



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:54 PM EST

PDB ID : 5JFN  
Title : Crystal structure of Rhodopseudomonas palustris propionaldehyde dehydrogenase with bound CoA and acylated Cys330  
Authors : Zarzycki, J.; Sutter, M.; Kerfeld, C.A.  
Deposited on : 2016-04-19  
Resolution : 1.90 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

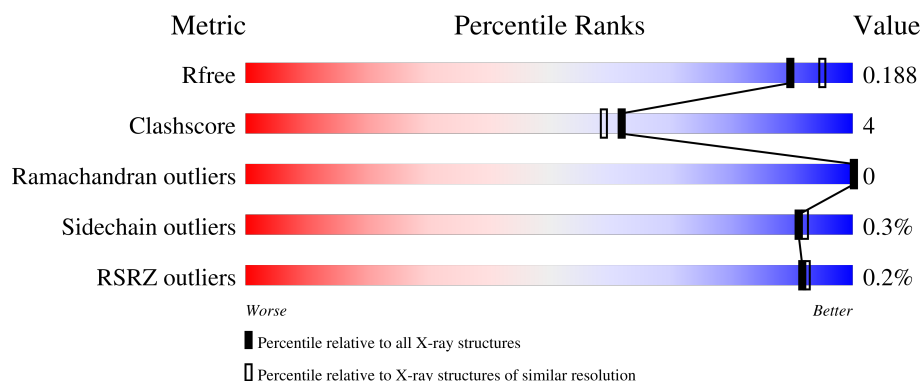
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 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	525	 78% 6% 16%
1	B	525	 78% 6% 16%
1	C	525	 79% 6% 15%
1	D	525	 77% 6% 16%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15377 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	2	0
			3308	2081	571	633	23			
1	B	439	Total	C	N	O	S	0	2	0
			3308	2081	571	633	23			
1	C	446	Total	C	N	O	S	0	2	0
			3357	2110	580	644	23			
1	D	439	Total	C	N	O	S	0	3	0
			3312	2084	571	634	23			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q21A49
A	2	ALA	-	expression tag	UNP Q21A49
A	3	TRP	-	expression tag	UNP Q21A49
A	4	SER	-	expression tag	UNP Q21A49
A	5	HIS	-	expression tag	UNP Q21A49
A	6	PRO	-	expression tag	UNP Q21A49
A	7	GLN	-	expression tag	UNP Q21A49
A	8	PHE	-	expression tag	UNP Q21A49
A	9	GLU	-	expression tag	UNP Q21A49
A	10	LYS	-	expression tag	UNP Q21A49
A	11	GLY	-	expression tag	UNP Q21A49
A	12	HIS	-	expression tag	UNP Q21A49
A	13	MET	-	expression tag	UNP Q21A49
A	14	ASN	-	expression tag	UNP Q21A49
A	15	ASP	-	expression tag	UNP Q21A49
A	16	ALA	-	expression tag	UNP Q21A49
A	17	ASN	-	expression tag	UNP Q21A49
A	18	ILE	-	expression tag	UNP Q21A49
A	19	ALA	-	expression tag	UNP Q21A49
A	20	ASP	-	expression tag	UNP Q21A49
A	21	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	VAL	-	expression tag	UNP Q21A49
A	23	THR	-	expression tag	UNP Q21A49
A	24	LYS	-	expression tag	UNP Q21A49
A	25	VAL	-	expression tag	UNP Q21A49
A	26	LEU	-	expression tag	UNP Q21A49
A	27	GLY	-	expression tag	UNP Q21A49
A	28	GLU	-	expression tag	UNP Q21A49
A	29	TYR	-	expression tag	UNP Q21A49
A	30	GLY	-	expression tag	UNP Q21A49
A	31	ALA	-	expression tag	UNP Q21A49
A	32	PRO	-	expression tag	UNP Q21A49
A	33	GLY	-	expression tag	UNP Q21A49
A	34	ALA	-	expression tag	UNP Q21A49
A	35	VAL	-	expression tag	UNP Q21A49
A	36	SER	-	expression tag	UNP Q21A49
A	37	VAL	-	expression tag	UNP Q21A49
A	38	ALA	-	expression tag	UNP Q21A49
A	39	ALA	-	expression tag	UNP Q21A49
A	40	LEU	-	expression tag	UNP Q21A49
A	41	THR	-	expression tag	UNP Q21A49
A	42	ALA	-	expression tag	UNP Q21A49
A	43	LYS	-	expression tag	UNP Q21A49
A	44	SER	-	expression tag	UNP Q21A49
A	45	PRO	-	expression tag	UNP Q21A49
A	46	ASP	-	expression tag	UNP Q21A49
A	47	GLY	-	expression tag	UNP Q21A49
A	48	LYS	-	expression tag	UNP Q21A49
A	49	SER	-	expression tag	UNP Q21A49
A	50	ASN	-	expression tag	UNP Q21A49
A	51	SER	-	expression tag	UNP Q21A49
A	52	SER	-	expression tag	UNP Q21A49
A	53	ALA	-	expression tag	UNP Q21A49
A	54	ASP	-	expression tag	UNP Q21A49
A	55	ALA	-	expression tag	UNP Q21A49
A	56	ASP	-	expression tag	UNP Q21A49
A	57	VAL	-	expression tag	UNP Q21A49
A	58	VAL	-	expression tag	UNP Q21A49
A	59	ALA	-	expression tag	UNP Q21A49
A	60	ARG	-	expression tag	UNP Q21A49
B	1	MET	-	initiating methionine	UNP Q21A49
B	2	ALA	-	expression tag	UNP Q21A49
B	3	TRP	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP Q21A49
B	5	HIS	-	expression tag	UNP Q21A49
B	6	PRO	-	expression tag	UNP Q21A49
B	7	GLN	-	expression tag	UNP Q21A49
B	8	PHE	-	expression tag	UNP Q21A49
B	9	GLU	-	expression tag	UNP Q21A49
B	10	LYS	-	expression tag	UNP Q21A49
B	11	GLY	-	expression tag	UNP Q21A49
B	12	HIS	-	expression tag	UNP Q21A49
B	13	MET	-	expression tag	UNP Q21A49
B	14	ASN	-	expression tag	UNP Q21A49
B	15	ASP	-	expression tag	UNP Q21A49
B	16	ALA	-	expression tag	UNP Q21A49
B	17	ASN	-	expression tag	UNP Q21A49
B	18	ILE	-	expression tag	UNP Q21A49
B	19	ALA	-	expression tag	UNP Q21A49
B	20	ASP	-	expression tag	UNP Q21A49
B	21	VAL	-	expression tag	UNP Q21A49
B	22	VAL	-	expression tag	UNP Q21A49
B	23	THR	-	expression tag	UNP Q21A49
B	24	LYS	-	expression tag	UNP Q21A49
B	25	VAL	-	expression tag	UNP Q21A49
B	26	LEU	-	expression tag	UNP Q21A49
B	27	GLY	-	expression tag	UNP Q21A49
B	28	GLU	-	expression tag	UNP Q21A49
B	29	TYR	-	expression tag	UNP Q21A49
B	30	GLY	-	expression tag	UNP Q21A49
B	31	ALA	-	expression tag	UNP Q21A49
B	32	PRO	-	expression tag	UNP Q21A49
B	33	GLY	-	expression tag	UNP Q21A49
B	34	ALA	-	expression tag	UNP Q21A49
B	35	VAL	-	expression tag	UNP Q21A49
B	36	SER	-	expression tag	UNP Q21A49
B	37	VAL	-	expression tag	UNP Q21A49
B	38	ALA	-	expression tag	UNP Q21A49
B	39	ALA	-	expression tag	UNP Q21A49
B	40	LEU	-	expression tag	UNP Q21A49
B	41	THR	-	expression tag	UNP Q21A49
B	42	ALA	-	expression tag	UNP Q21A49
B	43	LYS	-	expression tag	UNP Q21A49
B	44	SER	-	expression tag	UNP Q21A49
