



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2022 – 02:09 PM JST

PDB ID : 8GXK
Title : Pseudomonas jinjuensis N-acetyltransferase
Authors : Song, Y.J.; Bao, R.
Deposited on : 2022-09-20
Resolution : 1.78 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

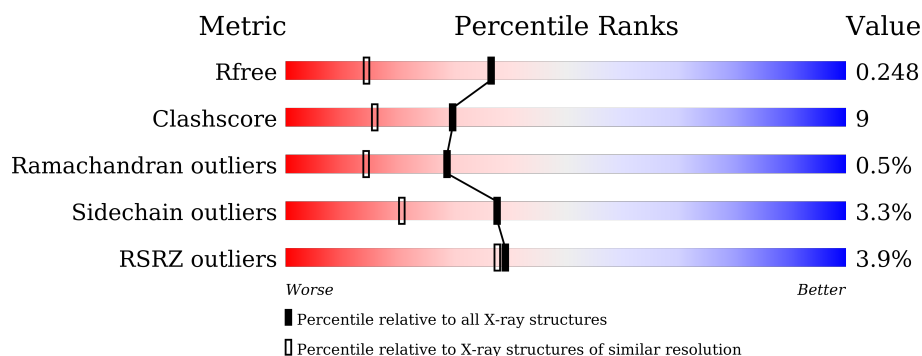
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	189	 4% 83% 13% ...
1	B	189	 4% 78% 20% ..
1	C	189	 3% 81% 17% ..
1	D	189	 4% 83% 14% ...

2 Entry composition ⓘ

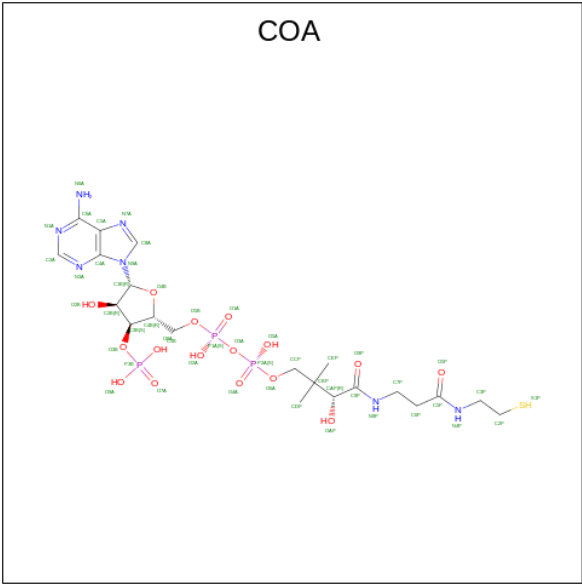
There are 3 unique types of molecules in this entry. The entry contains 12591 atoms, of which 6083 are hydrogens and 0 are deuteriums.

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 Protein N-acetyltransferase, RimJ/RimL family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	185	Total	C	H	N	O	S	0	0	0
			2930	916	1470	274	262	8			
1	B	188	Total	C	H	N	O	S	0	0	0
			2989	936	1500	280	265	8			
1	C	187	Total	C	H	N	O	S	0	0	0
			2971	927	1493	279	264	8			
1	D	187	Total	C	H	N	O	S	0	0	0
			2983	934	1498	279	264	8			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			78	21	30	7	16	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			79	21	31	7	16	3	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	S	0	0
			79	21	31	7	16	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			78	21	30	7	16	3	1		

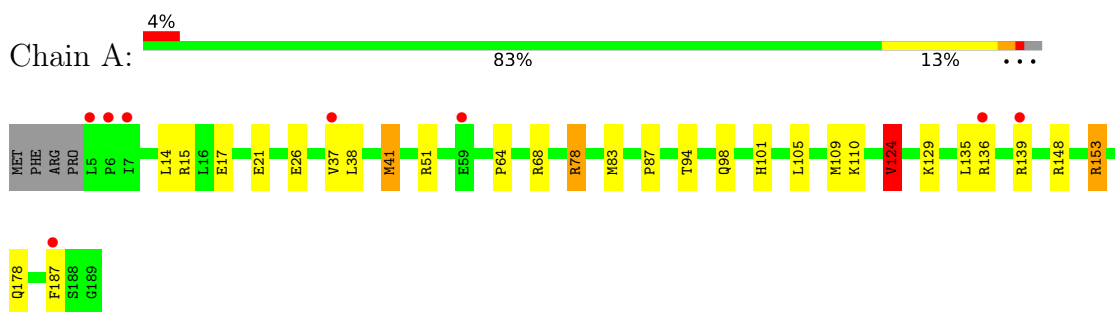
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	103	Total	O	0	0
			103	103		
3	C	101	Total	O	0	0
			101	101		
3	D	106	Total	O	0	0
			106	106		

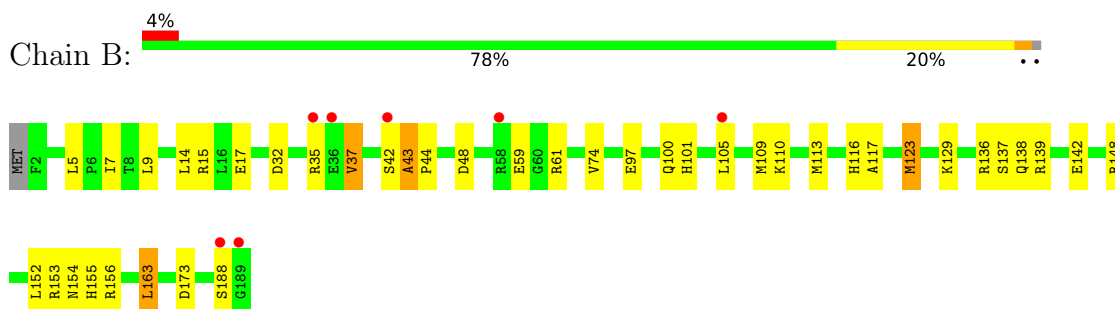
3 Residue-property plots [i](#)

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.

