-3.43	1.37	1.45
2	B	172	COA	P3B-O7A	3.21	1.60	1.50
2	A	200	COA	P3B-O7A	3.19	1.60	1.50
2	A	200	COA	OAP-CAP	2.70	1.47	1.42
3	B	173	B33	C9-C10	-2.48	1.41	1.51
2	B	172	COA	OAP-CAP	2.30	1.46	1.42
2	A	200	COA	C7P-C6P	-2.11	1.44	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	COA	C2P-C3P-N4P	24.40	168.06	112.31
2	B	172	COA	C7P-N8P-C9P	20.01	158.28	122.59
3	B	173	B33	C9-C10-N11	18.21	161.26	112.14
3	B	173	B33	C5-C4-N3	16.76	157.36	112.14
2	B	172	COA	OAP-CAP-CBP	16.07	148.07	110.25
2	A	200	COA	C2P-C3P-N4P	15.73	148.24	112.31
2	B	172	COA	C5B-C4B-C3B	15.45	165.59	114.40
2	B	172	COA	C7P-C6P-C5P	13.12	134.20	112.36
3	B	173	B33	C6-C5-C4	12.89	161.33	114.26
2	B	172	COA	O6A-CCP-CBP	11.64	129.26	110.55
2	B	172	COA	C3P-N4P-C5P	11.48	144.16	122.84
3	B	173	B33	C9-C8-N7	11.47	143.08	112.14
2	A	200	COA	O6A-CCP-CBP	9.40	125.66	110.55
2	A	200	COA	C6P-C7P-N8P	8.58	129.22	111.90
2	B	172	COA	CEP-CBP-CCP	-8.44	94.46	108.23
2	A	200	COA	C7P-N8P-C9P	8.32	137.42	122.59
2	B	172	COA	C6P-C7P-N8P	7.31	126.65	111.90
3	B	173	B33	C4-N3-C2	6.07	126.36	113.43
2	B	172	COA	CDP-CBP-CAP	5.78	118.84	108.82
2	B	172	COA	O4B-C4B-C5B	-5.63	90.87	109.37
2	B	172	COA	N3A-C2A-N1A	-5.18	120.59	128.68
2	A	200	COA	N3A-C2A-N1A	-5.16	120.61	128.68
2	B	172	COA	CEP-CBP-CDP	5.05	119.47	109.17
2	A	200	COA	O9P-C9P-CAP	-3.99	108.89	121.06
2	A	200	COA	C7P-C6P-C5P	-3.95	105.79	112.36
2	A	200	COA	CEP-CBP-CAP	3.88	115.55	108.82
2	B	172	COA	CEP-CBP-CAP	3.86	115.51	108.82
2	A	200	COA	O4B-C4B-C5B	3.85	122.03	109.37
2	B	172	COA	C6P-C5P-N4P	-3.76	110.09	116.42
3	B	173	B33	C8-N7-C6	-3.46	97.15	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	COA	P2A-O3A-P1A	3.39	144.44	132.83
2	A	200	COA	C5B-C4B-C3B	3.35	125.49	114.40
2	B	172	COA	O2A-P1A-O5B	3.16	122.42	107.75
2	A	200	COA	O6A-P2A-O4A	3.01	120.85	109.07
2	B	172	COA	C2B-C3B-C4B	-2.95	97.99	103.22
2	A	200	COA	C6P-C5P-N4P	-2.95	111.46	116.42
2	A	200	COA	C2B-C3B-C4B	-2.93	98.04	103.22
2	A	200	COA	O9A-P3B-O8A	2.85	118.53	107.64
2	B	172	COA	O9A-P3B-O8A	2.85	118.52	107.64
3	B	173	B33	C12-N11-C10	-2.81	100.20	113.45
2	A	200	COA	O2A-P1A-O5B	-2.75	94.97	107.75
2	B	172	COA	P1A-O5B-C5B	-2.68	105.95	121.68
2	A	200	COA	O9P-C9P-N8P	2.52	128.41	122.99
3	B	173	B33	C5-C6-N7	2.52	118.93	112.14
2	B	172	COA	O6A-P2A-O4A	2.52	118.89	109.07
2	B	172	COA	CDP-CBP-CCP	-2.43	104.26	108.23
2	A	200	COA	CAP-C9P-N8P	-2.35	111.91	116.58
2	B	172	COA	O5B-P1A-O1A	-2.25	100.27	109.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	172	COA	C4B
2	B	172	COA	CAP
2	A	200	COA	CAP