B	45	PRO	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	46	ASP	-	expression tag	UNP Q21A49
B	47	GLY	-	expression tag	UNP Q21A49
B	48	LYS	-	expression tag	UNP Q21A49
B	49	SER	-	expression tag	UNP Q21A49
B	50	ASN	-	expression tag	UNP Q21A49
B	51	SER	-	expression tag	UNP Q21A49
B	52	SER	-	expression tag	UNP Q21A49
B	53	ALA	-	expression tag	UNP Q21A49
B	54	ASP	-	expression tag	UNP Q21A49
B	55	ALA	-	expression tag	UNP Q21A49
B	56	ASP	-	expression tag	UNP Q21A49
B	57	VAL	-	expression tag	UNP Q21A49
B	58	VAL	-	expression tag	UNP Q21A49
B	59	ALA	-	expression tag	UNP Q21A49
B	60	ARG	-	expression tag	UNP Q21A49
C	1	MET	-	initiating methionine	UNP Q21A49
C	2	ALA	-	expression tag	UNP Q21A49
C	3	TRP	-	expression tag	UNP Q21A49
C	4	SER	-	expression tag	UNP Q21A49
C	5	HIS	-	expression tag	UNP Q21A49
C	6	PRO	-	expression tag	UNP Q21A49
C	7	GLN	-	expression tag	UNP Q21A49
C	8	PHE	-	expression tag	UNP Q21A49
C	9	GLU	-	expression tag	UNP Q21A49
C	10	LYS	-	expression tag	UNP Q21A49
C	11	GLY	-	expression tag	UNP Q21A49
C	12	HIS	-	expression tag	UNP Q21A49
C	13	MET	-	expression tag	UNP Q21A49
C	14	ASN	-	expression tag	UNP Q21A49
C	15	ASP	-	expression tag	UNP Q21A49
C	16	ALA	-	expression tag	UNP Q21A49
C	17	ASN	-	expression tag	UNP Q21A49
C	18	ILE	-	expression tag	UNP Q21A49
C	19	ALA	-	expression tag	UNP Q21A49
C	20	ASP	-	expression tag	UNP Q21A49
C	21	VAL	-	expression tag	UNP Q21A49
C	22	VAL	-	expression tag	UNP Q21A49
C	23	THR	-	expression tag	UNP Q21A49
C	24	LYS	-	expression tag	UNP Q21A49
C	25	VAL	-	expression tag	UNP Q21A49
C	26	LEU	-	expression tag	UNP Q21A49
C	27	GLY	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLU	-	expression tag	UNP Q21A49
C	29	TYR	-	expression tag	UNP Q21A49
C	30	GLY	-	expression tag	UNP Q21A49
C	31	ALA	-	expression tag	UNP Q21A49
C	32	PRO	-	expression tag	UNP Q21A49
C	33	GLY	-	expression tag	UNP Q21A49
C	34	ALA	-	expression tag	UNP Q21A49
C	35	VAL	-	expression tag	UNP Q21A49
C	36	SER	-	expression tag	UNP Q21A49
C	37	VAL	-	expression tag	UNP Q21A49
C	38	ALA	-	expression tag	UNP Q21A49
C	39	ALA	-	expression tag	UNP Q21A49
C	40	LEU	-	expression tag	UNP Q21A49
C	41	THR	-	expression tag	UNP Q21A49
C	42	ALA	-	expression tag	UNP Q21A49
C	43	LYS	-	expression tag	UNP Q21A49
C	44	SER	-	expression tag	UNP Q21A49
C	45	PRO	-	expression tag	UNP Q21A49
C	46	ASP	-	expression tag	UNP Q21A49
C	47	GLY	-	expression tag	UNP Q21A49
C	48	LYS	-	expression tag	UNP Q21A49
C	49	SER	-	expression tag	UNP Q21A49
C	50	ASN	-	expression tag	UNP Q21A49
C	51	SER	-	expression tag	UNP Q21A49
C	52	SER	-	expression tag	UNP Q21A49
C	53	ALA	-	expression tag	UNP Q21A49
C	54	ASP	-	expression tag	UNP Q21A49
C	55	ALA	-	expression tag	UNP Q21A49
C	56	ASP	-	expression tag	UNP Q21A49
C	57	VAL	-	expression tag	UNP Q21A49
C	58	VAL	-	expression tag	UNP Q21A49
C	59	ALA	-	expression tag	UNP Q21A49
C	60	ARG	-	expression tag	UNP Q21A49
D	1	MET	-	initiating methionine	UNP Q21A49
D	2	ALA	-	expression tag	UNP Q21A49
D	3	TRP	-	expression tag	UNP Q21A49
D	4	SER	-	expression tag	UNP Q21A49
D	5	HIS	-	expression tag	UNP Q21A49
D	6	PRO	-	expression tag	UNP Q21A49
D	7	GLN	-	expression tag	UNP Q21A49
D	8	PHE	-	expression tag	UNP Q21A49
D	9	GLU	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	10	LYS	-	expression tag	UNP Q21A49
D	11	GLY	-	expression tag	UNP Q21A49
D	12	HIS	-	expression tag	UNP Q21A49
D	13	MET	-	expression tag	UNP Q21A49
D	14	ASN	-	expression tag	UNP Q21A49
D	15	ASP	-	expression tag	UNP Q21A49
D	16	ALA	-	expression tag	UNP Q21A49
D	17	ASN	-	expression tag	UNP Q21A49
D	18	ILE	-	expression tag	UNP Q21A49
D	19	ALA	-	expression tag	UNP Q21A49
D	20	ASP	-	expression tag	UNP Q21A49
D	21	VAL	-	expression tag	UNP Q21A49
D	22	VAL	-	expression tag	UNP Q21A49
D	23	THR	-	expression tag	UNP Q21A49
D	24	LYS	-	expression tag	UNP Q21A49
D	25	VAL	-	expression tag	UNP Q21A49
D	26	LEU	-	expression tag	UNP Q21A49
D	27	GLY	-	expression tag	UNP Q21A49
D	28	GLU	-	expression tag	UNP Q21A49
D	29	TYR	-	expression tag	UNP Q21A49
D	30	GLY	-	expression tag	UNP Q21A49
D	31	ALA	-	expression tag	UNP Q21A49
D	32	PRO	-	expression tag	UNP Q21A49
D	33	GLY	-	expression tag	UNP Q21A49
D	34	ALA	-	expression tag	UNP Q21A49
D	35	VAL	-	expression tag	UNP Q21A49
D	36	SER	-	expression tag	UNP Q21A49
D	37	VAL	-	expression tag	UNP Q21A49
D	38	ALA	-	expression tag	UNP Q21A49
D	39	ALA	-	expression tag	UNP Q21A49
D	40	LEU	-	expression tag	UNP Q21A49
D	41	THR	-	expression tag	UNP Q21A49
D	42	ALA	-	expression tag	UNP Q21A49
D	43	LYS	-	expression tag	UNP Q21A49
D	44	SER	-	expression tag	UNP Q21A49
D	45	PRO	-	expression tag	UNP Q21A49
D	46	ASP	-	expression tag	UNP Q21A49
D	47	GLY	-	expression tag	UNP Q21A49
D	48	LYS	-	expression tag	UNP Q21A49
D	49	SER	-	expression tag	UNP Q21A49
D	50	ASN	-	expression tag	UNP Q21A49
D	51	SER	-	expression tag	UNP Q21A49