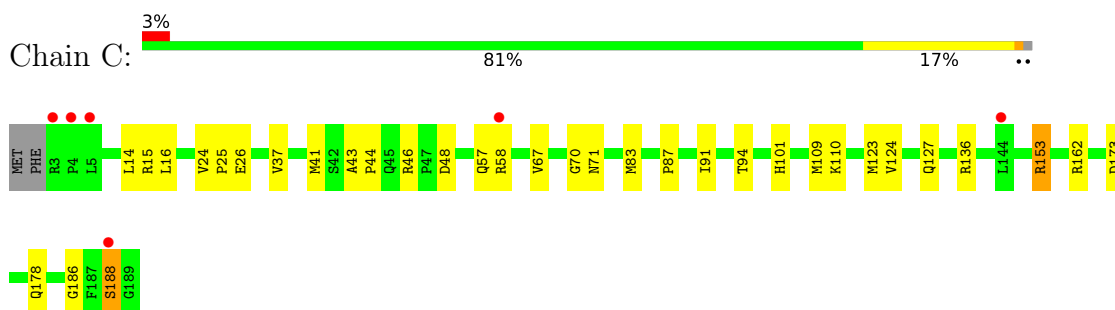
- Molecule 1: Protein N-acetyltransferase, RimJ/RimL family



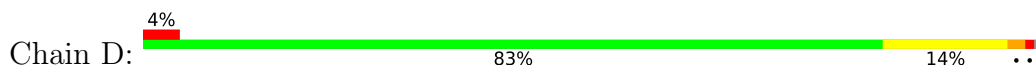
- Molecule 1: Protein N-acetyltransferase, RimJ/RimL family