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	172	COA	O4B-C4B-C5B-O5B
2	B	172	COA	CAP-CBP-CCP-O6A
2	B	172	COA	OAP-CAP-CBP-CCP
2	B	172	COA	OAP-CAP-CBP-CDP
2	B	172	COA	OAP-CAP-CBP-CEP
2	B	172	COA	C9P-CAP-CBP-CEP
2	B	172	COA	CAP-C9P-N8P-C7P
2	B	172	COA	C5P-C6P-C7P-N8P
3	B	173	B33	C9-C10-N11-C12
3	B	173	B33	C5-C4-N3-C2
3	B	173	B33	C9-C8-N7-C6
2	A	200	COA	C9P-CAP-CBP-CCP
2	A	200	COA	C9P-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
2	A	200	COA	C9P-CAP-CBP-CEP
2	A	200	COA	N8P-C9P-CAP-OAP
2	A	200	COA	CAP-C9P-N8P-C7P
2	B	172	COA	O9P-C9P-N8P-C7P
2	A	200	COA	C6P-C7P-N8P-C9P
3	B	173	B33	N3-C4-C5-C6
3	B	173	B33	N11-C10-C9-C8
3	B	173	B33	N7-C8-C9-C10
2	A	200	COA	O4B-C4B-C5B-O5B
2	B	172	COA	CDP-CBP-CCP-O6A
2	B	172	COA	CEP-CBP-CCP-O6A
2	B	172	COA	O5P-C5P-N4P-C3P
2	B	172	COA	O9P-C9P-CAP-OAP
2	B	172	COA	C6P-C5P-N4P-C3P
2	A	200	COA	OAP-CAP-CBP-CDP
2	A	200	COA	C3B-C4B-C5B-O5B
3	B	173	B33	C4-C5-C6-N7
2	A	200	COA	P2A-O3A-P1A-O1A
3	B	173	B33	N11-C12-C13-C14
2	A	200	COA	O9P-C9P-CAP-CBP
2	A	200	COA	O9P-C9P-CAP-OAP
2	B	172	COA	N8P-C9P-CAP-OAP
2	A	200	COA	O9P-C9P-N8P-C7P
2	A	200	COA	OAP-CAP-CBP-CEP
2	B	172	COA	P1A-O3A-P2A-O5A
2	B	172	COA	C9P-CAP-CBP-CCP