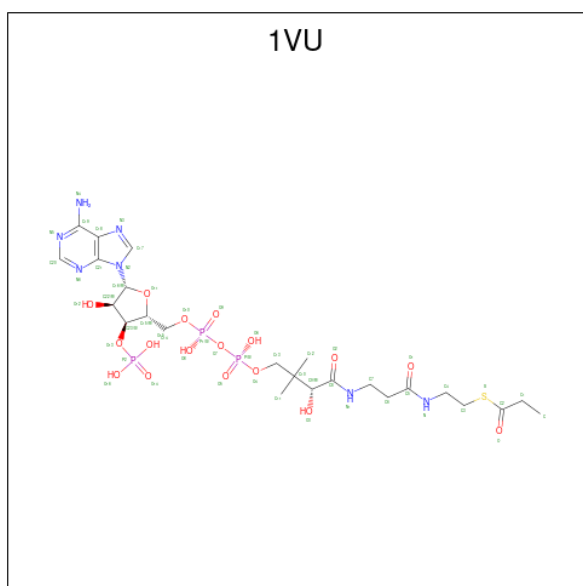
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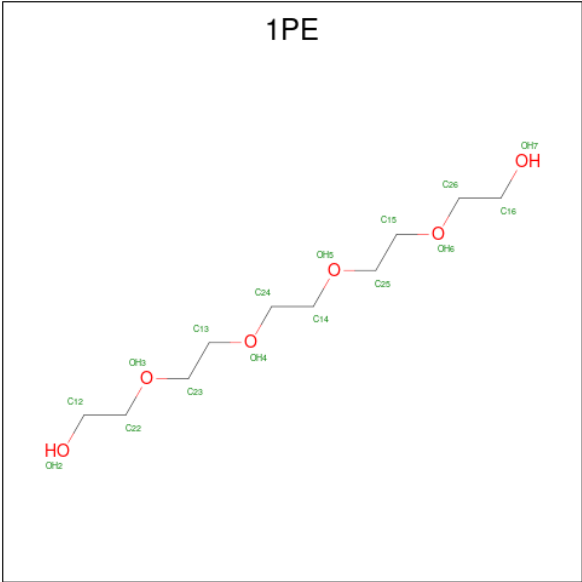
Chain	Residue	Modelled	Actual	Comment	Reference
D	52	SER	-	expression tag	UNP Q21A49
D	53	ALA	-	expression tag	UNP Q21A49
D	54	ASP	-	expression tag	UNP Q21A49
D	55	ALA	-	expression tag	UNP Q21A49
D	56	ASP	-	expression tag	UNP Q21A49
D	57	VAL	-	expression tag	UNP Q21A49
D	58	VAL	-	expression tag	UNP Q21A49
D	59	ALA	-	expression tag	UNP Q21A49
D	60	ARG	-	expression tag	UNP Q21A49

- Molecule 2 is propionyl Coenzyme A (three-letter code: 1VU) (formula:  $C_{24}H_{40}N_7O_{17}P_3S$ ).