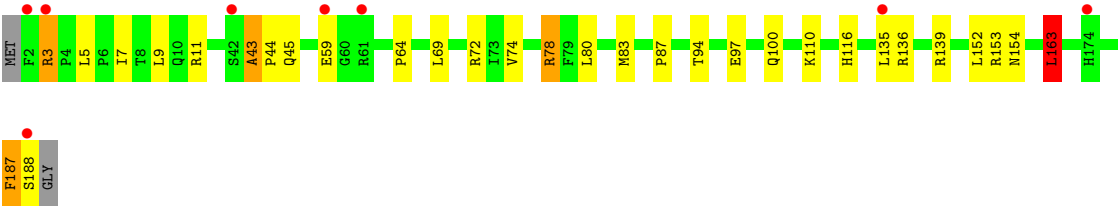


- Molecule 1: Protein N-acetyltransferase, RimJ/RimL family



- Molecule 1: Protein N-acetyltransferase, RimJ/RimL family





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.88Å 100.69Å 94.62Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	33.43 – 1.78 47.03 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.43-1.78) 96.1 (47.03-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.205 , 0.247 0.205 , 0.248	Depositor DCC
R_{free} test set	1999 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12591	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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	0.62	0/1488	0.82	3/2013 (0.1%)
1	B	0.63	0/1519	0.86	6/2055 (0.3%)
1	C	0.64	0/1507	0.79	2/2039 (0.1%)
1	D	0.60	0/1515	0.82	2/2050 (0.1%)
All	All	0.62	0/6029	0.82	13/8157 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	MET	CG-SD-CE	6.94	111.31	100.20
1	A	153	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	B	152	LEU	CB-CG-CD2	6.56	122.15	111.00
1	C	41	MET	CA-CB-CG	-6.48	102.28	113.30
1	B	163	LEU	CA-CB-CG	6.36	129.92	115.30
1	B	173	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	136	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	163	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	123	MET	CG-SD-CE	5.56	109.10	100.20
1	A	124	VAL	CG1-CB-CG2	5.35	119.45	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	136	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	123	MET	CG-SD-CE	5.13	108.40	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	PHE	Mainchain
1	D	187	PHE	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	1460	1470	1471	28	0
1	B	1489	1500	1500	21	0
1	C	1478	1493	1491	33	0
1	D	1485	1498	1497	28	0
2	A	48	30	29	9	0
2	B	48	31	31	3	0
2	C	48	31	32	9	0
2	D	48	30	30	8	0
3	A	94	0	0	5	0
3	B	103	0	0	2	0
3	C	101	0	0	7	0
3	D	106	0	0	2	0
All	All	6508	6083	6081	115	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 (115) 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:B:201:COA:C1B	2:B:201:COA:O4B	1.65	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:COA:C1B	2:C:201:COA:O4B	1.66	1.26
2:D:201:COA:O4B	2:D:201:COA:C1B	1.69	1.20
2:A:201:COA:O4B	2:A:201:COA:C1B	1.70	1.14
1:C:124:VAL:HG11	1:D:163:LEU:HD11	1.45	0.95
1:C:57:GLN:OE1	3:C:301:HOH:O	1.87	0.92
1:A:15:ARG:NH2	3:A:302:HOH:O	2.07	0.88
1:C:173:ASP:OD1	3:C:302:HOH:O	1.97	0.83
1:A:26:GLU:OE2	3:A:301:HOH:O	1.96	0.82
1:C:124:VAL:HG12	1:D:154:ASN:HB3	1.63	0.79
1:A:139:ARG:CG	2:A:201:COA:H8A	2.14	0.78
1:D:7:ILE:HD12	1:D:9:LEU:HD21	1.69	0.74
1:C:46:ARG:NE	1:C:48:ASP:OD1	2.22	0.73
1:A:178:GLN:NE2	3:A:304:HOH:O	2.23	0.72
1:C:101:HIS:CD2	2:C:201:COA:H142	2.26	0.71
1:C:48:ASP:OD2	3:C:303:HOH:O	2.08	0.71
1:D:110:LYS:HE3	3:D:321:HOH:O	1.89	0.71
1:B:74:VAL:HG21	1:B:100:GLN:HG3	1.71	0.71
1:A:124:VAL:HG13	1:B:154:ASN:HB3	1.74	0.70
1:A:21:GLU:OE1	1:A:51:ARG:NH1	2.23	0.70
1:D:64:PRO:HA	1:D:78:ARG:HB2	1.73	0.69
1:A:136:ARG:HG3	2:A:201:COA:H52A	1.75	0.69
1:B:110:LYS:HE3	3:B:326:HOH:O	1.91	0.69
2:D:201:COA:O4B	2:D:201:COA:N9A	2.26	0.67
1:C:14:LEU:HD12	1:C:15:ARG:N	2.12	0.65
1:A:101:HIS:CE1	2:A:201:COA:O9P	2.50	0.65
1:A:139:ARG:HG2	2:A:201:COA:H8A	1.78	0.64
1:B:14:LEU:HD13	1:B:105:LEU:HD11	1.79	0.64
1:A:94:THR:O	2:A:201:COA:H61	1.99	0.63
1:A:148:ARG:NH2	3:A:303:HOH:O	2.14	0.61
1:B:59:GLU:HG3	1:B:61:ARG:HG3	1.81	0.61
1:C:26:GLU:OE2	3:C:304:HOH:O	2.16	0.60
1:A:139:ARG:HG3	2:A:201:COA:H8A	1.84	0.59
1:A:15:ARG:NH2	1:A:17:GLU:OE1	2.35	0.59
1:B:37:VAL:HG21	1:B:101:HIS:CE1	2.38	0.59
1:C:110:LYS:HE3	3:C:312:HOH:O	2.03	0.58
2:A:201:COA:O5A	2:A:201:COA:H132	2.06	0.56
1:D:187:PHE:O	1:D:188:SER:HB2	2.06	0.55
1:A:37:VAL:HG11	1:A:101:HIS:CE1	2.41	0.55
2:C:201:COA:O5A	2:C:201:COA:H143	2.07	0.55
1:D:110:LYS:NZ	2:D:201:COA:H21	2.21	0.55
1:A:135:LEU:O	1:A:139:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:COA:O5A	2:C:201:COA:H132	2.07	0.54
2:D:201:COA:O4B	2:D:201:COA:C8A	2.56	0.53
1:A:37:VAL:CG1	1:A:101:HIS:HE1	2.21	0.53
3:B:343:HOH:O	1:C:178:GLN:HG3	2.09	0.53
1:C:70:GLY:O	1:C:71:ASN:HB2	2.07	0.53
1:D:74:VAL:HG21	1:D:100:GLN:HG3	1.89	0.53
1:B:74:VAL:CG2	1:B:100:GLN:HG3	2.37	0.52
1:B:32:ASP:O	1:B:35:ARG:HG3	2.10	0.52
1:C:94:THR:HB	2:C:201:COA:H32	1.92	0.52
1:D:72:ARG:NH1	1:D:97:GLU:OE1	2.43	0.52
1:B:43:ALA:N	1:B:44:PRO:CD	2.73	0.52
1:B:15:ARG:HD3	1:B:17:GLU:OE1	2.09	0.52
1:A:129:LYS:O	2:A:201:COA:H21	2.10	0.52
1:A:37:VAL:HG11	1:A:101:HIS:HE1	1.76	0.51
1:B:7:ILE:HD13	1:B:116:HIS:CD2	2.45	0.51
1:A:14:LEU:HD12	1:A:105:LEU:CD1	2.41	0.50
1:D:94:THR:HB	2:D:201:COA:H22	1.93	0.50
1:A:64:PRO:HA	1:A:78:ARG:HB2	1.93	0.49
1:C:124:VAL:CG1	1:D:154:ASN:HB3	2.40	0.49
1:C:136:ARG:NH2	2:C:201:COA:H8A	2.28	0.49
1:B:37:VAL:CG2	1:B:101:HIS:HE1	2.25	0.49
1:D:139:ARG:HG3	2:D:201:COA:H8A	1.94	0.49
1:B:137:SER:OG	2:B:201:COA:H31	2.12	0.48
1:A:17:GLU:OE1	1:A:68:ARG:HD2	2.13	0.48
1:B:138:GLN:O	1:B:142:GLU:HG3	2.13	0.48
1:C:14:LEU:HD11	1:C:67:VAL:HG13	1.95	0.48
1:A:37:VAL:HG21	1:A:98:GLN:HB2	1.95	0.47
1:C:124:VAL:CG1	1:D:163:LEU:HD11	2.32	0.47
1:A:83:MET:O	1:A:87:PRO:HA	2.14	0.47
1:B:7:ILE:HD12	1:B:9:LEU:HD21	1.97	0.47
2:B:201:COA:O4B	2:B:201:COA:N9A	2.41	0.47
1:C:83:MET:O	1:C:87:PRO:HA	2.15	0.47
1:C:46:ARG:NH2	1:C:48:ASP:OD1	2.48	0.47
1:B:117:ALA:O	1:B:123:MET:HG3	2.15	0.47
1:B:129:LYS:HE3	1:B:155:HIS:HE1	1.80	0.47
1:A:14:LEU:C	1:A:14:LEU:HD23	2.35	0.47
1:A:110:LYS:HE3	3:A:305:HOH:O	2.15	0.46
2:C:201:COA:H143	2:C:201:COA:P2A	2.56	0.46
1:C:24:VAL:HB	1:C:25:PRO:HD3	1.97	0.46
1:C:37:VAL:HG11	1:C:101:HIS:CE1	2.51	0.46
1:D:74:VAL:CG2	1:D:100:GLN:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:CG1	1:C:101:HIS:HE1	2.28	0.45
1:C:58:ARG:NH2	3:C:310:HOH:O	2.49	0.45
1:D:135:LEU:O	1:D:139:ARG:HG2	2.16	0.45
1:A:37:VAL:HG12	1:A:38:LEU:HD23	1.98	0.45
1:D:83:MET:O	1:D:87:PRO:HA	2.17	0.44
1:D:7:ILE:HD13	1:D:116:HIS:CD2	2.51	0.44
1:B:42:SER:O	1:B:43:ALA:HB3	2.17	0.44
1:C:16:LEU:CD2	1:C:67:VAL:HG22	2.47	0.44
1:C:14:LEU:HD21	1:C:109:MET:HG3	2.00	0.44
1:B:37:VAL:CG2	1:B:101:HIS:CE1	3.01	0.43
1:A:14:LEU:HD23	1:A:15:ARG:N	2.33	0.43
1:C:136:ARG:HG3	2:C:201:COA:H52A	2.00	0.43
1:B:109:MET:O	1:B:113:MET:HG3	2.18	0.43
1:D:110:LYS:HZ3	2:D:201:COA:H21	1.84	0.43
1:D:74:VAL:HG22	1:D:97:GLU:HG2	2.01	0.43
1:A:14:LEU:HD11	1:A:109:MET:HG3	2.01	0.42
1:C:124:VAL:HG13	1:D:154:ASN:ND2	2.34	0.42
1:D:7:ILE:HD12	1:D:9:LEU:CD2	2.44	0.42
1:D:152:LEU:N	1:D:152:LEU:HD23	2.35	0.42
1:C:94:THR:O	2:C:201:COA:H71	2.18	0.42
1:D:43:ALA:N	1:D:44:PRO:CD	2.84	0.41
1:D:110:LYS:HZ1	2:D:201:COA:H21	1.86	0.41
1:C:153:ARG:HD2	3:C:381:HOH:O	2.20	0.41
1:D:59:GLU:O	1:D:59:GLU:HG3	2.20	0.41
1:C:43:ALA:N	1:C:44:PRO:CD	2.84	0.41
1:D:3:ARG:HB3	1:D:5:LEU:HG	2.03	0.41
1:C:46:ARG:CZ	1:C:48:ASP:OD1	2.69	0.41
1:C:186:GLY:C	1:C:188:SER:H	2.23	0.41
1:D:11:ARG:NH2	1:D:187:PHE:HB3	2.36	0.41
1:D:45:GLN:HB2	3:D:348:HOH:O	2.20	0.41
1:B:74:VAL:HG22	1:B:97:GLU:HG2	2.03	0.40
1:C:91:ILE:HG21	1:C:110:LYS:HE2	2.04	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	183/189 (97%)	180 (98%)	3 (2%)	0	100	100
1	B	186/189 (98%)	182 (98%)	2 (1%)	2 (1%)	14	4
1	C	185/189 (98%)	182 (98%)	3 (2%)	0	100	100
1	D	185/189 (98%)	180 (97%)	3 (2%)	2 (1%)	14	4
All	All	739/756 (98%)	724 (98%)	11 (2%)	4 (0%)	29	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	ALA
1	B	188	SER
1	D	43	ALA
1	D	3	ARG

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	151/155 (97%)	147 (97%)	4 (3%)	46	29
1	B	154/155 (99%)	147 (96%)	7 (4%)	27	11
1	C	153/155 (99%)	149 (97%)	4 (3%)	46	29
1	D	154/155 (99%)	149 (97%)	5 (3%)	39	22
All	All	612/620 (99%)	592 (97%)	20 (3%)	38	21