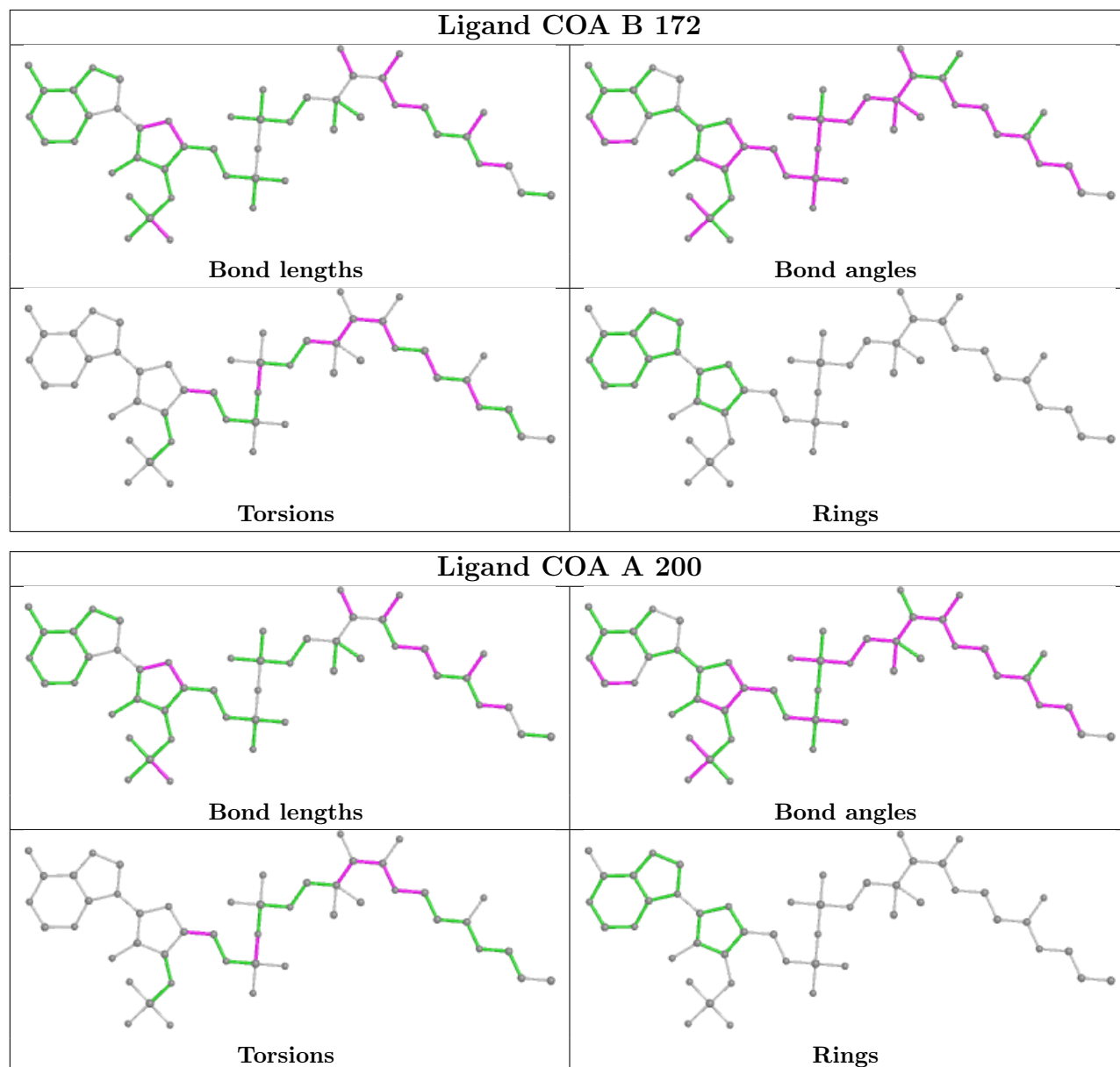
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	172	COA	3	0
3	B	173	B33	5	1
2	A	200	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.



## 5.7 Other polymers ⓘ

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	160/171 (93%)	0.48	7 (4%) 34 33	16, 29, 48, 55	0
1	B	164/171 (95%)	0.29	11 (6%) 17 17	14, 27, 49, 64	0
All	All	324/342 (94%)	0.38	18 (5%) 24 23	14, 28, 49, 64	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	6.1
1	B	29	TYR	5.8
1	A	103	PHE	5.0
1	B	48	GLU	4.8
1	B	64	TRP	4.4
1	B	171	GLU	3.6
1	B	65	THR	3.6
1	B	61	LYS	3.5
1	B	49	HIS	3.2
1	B	32	GLU	2.9
1	A	63	HIS	2.8
1	B	68	GLY	2.8
1	A	42	LEU	2.6
1	A	59	VAL	2.2
1	B	66	PRO	2.2
1	A	68	GLY	2.2
1	A	84	TRP	2.2
1	B	63	HIS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

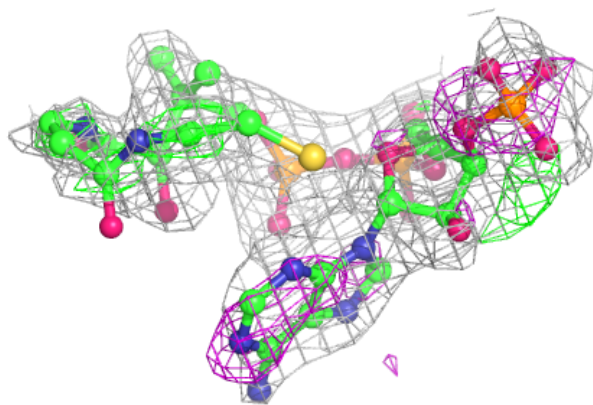
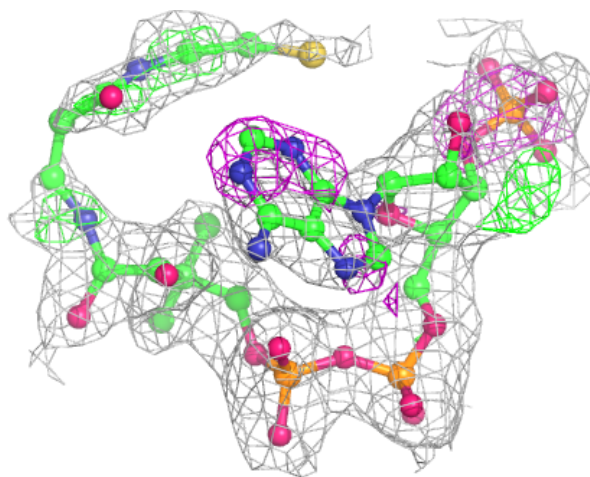
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