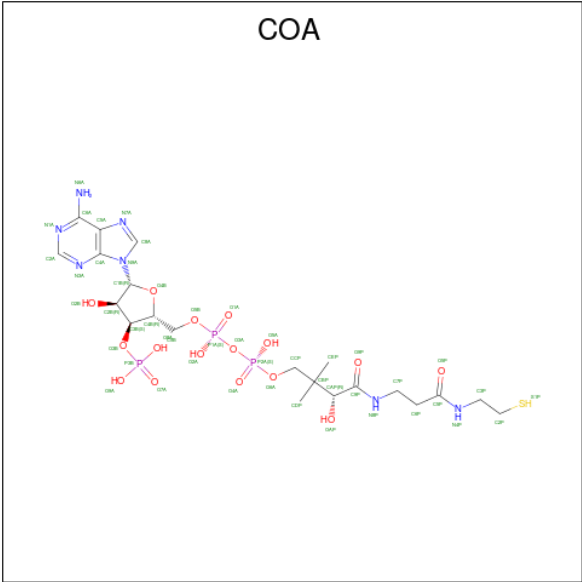
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			52	24	7	17	3	1	

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 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
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

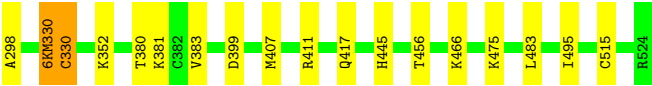
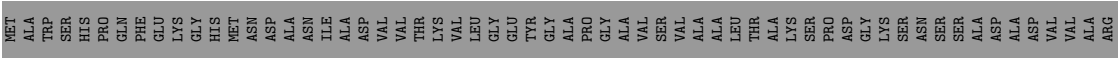
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	480	Total	O	0	0
			480	480		
5	B	431	Total	O	0	0
			431	431		
5	C	500	Total	O	0	0
			500	500		
5	D	373	Total	O	0	0
			373	373		





● Molecule 1: Aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.19Å 106.45Å 125.73Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	39.20 – 1.90 39.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.20-1.90) 92.7 (39.20-1.90)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, $R_{free}$	0.162 , 0.186 0.163 , 0.188	Depositor DCC
$R_{free}$ test set	1994 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: 1VU, 1PE, 6KM, 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	0.31	0/3344	0.50	0/4532
1	B	0.31	0/3344	0.50	0/4532
1	C	0.31	0/3393	0.49	0/4595
1	D	0.29	0/3351	0.48	0/4542
All	All	0.30	0/13432	0.49	0/18201

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3308	0	3387	22	0
1	B	3308	0	3387	28	0
1	C	3357	0	3436	25	0
1	D	3312	0	3394	26	0
2	A	52	0	38	7	0
3	A	16	0	22	1	0
3	B	32	0	44	2	0
3	C	32	0	44	1	0
3	D	32	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	48	0	32	6	0
4	C	48	0	32	7	0
4	D	48	0	32	8	0
5	A	480	0	0	3	1
5	B	431	0	0	8	1
5	C	500	0	0	15	1
5	D	373	0	0	7	0
All	All	15377	0	13892	107	2

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 4.