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	124	VAL
1	A	153	ARG
1	B	5	LEU
1	B	37	VAL
1	B	48	ASP
1	B	139	ARG
1	B	148	ARG
1	B	153	ARG
1	B	163	LEU
1	C	127	GLN
1	C	153	ARG
1	C	162	ARG
1	C	188	SER
1	D	69	LEU
1	D	78	ARG
1	D	80	LEU
1	D	153	ARG
1	D	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	C	201	-	41,50,50	4.58	17 (41%)	52,75,75	4.62	23 (44%)
2	COA	A	201	-	41,50,50	4.84	19 (46%)	52,75,75	3.75	25 (48%)
2	COA	D	201	-	41,50,50	5.01	23 (56%)	52,75,75	3.43	21 (40%)
2	COA	B	201	-	41,50,50	4.10	16 (39%)	52,75,75	2.51	6 (11%)

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	C	201	-	-	23/44/64/64	0/3/3/3
2	COA	A	201	-	-	18/44/64/64	0/3/3/3
2	COA	D	201	-	-	16/44/64/64	0/3/3/3
2	COA	B	201	-	-	4/44/64/64	0/3/3/3

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	COA	O4B-C1B	21.13	1.70	1.41
2	D	201	COA	O4B-C1B	20.14	1.69	1.41
2	C	201	COA	O4B-C1B	18.16	1.66	1.41
2	B	201	COA	O4B-C1B	17.52	1.65	1.41
2	D	201	COA	C2B-C1B	-15.28	1.30	1.53
2	A	201	COA	C2B-C1B	-15.01	1.31	1.53
2	C	201	COA	C2B-C1B	-13.78	1.32	1.53
2	B	201	COA	C2B-C1B	-13.37	1.33	1.53
2	C	201	COA	C9P-N8P	10.64	1.56	1.33
2	D	201	COA	C9P-N8P	10.20	1.55	1.33
2	A	201	COA	C9P-N8P	10.10	1.55	1.33
2	B	201	COA	C9P-N8P	6.94	1.48	1.33
2	D	201	COA	C6P-C5P	5.67	1.62	1.51
2	D	201	COA	C7P-N8P	5.62	1.59	1.46
2	C	201	COA	C6P-C5P	5.52	1.61	1.51
2	B	201	COA	O4B-C4B	-5.39	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	COA	O4B-C4B	-5.04	1.33	1.45
2	C	201	COA	O5P-C5P	-4.93	1.13	1.23
2	D	201	COA	O4B-C4B	-4.87	1.34	1.45
2	D	201	COA	C7P-C6P	4.77	1.66	1.51
2	C	201	COA	C5P-N4P	4.75	1.44	1.33
2	A	201	COA	C7P-N8P	4.63	1.56	1.46
2	A	201	COA	C5P-N4P	4.61	1.43	1.33
2	A	201	COA	O4B-C4B	-4.57	1.34	1.45
2	D	201	COA	C5P-N4P	4.54	1.43	1.33
2	D	201	COA	O5P-C5P	-4.53	1.14	1.23
2	C	201	COA	OAP-CAP	4.33	1.50	1.42
2	A	201	COA	C6P-C5P	3.81	1.58	1.51
2	B	201	COA	O5P-C5P	-3.68	1.15	1.23
2	A	201	COA	O5P-C5P	-3.64	1.15	1.23
2	C	201	COA	P2A-O6A	3.60	1.73	1.59
2	D	201	COA	P2A-O6A	3.41	1.73	1.59
2	D	201	COA	C6A-C5A	-3.35	1.30	1.43
2	A	201	COA	C3B-C4B	3.34	1.61	1.52
2	D	201	COA	C5A-C4A	-3.27	1.32	1.40
2	B	201	COA	C3B-C4B	3.26	1.61	1.52
2	B	201	COA	C5P-N4P	3.17	1.40	1.33
2	C	201	COA	C3B-C4B	3.15	1.61	1.52
2	D	201	COA	C3B-C4B	3.15	1.61	1.52
2	B	201	COA	C5A-C4A	-3.13	1.32	1.40
2	B	201	COA	C2A-N3A	3.10	1.37	1.32
2	C	201	COA	CEP-CBP	2.97	1.60	1.53
2	D	201	COA	P3B-O3B	2.97	1.64	1.59
2	C	201	COA	C7P-N8P	2.92	1.52	1.46
2	C	201	COA	O6A-CCP	2.90	1.53	1.43
2	D	201	COA	O6A-CCP	2.85	1.53	1.43
2	C	201	COA	C5A-C4A	-2.84	1.33	1.40
2	D	201	COA	OAP-CAP	2.79	1.47	1.42
2	D	201	COA	CEP-CBP	2.68	1.59	1.53
2	C	201	COA	O3B-C3B	-2.65	1.34	1.44
2	B	201	COA	C6P-C5P	2.64	1.56	1.51
2	B	201	COA	O3B-C3B	-2.64	1.34	1.44
2	D	201	COA	C2A-N3A	2.59	1.36	1.32
2	B	201	COA	CDP-CBP	2.51	1.59	1.53
2	B	201	COA	O2B-C2B	2.50	1.48	1.43
2	C	201	COA	C6A-N6A	2.46	1.43	1.34
2	A	201	COA	C5A-C4A	-2.46	1.34	1.40
2	D	201	COA	CDP-CBP	2.44	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	COA	CEP-CBP	2.41	1.59	1.53
2	A	201	COA	C6A-N6A	2.40	1.42	1.34
2	A	201	COA	P2A-O6A	2.39	1.69	1.59
2	A	201	COA	P3B-O3B	2.38	1.63	1.59
2	D	201	COA	O2B-C2B	2.37	1.48	1.43
2	B	201	COA	C7P-N8P	2.37	1.51	1.46
2	A	201	COA	C3P-N4P	2.36	1.51	1.46
2	D	201	COA	O3B-C3B	-2.35	1.35	1.44
2	A	201	COA	O3B-C3B	-2.24	1.35	1.44
2	A	201	COA	C2A-N3A	2.23	1.35	1.32
2	D	201	COA	C5A-N7A	-2.22	1.31	1.39
2	B	201	COA	C6A-C5A	-2.20	1.35	1.43
2	C	201	COA	C2A-N3A	2.18	1.35	1.32
2	A	201	COA	OAP-CAP	2.18	1.46	1.42
2	D	201	COA	P3B-O9A	-2.16	1.46	1.54
2	A	201	COA	C6A-C5A	-2.11	1.35	1.43
2	B	201	COA	P3B-O9A	-2.07	1.46	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	C6P-C5P-N4P	14.51	140.85	116.42
2	C	201	COA	C5A-C6A-N6A	12.93	140.01	120.35
2	A	201	COA	C5A-C6A-N6A	12.59	139.49	120.35
2	B	201	COA	C5A-C6A-N6A	12.17	138.85	120.35
2	A	201	COA	CEP-CBP-CAP	-10.71	90.25	108.82
2	C	201	COA	C7P-C6P-C5P	10.37	129.62	112.36
2	B	201	COA	N6A-C6A-N1A	-9.32	99.23	118.57
2	C	201	COA	O5P-C5P-N4P	-9.22	105.62	123.01
2	C	201	COA	N6A-C6A-N1A	-9.18	99.52	118.57
2	C	201	COA	CAP-C9P-N8P	8.74	133.99	116.58
2	D	201	COA	C1B-N9A-C4A	8.59	141.74	126.64
2	A	201	COA	N6A-C6A-N1A	-8.49	100.95	118.57
2	D	201	COA	C6P-C5P-N4P	8.31	130.41	116.42
2	D	201	COA	CEP-CBP-CAP	-7.92	95.08	108.82
2	D	201	COA	C5A-C6A-N6A	7.82	132.24	120.35
2	A	201	COA	CAP-C9P-N8P	7.49	131.50	116.58
2	D	201	COA	O5P-C5P-N4P	-7.30	109.25	123.01
2	C	201	COA	OAP-CAP-CBP	-7.22	93.26	110.25
2	D	201	COA	N6A-C6A-N1A	-6.64	104.78	118.57
2	A	201	COA	C1B-N9A-C4A	6.35	137.80	126.64
2	D	201	COA	C7P-C6P-C5P	6.19	122.66	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	OAP-CAP-C9P	-6.15	79.81	109.42
2	A	201	COA	O9P-C9P-N8P	-5.97	110.18	122.99
2	A	201	COA	O4B-C1B-C2B	-5.60	98.74	106.93
2	D	201	COA	C7P-N8P-C9P	5.49	132.38	122.59
2	C	201	COA	C6P-C7P-N8P	5.35	122.69	111.90
2	C	201	COA	CEP-CBP-CCP	-5.31	99.57	108.23
2	A	201	COA	OAP-CAP-CBP	5.23	122.57	110.25
2	A	201	COA	OAP-CAP-C9P	-5.22	84.31	109.42
2	C	201	COA	N3A-C2A-N1A	-5.14	120.64	128.68
2	C	201	COA	CDP-CBP-CAP	-4.97	100.21	108.82
2	C	201	COA	O5P-C5P-C6P	-4.89	113.07	122.02
2	C	201	COA	O9P-C9P-N8P	-4.89	112.50	122.99
2	B	201	COA	N3A-C2A-N1A	-4.84	121.12	128.68
2	C	201	COA	O6A-CCP-CBP	4.76	118.19	110.55
2	A	201	COA	O3B-C3B-C4B	-4.68	93.16	110.08
2	C	201	COA	CDP-CBP-CCP	4.41	115.42	108.23
2	A	201	COA	N3A-C2A-N1A	-4.26	122.02	128.68
2	C	201	COA	C3P-N4P-C5P	4.04	130.33	122.84
2	D	201	COA	C6P-C7P-N8P	3.92	119.80	111.90
2	D	201	COA	C4A-C5A-N7A	3.89	113.45	109.40
2	C	201	COA	O6A-P2A-O4A	3.79	123.86	109.07
2	A	201	COA	C7P-N8P-C9P	3.75	129.28	122.59
2	D	201	COA	OAP-CAP-CBP	-3.70	101.53	110.25
2	A	201	COA	O6A-P2A-O4A	3.54	122.89	109.07
2	D	201	COA	CDP-CBP-CCP	-3.53	102.48	108.23
2	D	201	COA	O5A-P2A-O6A	3.52	124.08	107.75
2	D	201	COA	N3A-C2A-N1A	-3.50	123.21	128.68
2	A	201	COA	C5B-C4B-C3B	3.45	125.84	114.40
2	D	201	COA	CEP-CBP-CCP	-3.35	102.77	108.23
2	A	201	COA	CDP-CBP-CCP	3.31	113.63	108.23
2	D	201	COA	O6A-P2A-O4A	-3.24	96.40	109.07
2	A	201	COA	O4B-C4B-C3B	-3.21	97.98	104.87
2	D	201	COA	C3P-N4P-C5P	3.19	128.75	122.84
2	C	201	COA	O3B-C3B-C4B	-3.06	99.01	110.08
2	A	201	COA	C2P-C3P-N4P	-2.85	105.79	112.31
2	A	201	COA	C2B-C3B-C4B	2.81	108.21	103.22
2	D	201	COA	CDP-CBP-CAP	2.72	113.54	108.82
2	C	201	COA	O9P-C9P-CAP	-2.51	113.41	121.06
2	D	201	COA	C2A-N1A-C6A	-2.47	114.53	118.75
2	A	201	COA	C6P-C7P-N8P	2.43	116.80	111.90
2	B	201	COA	O4B-C1B-C2B	-2.42	103.39	106.93
2	C	201	COA	O5A-P2A-O4A	-2.40	100.37	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	COA	C6P-C5P-N4P	2.36	120.39	116.42
2	C	201	COA	C7P-N8P-C9P	2.26	126.62	122.59
2	D	201	COA	O4B-C1B-C2B	-2.25	103.63	106.93
2	B	201	COA	CEP-CBP-CCP	2.14	111.73	108.23
2	A	201	COA	O4B-C4B-C5B	2.14	116.41	109.37
2	A	201	COA	O9P-C9P-CAP	-2.14	114.55	121.06
2	C	201	COA	O4B-C1B-C2B	-2.10	103.86	106.93
2	A	201	COA	O3B-C3B-C2B	2.09	119.25	111.68
2	B	201	COA	P2A-O3A-P1A	-2.07	125.73	132.83
2	A	201	COA	CEP-CBP-CDP	2.05	113.35	109.17
2	D	201	COA	O5B-P1A-O1A	-2.02	101.19	109.07
2	A	201	COA	O5P-C5P-N4P	-2.00	119.23	123.01