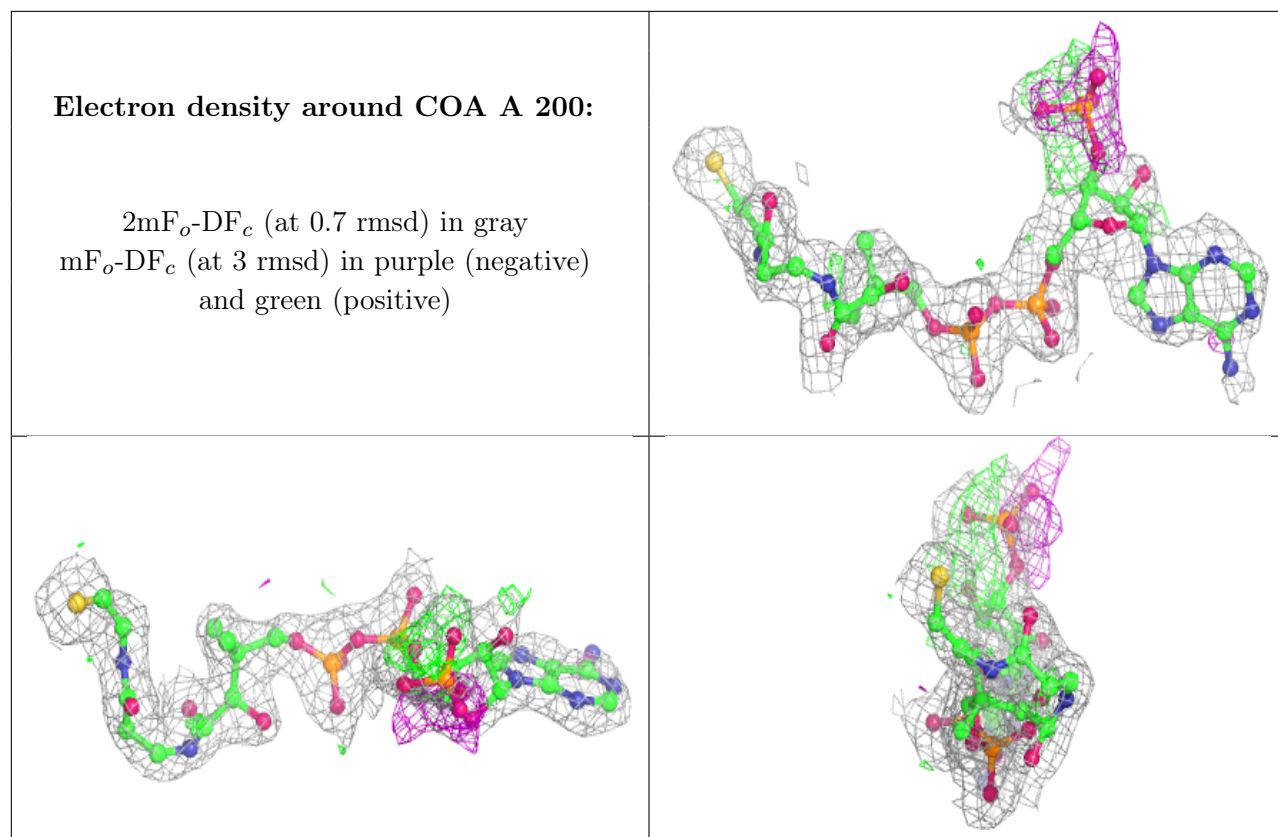
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	COA	B	172	48/48	0.80	0.24	28,38,48,49	9
3	B33	B	173	14/14	0.81	0.39	51,54,55,55	7
2	COA	A	200	48/48	0.83	0.20	24,34,40,41	0

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 B 172:**

$2mF_o-DF_c$  (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.