All (107) 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)
4:D:601:COA:C1B	4:D:601:COA:O4B	1.65	1.24
4:C:601:COA:O4B	4:C:601:COA:C1B	1.65	1.23
4:B:601:COA:O4B	4:B:601:COA:C1B	1.65	1.09
2:A:601:1VU:O16	5:A:701:HOH:O	1.84	0.92
1:A:199:ASN:HD22	2:A:601:1VU:H34	1.40	0.85
1:D:399:ASP:OD2	5:D:701:HOH:O	1.95	0.83
1:C:111:CYS:SG	5:C:1069:HOH:O	2.37	0.83
1:A:515:CYS:SG	1:C:475:LYS:NZ	2.52	0.82
1:D:142:GLU:OE1	5:D:702:HOH:O	1.99	0.80
1:B:475:LYS:NZ	1:D:515:CYS:SG	2.53	0.78
1:C:277:THR:HG22	4:C:601:COA:H31	1.70	0.74
4:C:601:COA:O7A	5:C:701:HOH:O	2.07	0.72
1:A:483:LEU:HD11	2:A:601:1VU:H38	1.70	0.71
1:B:196:PRO:HG3	4:B:601:COA:H22	1.69	0.71
1:B:515:CYS:SG	1:D:475:LYS:NZ	2.58	0.69
1:B:499:THR:HA	1:D:292:LYS:HG2	1.75	0.68
1:C:259:ILE:HA	4:C:601:COA:H2A	1.74	0.68
1:B:240:LYS:HD3	3:B:603:1PE:H141	1.74	0.68
1:D:90:VAL:O	5:D:703:HOH:O	2.13	0.67
1:B:198:THR:HG21	1:B:421:MET:HE1	1.77	0.66
3:B:603:1PE:H142	5:B:1026:HOH:O	1.99	0.62
1:D:223:HIS:NE2	4:D:601:COA:O2A	2.32	0.62
1:D:466:LYS:HE2	5:D:936:HOH:O	1.98	0.62
1:B:86:VAL:N	5:B:706:HOH:O	2.33	0.61
4:D:601:COA:S1P	5:D:952:HOH:O	2.56	0.60
1:B:225:ARG:NE	5:B:702:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLN:NE2	5:B:705:HOH:O	2.29	0.60
1:C:483:LEU:HD21	1:C:495:ILE:HD11	1.84	0.60
1:A:438:ASP:HB3	3:A:602:1PE:H221	1.84	0.59
3:C:602:1PE:OH2	5:C:703:HOH:O	2.17	0.59
1:D:227:ARG:NH2	1:D:255:GLU:OE2	2.38	0.57
1:D:411:ARG:HH22	3:D:602:1PE:H241	1.68	0.57
1:C:434:ASP:OD2	5:C:704:HOH:O	2.17	0.56
1:C:43:LYS:HA	5:C:921:HOH:O	2.05	0.56
4:D:601:COA:O1A	4:D:601:COA:H4B	2.05	0.56
1:B:172:ASP:OD2	1:B:512[B]:ARG:NH1	2.39	0.56
1:B:483:LEU:HD21	1:B:495:ILE:HD11	1.87	0.56
1:A:86:VAL:N	5:A:705:HOH:O	2.39	0.55
1:A:227:ARG:NH2	1:A:256:LYS:HG2	2.22	0.55
1:D:144:THR:HB	1:D:146:MET:HE2	1.89	0.55
1:A:227:ARG:HG3	1:A:257:PRO:HD2	1.89	0.54
1:A:221:SER:HG	1:A:262:THR:HG1	1.54	0.54
1:C:368:GLN:NE2	5:C:702:HOH:O	2.10	0.54
4:D:601:COA:H8A	5:D:833:HOH:O	2.08	0.54
1:B:172:ASP:HB2	1:B:183:VAL:HB	1.90	0.54
1:D:196:PRO:HG3	4:D:601:COA:H22	1.90	0.53
1:D:483:LEU:HD21	1:D:495:ILE:HD11	1.90	0.52
1:C:498:PRO:HG3	5:C:1025:HOH:O	2.10	0.51
1:C:135:LYS:NZ	5:C:715:HOH:O	2.44	0.51
1:D:381:LYS:HG3	5:D:744:HOH:O	2.11	0.51
1:B:466:LYS:HE2	5:B:893:HOH:O	2.11	0.51
1:B:287:LEU:HD23	1:B:293:ALA:HB3	1.94	0.50
1:B:298:ALA:HA	1:B:330[A]:6KM:CA3	2.42	0.49
1:C:248:GLU:OE2	5:C:705:HOH:O	2.20	0.49
1:A:120:VAL:HG13	1:A:209:ILE:HG23	1.95	0.49
1:B:375:LYS:HG2	1:B:375:LYS:O	2.12	0.49
1:D:172:ASP:HB2	1:D:183:VAL:HB	1.94	0.49
1:A:155:LYS:NZ	1:A:199:ASN:OD1	2.19	0.48
1:B:364:LEU:O	1:B:368:GLN:HG3	2.13	0.48
1:D:197[B]:THR:HG21	1:D:225:ARG:HB2	1.95	0.48
1:B:497:GLY:HA3	5:B:756:HOH:O	2.15	0.47
1:D:120:VAL:HG13	1:D:209:ILE:HG23	1.97	0.47
1:B:198:THR:HG21	1:B:421:MET:CE	2.44	0.46
1:C:196:PRO:HG3	4:C:601:COA:H22	1.97	0.46
1:D:380:THR:HG23	4:D:601:COA:H121	1.95	0.46
3:D:602:1PE:H262	3:D:602:1PE:H251	1.65	0.46
1:A:194:ILE:HG23	2:A:601:1VU:N4	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:CD	5:C:705:HOH:O	2.56	0.45
1:A:199:ASN:ND2	2:A:601:1VU:H34	2.21	0.45
1:A:141:VAL:HG23	1:A:152:LYS:HD2	1.98	0.44
1:A:483:LEU:HD21	1:A:495:ILE:HD11	2.00	0.44
1:C:368:GLN:HB3	5:C:702:HOH:O	2.17	0.44
1:A:277:THR:HG22	2:A:601:1VU:H32	1.99	0.44
1:B:499:THR:HA	1:D:292:LYS:CG	2.45	0.44
1:C:141:VAL:HG23	1:C:152:LYS:HD2	1.98	0.44
1:D:199:ASN:ND2	4:D:601:COA:S1P	2.91	0.44
1:B:196:PRO:HB3	4:B:601:COA:HN4	1.82	0.44
1:C:256:LYS:HE2	5:C:980:HOH:O	2.18	0.44
1:A:276:ALA:HB2	1:A:286:VAL:HG11	1.98	0.43
1:A:287:LEU:HD23	1:A:293:ALA:HB3	2.00	0.43
1:A:461:LEU:HD22	1:A:475:LYS:HG2	2.00	0.43
1:D:298:ALA:HA	1:D:330[A]:6KM:CA3	2.47	0.43
1:A:266:MET:HB3	1:A:289:THR:HG21	2.01	0.43
1:A:330[A]:6KM:N	2:A:601:1VU:H40	2.34	0.43
1:A:172:ASP:HB2	1:A:183:VAL:HB	2.00	0.43
1:A:417:GLN:O	1:A:445:HIS:HE1	2.02	0.42
1:B:197:THR:HG22	4:B:601:COA:H131	2.00	0.42
1:B:297:GLY:HA2	5:B:704:HOH:O	2.19	0.42
1:C:431:GLU:OE2	5:C:706:HOH:O	2.22	0.42
1:C:364:LEU:O	1:C:368:GLN:HG3	2.19	0.42
5:A:1045:HOH:O	1:C:174:PHE:HB3	2.18	0.42
1:B:146:MET:HE1	4:B:601:COA:H141	2.01	0.42
1:B:330[A]:6KM:CA1	4:B:601:COA:H32	2.49	0.42
1:D:146:MET:HG2	1:D:383:VAL:O	2.19	0.41
4:C:601:COA:H141	4:C:601:COA:HN8	1.86	0.41
1:B:446:ASP:OD2	1:D:272:ARG:NH2	2.49	0.41
1:C:459:ARG:CZ	1:D:456:THR:HG21	2.50	0.41
1:B:276:ALA:HB2	1:B:286:VAL:HG11	2.02	0.41
1:C:333:GLU:HG3	1:C:452:ILE:HD13	2.01	0.41
5:B:781:HOH:O	1:C:466:LYS:HE3	2.21	0.41
1:C:146:MET:HG2	1:C:383:VAL:O	2.20	0.41
4:C:601:COA:H8A	5:C:835:HOH:O	2.20	0.41
1:D:417:GLN:O	1:D:445:HIS:HE1	2.04	0.41
1:B:277:THR:HA	1:B:296:ALA:HB3	2.03	0.40
1:C:135:LYS:O	1:C:139:MET:HB2	2.22	0.40
1:C:512[B]:ARG:NH1	5:C:711:HOH:O	2.35	0.40
1:D:352:LYS:HB3	1:D:352:LYS:HE3	1.77	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:913:HOH:O	5:C:1003:HOH:O[2_546]	1.88	0.32
5:A:987:HOH:O	5:A:1082:HOH:O[2_545]	2.06	0.14

## 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	437/525 (83%)	432 (99%)	5 (1%)	0	100	100
1	B	437/525 (83%)	432 (99%)	5 (1%)	0	100	100
1	C	442/525 (84%)	437 (99%)	5 (1%)	0	100	100
1	D	438/525 (83%)	433 (99%)	5 (1%)	0	100	100
All	All	1754/2100 (84%)	1734 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	359/417 (86%)	359 (100%)	0	100	100
1	B	359/417 (86%)	358 (100%)	1 (0%)	91	92
1	C	365/417 (88%)	364 (100%)	1 (0%)	91	92
1	D	360/417 (86%)	358 (99%)	2 (1%)	84	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1443/1668 (86%)	1439 (100%)	4 (0%)	91	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	352	LYS
1	C	341	GLN
1	D	292	LYS
1	D	407	MET