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	COA	O4B-C4B-C5B-O5B
2	A	201	COA	CCP-O6A-P2A-O4A
2	A	201	COA	CBP-CCP-O6A-P2A
2	A	201	COA	C9P-CAP-CBP-CCP
2	A	201	COA	OAP-CAP-CBP-CDP
2	A	201	COA	C9P-CAP-CBP-CDP
2	A	201	COA	C9P-CAP-CBP-CEP
2	A	201	COA	O9P-C9P-CAP-OAP
2	A	201	COA	CAP-C9P-N8P-C7P
2	C	201	COA	O4B-C4B-C5B-O5B
2	C	201	COA	CBP-CCP-O6A-P2A
2	C	201	COA	CAP-CBP-CCP-O6A
2	C	201	COA	OAP-CAP-CBP-CCP
2	C	201	COA	OAP-CAP-CBP-CEP
2	C	201	COA	CAP-C9P-N8P-C7P
2	C	201	COA	C5P-C6P-C7P-N8P
2	C	201	COA	S1P-C2P-C3P-N4P
2	D	201	COA	CCP-O6A-P2A-O4A
2	D	201	COA	CCP-O6A-P2A-O5A
2	D	201	COA	CDP-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	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	A	201	COA	C6P-C7P-N8P-C9P
2	C	201	COA	C6P-C5P-N4P-C3P
2	D	201	COA	C6P-C5P-N4P-C3P
2	A	201	COA	C3B-C4B-C5B-O5B
2	A	201	COA	O9P-C9P-N8P-C7P
2	C	201	COA	O9P-C9P-N8P-C7P
2	C	201	COA	O5P-C5P-N4P-C3P
2	D	201	COA	O5P-C5P-N4P-C3P
2	C	201	COA	C3B-C4B-C5B-O5B
2	D	201	COA	CEP-CBP-CCP-O6A
2	D	201	COA	C5P-C6P-C7P-N8P
2	C	201	COA	O5P-C5P-C6P-C7P
2	C	201	COA	CEP-CBP-CCP-O6A
2	A	201	COA	OAP-CAP-CBP-CEP
2	C	201	COA	N8P-C9P-CAP-OAP
2	A	201	COA	C5P-C6P-C7P-N8P
2	D	201	COA	C9P-CAP-CBP-CEP
2	C	201	COA	P2A-O3A-P1A-O1A
2	D	201	COA	P2A-O3A-P1A-O2A
2	C	201	COA	CCP-O6A-P2A-O4A
2	A	201	COA	CEP-CBP-CCP-O6A
2	C	201	COA	CDP-CBP-CCP-O6A
2	A	201	COA	N8P-C9P-CAP-CBP
2	C	201	COA	P2A-O3A-P1A-O2A
2	A	201	COA	C3B-O3B-P3B-O7A
2	C	201	COA	C9P-CAP-CBP-CDP
2	A	201	COA	C3B-O3B-P3B-O8A
2	B	201	COA	C3B-O3B-P3B-O9A
2	C	201	COA	C3B-O3B-P3B-O9A
2	C	201	COA	OAP-CAP-CBP-CDP
2	C	201	COA	N4P-C5P-C6P-C7P
2	D	201	COA	CCP-O6A-P2A-O3A
2	D	201	COA	O4B-C4B-C5B-O5B
2	B	201	COA	P2A-O3A-P1A-O1A
2	B	201	COA	P2A-O3A-P1A-O2A
2	B	201	COA	O4B-C4B-C5B-O5B