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

Mol	Chain	Res	Type
1	C	106	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	6KM	D	330[A]	1	8,9,10	1.03	1 (12%)	5,10,12	2.56	3 (60%)
1	6KM	B	330[A]	1	8,9,10	0.93	0	5,10,12	2.57	3 (60%)
1	6KM	A	330[A]	1	8,9,10	1.03	1 (12%)	5,10,12	3.38	3 (60%)
1	6KM	C	330[A]	1	8,9,10	1.13	1 (12%)	5,10,12	3.34	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6KM	D	330[A]	1	-	5/7/9/11	-
1	6KM	B	330[A]	1	-	3/7/9/11	-
1	6KM	A	330[A]	1	-	3/7/9/11	-
1	6KM	C	330[A]	1	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330[A]	6KM	CA1-SG	2.44	1.82	1.76
1	D	330[A]	6KM	CA1-SG	2.41	1.81	1.76
1	A	330[A]	6KM	CA1-SG	2.35	1.81	1.76

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330[A]	6KM	CB-SG-CA1	5.32	108.07	100.76
1	C	330[A]	6KM	CA2-CA1-SG	5.08	119.97	113.56
1	A	330[A]	6KM	CA2-CA1-SG	4.38	119.09	113.56
1	C	330[A]	6KM	CB-SG-CA1	4.30	106.67	100.76
1	B	330[A]	6KM	CB-SG-CA1	4.05	106.33	100.76
1	D	330[A]	6KM	CA2-CA1-SG	3.84	118.41	113.56
1	D	330[A]	6KM	CB-SG-CA1	3.08	104.99	100.76
1	B	330[A]	6KM	CA2-CA1-SG	2.81	117.11	113.56
1	C	330[A]	6KM	OA1-CA1-CA2	-2.78	119.56	123.72
1	D	330[A]	6KM	OA1-CA1-CA2	-2.52	119.94	123.72
1	B	330[A]	6KM	OA1-CA1-CA2	-2.25	120.35	123.72
1	A	330[A]	6KM	OA1-CA1-CA2	-2.13	120.53	123.72

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	330[A]	6KM	CA2-CA1-SG-CB
1	A	330[A]	6KM	OA1-CA1-SG-CB
1	A	330[A]	6KM	CA-CB-SG-CA1
1	B	330[A]	6KM	CA2-CA1-SG-CB
1	B	330[A]	6KM	OA1-CA1-SG-CB
1	C	330[A]	6KM	CA2-CA1-SG-CB
1	C	330[A]	6KM	OA1-CA1-SG-CB

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Mol	Chain	Res	Type	Atoms
1	D	330[A]	6KM	SG-CA1-CA2-CA3
1	D	330[A]	6KM	CA2-CA1-SG-CB
1	D	330[A]	6KM	OA1-CA1-SG-CB
1	D	330[A]	6KM	CA-CB-SG-CA1
1	B	330[A]	6KM	CA-CB-SG-CA1
1	C	330[A]	6KM	CA-CB-SG-CA1
1	D	330[A]	6KM	OA1-CA1-CA2-CA3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	330[A]	6KM	1	0
1	B	330[A]	6KM	2	0
1	A	330[A]	6KM	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	$\# Z  > 2$
3	1PE	D	603	-	15,15,15	0.64	0	14,14,14	0.22	0
4	COA	B	601	-	43,50,50	3.64	13 (30%)	56,75,75	1.96	9 (16%)
3	1PE	B	603	-	15,15,15	0.65	0	14,14,14	0.23	0
3	1PE	A	602	-	15,15,15	0.64	0	14,14,14	0.22	0
3	1PE	D	602	-	15,15,15	0.64	0	14,14,14	0.23	0
3	1PE	C	602	-	15,15,15	0.65	0	14,14,14	0.26	0
2	1VU	A	601	-	48,54,54	2.99	12 (25%)	60,80,80	1.66	9 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1PE	C	603	-	15,15,15	0.66	0	14,14,14	0.25	0
4	COA	C	601	-	43,50,50	3.67	13 (30%)	56,75,75	1.99	10 (17%)
4	COA	D	601	-	43,50,50	3.71	14 (32%)	56,75,75	1.90	10 (17%)
3	1PE	B	602	-	15,15,15	0.67	0	14,14,14	0.58	0