There are no ring outliers.

4 monomers are involved in 29 short contacts:

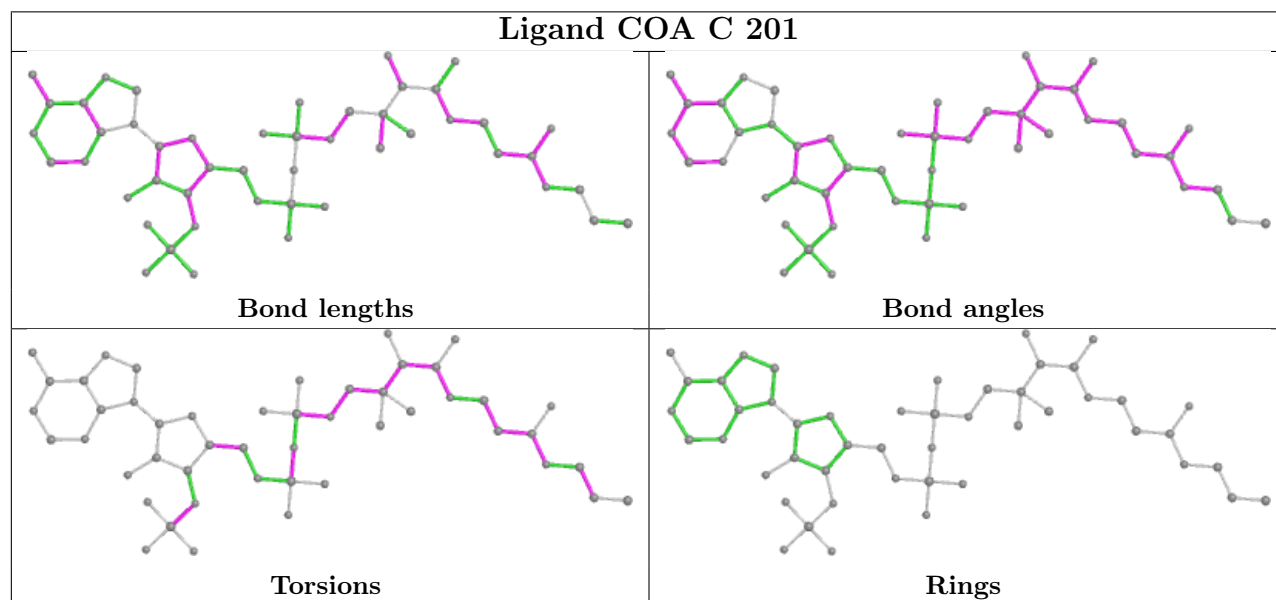
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	COA	9	0

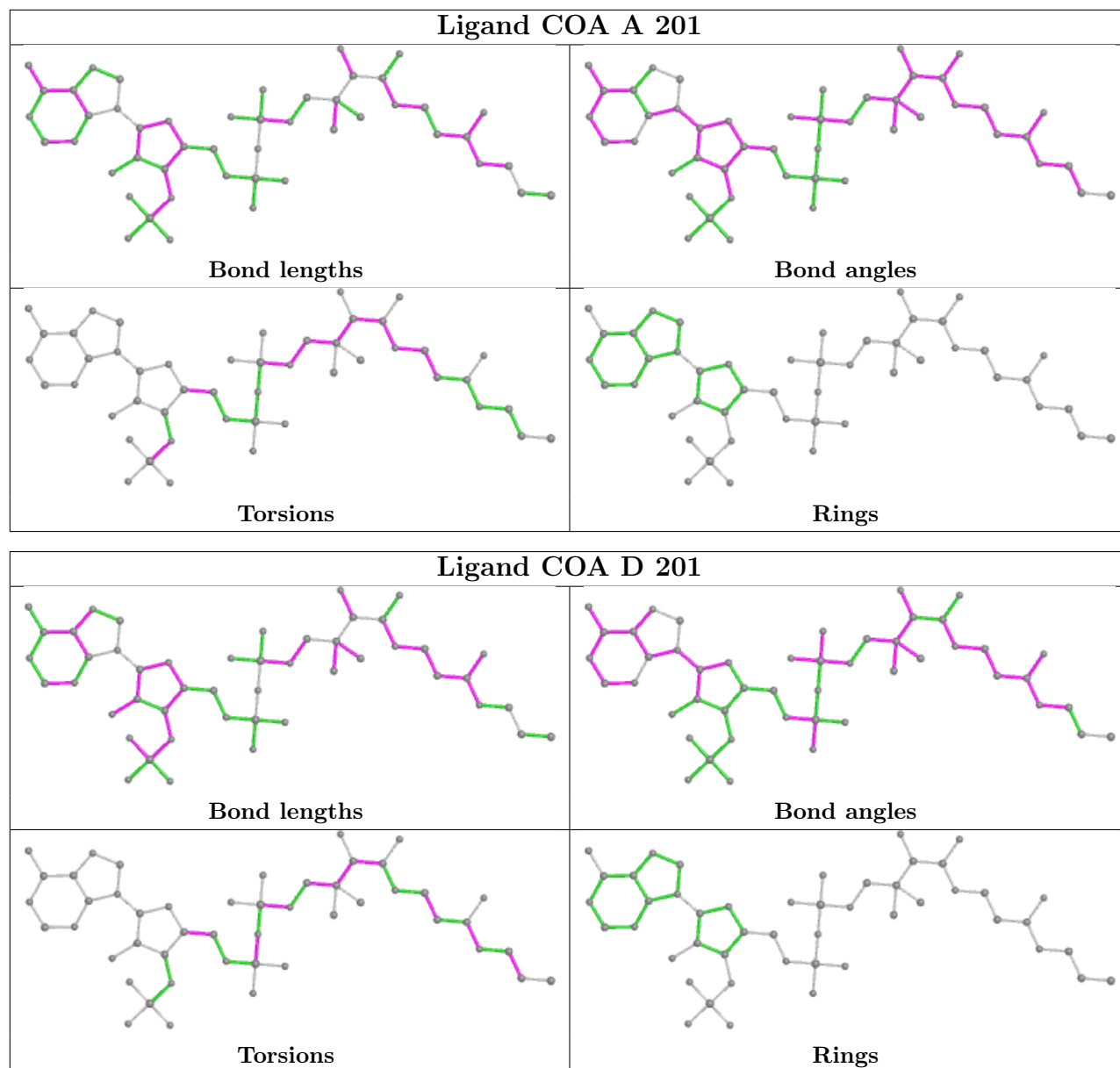
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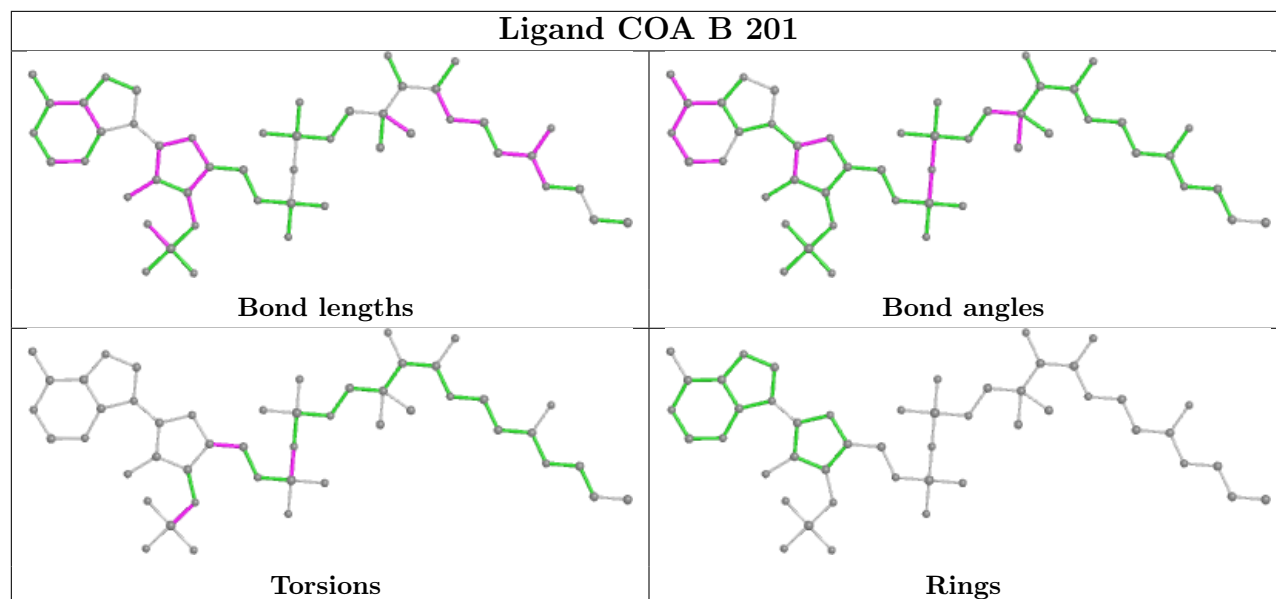
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	COA	9	0
2	D	201	COA	8	0
2	B	201	COA	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	185/189 (97%)	0.49	8 (4%) 35 33	13, 21, 35, 48	0
1	B	188/189 (99%)	0.46	7 (3%) 41 40	13, 19, 34, 47	0
1	C	187/189 (98%)	0.45	6 (3%) 47 46	13, 20, 36, 44	0
1	D	187/189 (98%)	0.47	8 (4%) 35 33	13, 20, 35, 46	0
All	All	747/756 (98%)	0.47	29 (3%) 39 38	13, 20, 36, 48	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	6.7
1	C	3	ARG	5.3
1	A	6	PRO	3.6
1	B	42	SER	3.3
1	D	174	HIS	3.3
1	C	4	PRO	3.2
1	D	3	ARG	3.0
1	A	59	GLU	2.9
1	B	189	GLY	2.9
1	D	188	SER	2.8
1	C	144	LEU	2.8
1	C	188	SER	2.8
1	B	35	ARG	2.7
1	B	188	SER	2.7
1	B	58	ARG	2.6
1	A	7	ILE	2.6
1	C	5	LEU	2.5
1	C	58	ARG	2.4
1	D	135	LEU	2.4
1	D	2	PHE	2.3
1	A	139	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	61	ARG	2.2
1	A	187	PHE	2.2
1	A	37	VAL	2.1
1	B	36	GLU	2.1
1	B	105	LEU	2.1
1	A	136	ARG	2.1
1	D	59	GLU	2.1
1	D	42	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

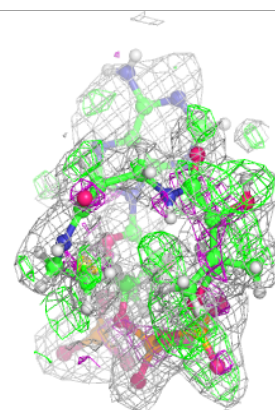
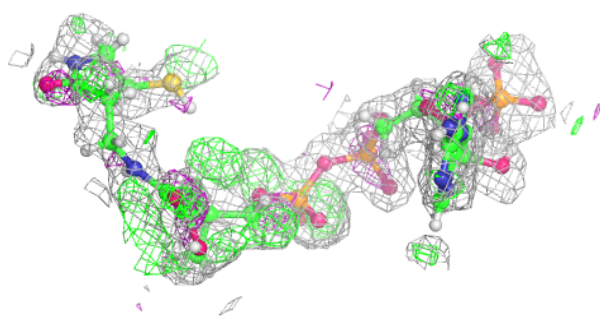
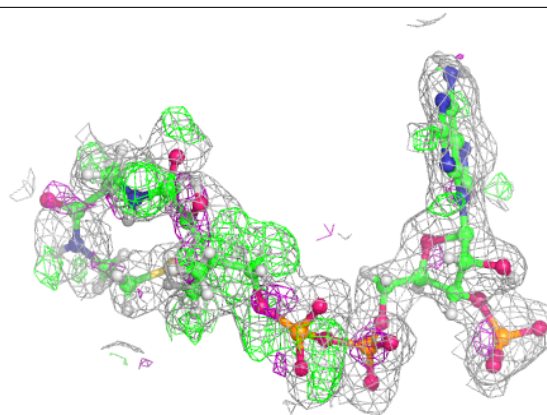
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COA	D	201	48/48	0.78	0.23	17,34,51,64	0
2	COA	C	201	48/48	0.80	0.25	11,41,55,65	0
2	COA	A	201	48/48	0.88	0.22	9,33,62,74	0
2	COA	B	201	48/48	0.95	0.11	12,20,33,37	0