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
3	1PE	D	603	-	-	2/13/13/13	-
4	COA	B	601	-	-	10/44/64/64	0/3/3/3
3	1PE	B	603	-	-	3/13/13/13	-
3	1PE	A	602	-	-	7/13/13/13	-
3	1PE	D	602	-	-	5/13/13/13	-
3	1PE	C	602	-	-	2/13/13/13	-
2	1VU	A	601	-	-	18/49/69/69	0/3/3/3
3	1PE	C	603	-	-	2/13/13/13	-
4	COA	C	601	-	-	13/44/64/64	0/3/3/3
4	COA	D	601	-	-	17/44/64/64	0/3/3/3
3	1PE	B	602	-	-	7/13/13/13	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	COA	O4B-C1B	18.66	1.65	1.40
4	D	601	COA	O4B-C1B	18.59	1.65	1.40
4	B	601	COA	O4B-C1B	18.54	1.65	1.40
2	A	601	1VU	O11-C16	14.93	1.60	1.40
4	D	601	COA	C9P-N8P	6.80	1.49	1.33
4	C	601	COA	C9P-N8P	6.54	1.48	1.33
4	B	601	COA	C9P-N8P	6.38	1.48	1.33
4	C	601	COA	O4B-C4B	-6.33	1.30	1.45
4	D	601	COA	O4B-C4B	-6.29	1.31	1.45
4	B	601	COA	O4B-C4B	-6.11	1.31	1.45
2	A	601	1VU	O11-C15	-5.83	1.32	1.45
2	A	601	1VU	C13-C10	5.37	1.61	1.52
2	A	601	1VU	C5-N	5.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	COA	CCP-CBP	5.03	1.60	1.52
4	B	601	COA	CCP-CBP	4.93	1.60	1.52
4	D	601	COA	CCP-CBP	4.70	1.60	1.52
2	A	601	1VU	C8-N1	4.43	1.44	1.33
4	C	601	COA	C6A-N6A	4.08	1.48	1.34
4	D	601	COA	C6A-N6A	4.02	1.48	1.34
4	D	601	COA	C5P-N4P	4.01	1.42	1.33
4	B	601	COA	C6A-N6A	3.97	1.48	1.34
4	B	601	COA	O9P-C9P	-3.87	1.16	1.23
4	D	601	COA	O9P-C9P	-3.87	1.16	1.23
4	C	601	COA	C5P-N4P	3.76	1.42	1.33
4	D	601	COA	C1B-N9A	-3.76	1.40	1.49
4	B	601	COA	C5P-N4P	3.74	1.42	1.33
4	C	601	COA	O9P-C9P	-3.72	1.16	1.23
2	A	601	1VU	P1-O7	3.55	1.63	1.59
4	B	601	COA	C1B-N9A	-3.50	1.41	1.49
2	A	601	1VU	C19-N4	3.48	1.46	1.34
4	C	601	COA	C1B-N9A	-3.47	1.41	1.49
4	D	601	COA	C2A-N3A	3.30	1.37	1.32
4	B	601	COA	C2A-N3A	3.23	1.37	1.32
2	A	601	1VU	C16-N2	-3.22	1.42	1.49
4	C	601	COA	C2A-N3A	3.20	1.37	1.32
2	A	601	1VU	P-O7	3.01	1.62	1.59
2	A	601	1VU	O3-C9	-2.81	1.37	1.42
2	A	601	1VU	C20-N6	2.78	1.36	1.32
4	B	601	COA	O3B-C3B	-2.64	1.35	1.44
4	D	601	COA	C6P-C5P	2.63	1.56	1.51
4	D	601	COA	O3B-C3B	-2.55	1.35	1.44
4	D	601	COA	P1A-O3A	-2.48	1.56	1.59
4	B	601	COA	OAP-CAP	-2.48	1.37	1.42
4	D	601	COA	OAP-CAP	-2.47	1.38	1.42
4	C	601	COA	O3B-C3B	-2.45	1.35	1.44
4	C	601	COA	C6P-C5P	2.40	1.56	1.51
4	B	601	COA	C6P-C5P	2.36	1.56	1.51
4	C	601	COA	OAP-CAP	-2.36	1.38	1.42
2	A	601	1VU	O13-C23	-2.28	1.36	1.44
4	C	601	COA	P3B-O8A	-2.22	1.46	1.54
4	D	601	COA	P3B-O8A	-2.22	1.46	1.54
4	B	601	COA	P3B-O8A	-2.19	1.46	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	COA	C5A-C6A-N6A	6.97	130.93	120.31
4	B	601	COA	C5A-C6A-N6A	6.71	130.53	120.31
4	D	601	COA	C5A-C6A-N6A	6.54	130.27	120.31
4	D	601	COA	N3A-C2A-N1A	-6.46	119.91	128.67
2	A	601	1VU	N6-C20-N5	-6.42	119.96	128.67
4	C	601	COA	C4B-O4B-C1B	-6.36	104.11	109.92
2	A	601	1VU	C1-C2-S	6.19	121.37	113.56
4	B	601	COA	N3A-C2A-N1A	-6.14	120.34	128.67
4	C	601	COA	N3A-C2A-N1A	-5.85	120.73	128.67
4	B	601	COA	C4B-O4B-C1B	-5.58	104.82	109.92
4	D	601	COA	C4B-O4B-C1B	-4.78	105.55	109.92
4	C	601	COA	N6A-C6A-N1A	-4.26	109.23	118.33
4	B	601	COA	N6A-C6A-N1A	-4.12	109.53	118.33
2	A	601	1VU	C16-N2-C21	-4.05	119.53	126.64
4	B	601	COA	C7P-C6P-C5P	-4.01	105.72	112.39
4	D	601	COA	N6A-C6A-N1A	-3.89	110.03	118.33
2	A	601	1VU	O-C2-S	-3.24	118.56	122.68
4	D	601	COA	C7P-C6P-C5P	-3.12	107.19	112.39
4	C	601	COA	CDP-CBP-CAP	2.96	113.82	108.77
4	C	601	COA	C7P-C6P-C5P	-2.94	107.50	112.39
4	B	601	COA	O4B-C1B-N9A	2.89	112.58	108.75
4	C	601	COA	C2P-C3P-N4P	-2.89	105.75	112.31
4	C	601	COA	C3B-C2B-C1B	2.85	106.16	99.89
4	D	601	COA	C3P-N4P-C5P	-2.76	117.69	122.82
4	D	601	COA	C6P-C5P-N4P	2.72	121.30	116.34
4	B	601	COA	C7P-N8P-C9P	-2.63	117.82	122.55
4	D	601	COA	CDP-CBP-CAP	2.48	112.99	108.77
2	A	601	1VU	O-C2-C1	-2.43	120.07	123.72
4	C	601	COA	C6P-C7P-N8P	-2.41	106.86	112.00
4	C	601	COA	C1B-N9A-C4A	-2.41	122.40	126.64
4	D	601	COA	C1B-N9A-C4A	-2.35	122.51	126.64
4	D	601	COA	C3B-C2B-C1B	2.30	104.95	99.89
2	A	601	1VU	C6-C7-N1	-2.30	107.11	112.00
2	A	601	1VU	C15-O11-C16	-2.30	107.82	109.92
4	B	601	COA	C6P-C7P-N8P	-2.27	107.17	112.00
2	A	601	1VU	C3-S-C2	2.24	108.47	101.84
4	B	601	COA	C6P-C5P-N4P	2.08	120.13	116.34
2	A	601	1VU	C18-C19-N4	2.07	123.46	120.31