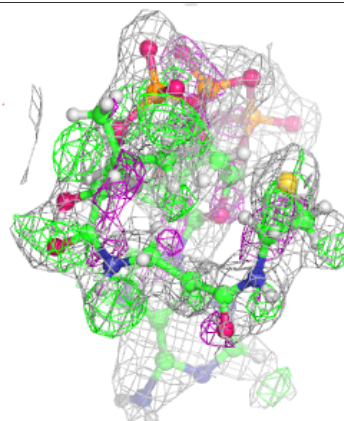
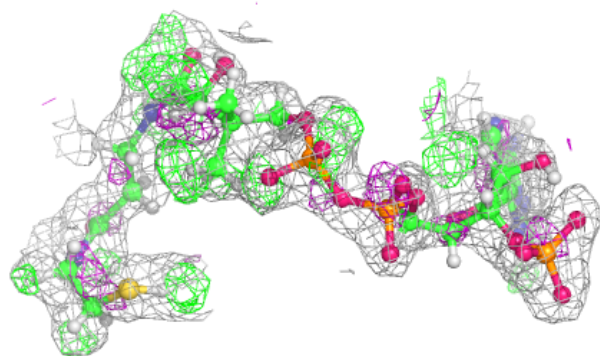
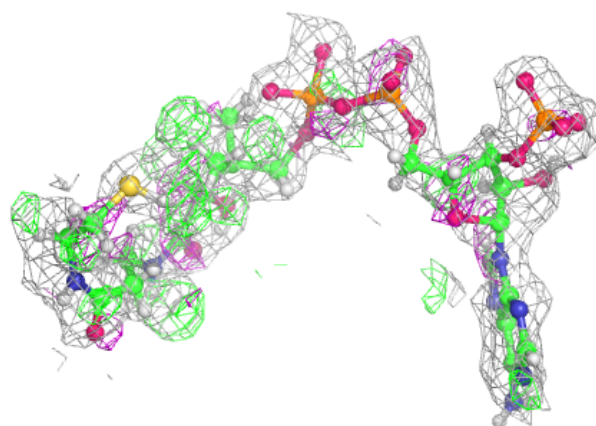
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA 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)

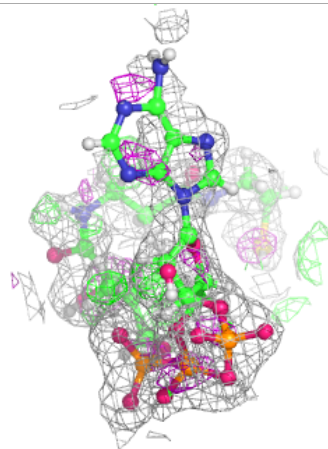
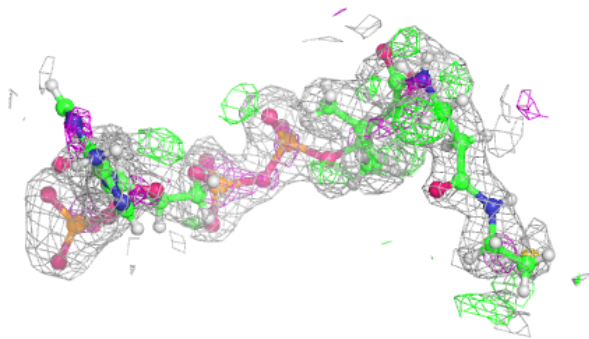
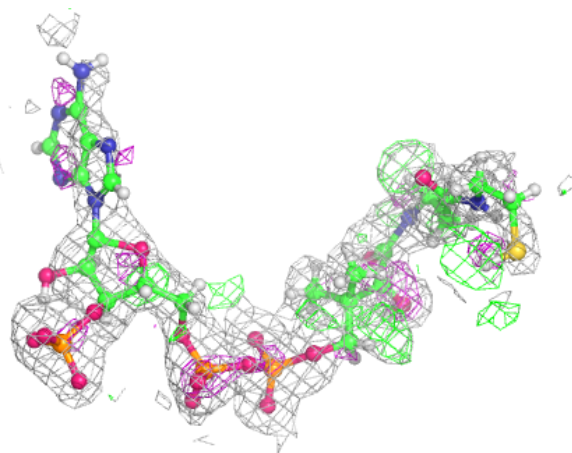
**Electron density around COA C 201:**

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



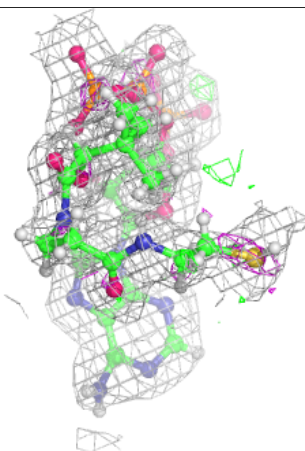
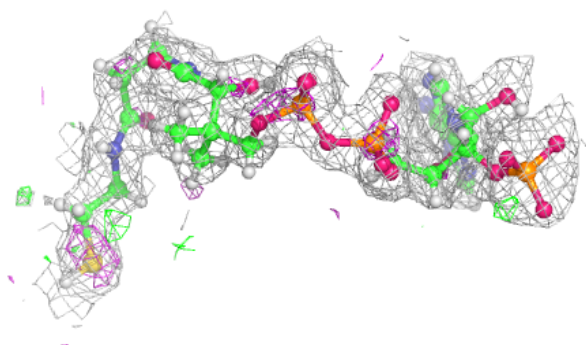
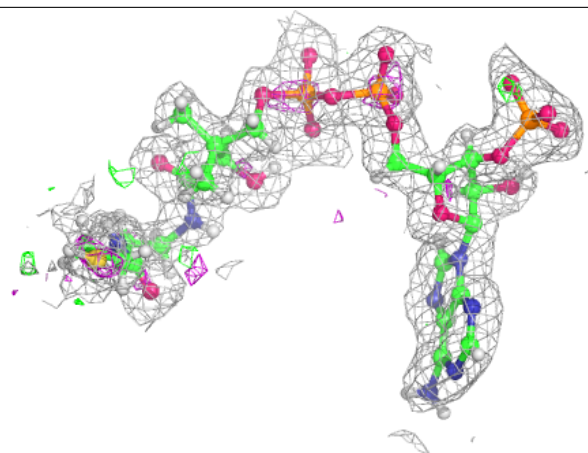
Electron density around COA A 201:

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



Electron density around COA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.