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	1VU	C14-O10-P1-O8
2	A	601	1VU	C14-O10-P1-O9
2	A	601	1VU	C14-O10-P1-O7
2	A	601	1VU	C13-C10-C9-O3
2	A	601	1VU	C13-C10-C9-C8
2	A	601	1VU	C11-C10-C9-O3
2	A	601	1VU	C11-C10-C9-C8
2	A	601	1VU	C5-C6-C7-N1
2	A	601	1VU	S-C3-C4-N
2	A	601	1VU	O-C2-S-C3
2	A	601	1VU	C1-C2-S-C3
2	A	601	1VU	C-C1-C2-S
4	B	601	COA	C5B-O5B-P1A-O1A
4	B	601	COA	C5B-O5B-P1A-O2A
4	B	601	COA	C5B-O5B-P1A-O3A
4	B	601	COA	CDP-CBP-CCP-O6A
4	B	601	COA	CEP-CBP-CCP-O6A
4	B	601	COA	CAP-CBP-CCP-O6A
4	B	601	COA	C5P-C6P-C7P-N8P
4	C	601	COA	O4B-C4B-C5B-O5B
4	C	601	COA	C5B-O5B-P1A-O1A
4	C	601	COA	C5B-O5B-P1A-O3A
4	C	601	COA	CDP-CBP-CCP-O6A
4	C	601	COA	CEP-CBP-CCP-O6A
4	C	601	COA	CAP-CBP-CCP-O6A
4	C	601	COA	O9P-C9P-CAP-CBP
4	C	601	COA	N8P-C9P-CAP-CBP
4	C	601	COA	N8P-C9P-CAP-OAP
4	D	601	COA	C4B-C5B-O5B-P1A
4	D	601	COA	OAP-CAP-CBP-CCP
4	D	601	COA	OAP-CAP-CBP-CDP
4	D	601	COA	C3B-C4B-C5B-O5B
4	D	601	COA	C6P-C7P-N8P-C9P
3	B	602	1PE	OH5-C14-C24-OH4
3	B	603	1PE	OH5-C14-C24-OH4
4	C	601	COA	C3B-C4B-C5B-O5B
4	D	601	COA	O4B-C4B-C5B-O5B
3	B	603	1PE	OH2-C12-C22-OH3
3	B	602	1PE	OH7-C16-C26-OH6
3	C	603	1PE	OH5-C14-C24-OH4
3	A	602	1PE	C13-C23-OH3-C22
3	D	602	1PE	OH2-C12-C22-OH3
3	B	602	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
3	B	602	1PE	OH2-C12-C22-OH3
3	D	602	1PE	C25-C15-OH6-C26
3	D	603	1PE	OH5-C14-C24-OH4
2	A	601	1VU	O10-C14-C15-O11
4	D	601	COA	C2B-C3B-O3B-P3B
2	A	601	1VU	O10-C14-C15-C23
2	A	601	1VU	C12-C10-C9-O3
4	D	601	COA	OAP-CAP-CBP-CEP
4	B	601	COA	C4B-C5B-O5B-P1A
3	D	602	1PE	OH6-C15-C25-OH5
4	D	601	COA	N8P-C9P-CAP-CBP
3	A	602	1PE	OH6-C15-C25-OH5
3	D	603	1PE	C24-C14-OH5-C25
3	B	602	1PE	OH6-C15-C25-OH5
3	D	602	1PE	C24-C14-OH5-C25
2	A	601	1VU	C12-C10-C9-C8
4	D	601	COA	C9P-CAP-CBP-CDP
3	C	602	1PE	C12-C22-OH3-C23
3	A	602	1PE	C15-C25-OH5-C14
2	A	601	1VU	C12-C10-C13-O4
4	D	601	COA	C5B-O5B-P1A-O1A
4	D	601	COA	C4B-C3B-O3B-P3B
3	B	602	1PE	C15-C25-OH5-C14
3	C	603	1PE	C12-C22-OH3-C23
4	D	601	COA	C5P-C6P-C7P-N8P
4	D	601	COA	C3B-O3B-P3B-O9A
3	C	602	1PE	OH4-C13-C23-OH3
3	A	602	1PE	C12-C22-OH3-C23
4	C	601	COA	C4B-C5B-O5B-P1A
3	A	602	1PE	C24-C14-OH5-C25
3	D	602	1PE	C12-C22-OH3-C23
3	B	603	1PE	C25-C15-OH6-C26
4	D	601	COA	C9P-CAP-CBP-CEP
4	D	601	COA	P1A-O3A-P2A-O5A
4	D	601	COA	O9P-C9P-CAP-CBP
3	B	602	1PE	C16-C26-OH6-C15
3	A	602	1PE	C16-C26-OH6-C15
2	A	601	1VU	C11-C10-C13-O4
4	C	601	COA	N4P-C5P-C6P-C7P
4	C	601	COA	O5P-C5P-C6P-C7P
3	A	602	1PE	C25-C15-OH6-C26
4	B	601	COA	N8P-C9P-CAP-OAP

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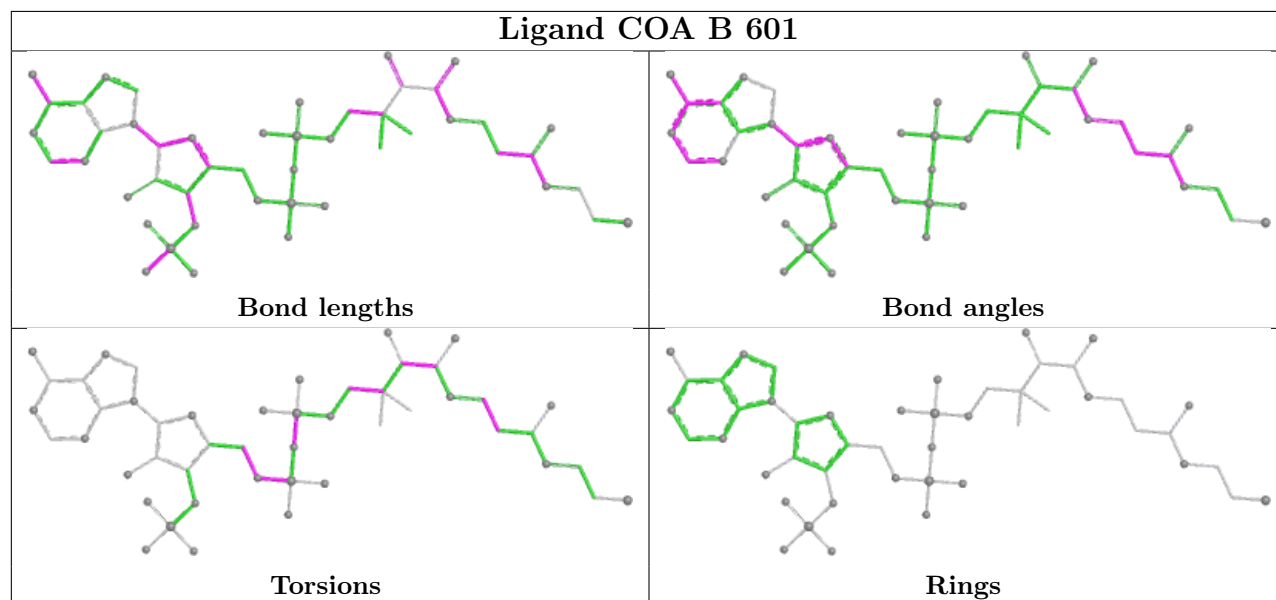
Mol	Chain	Res	Type	Atoms
4	B	601	COA	P1A-O3A-P2A-O5A

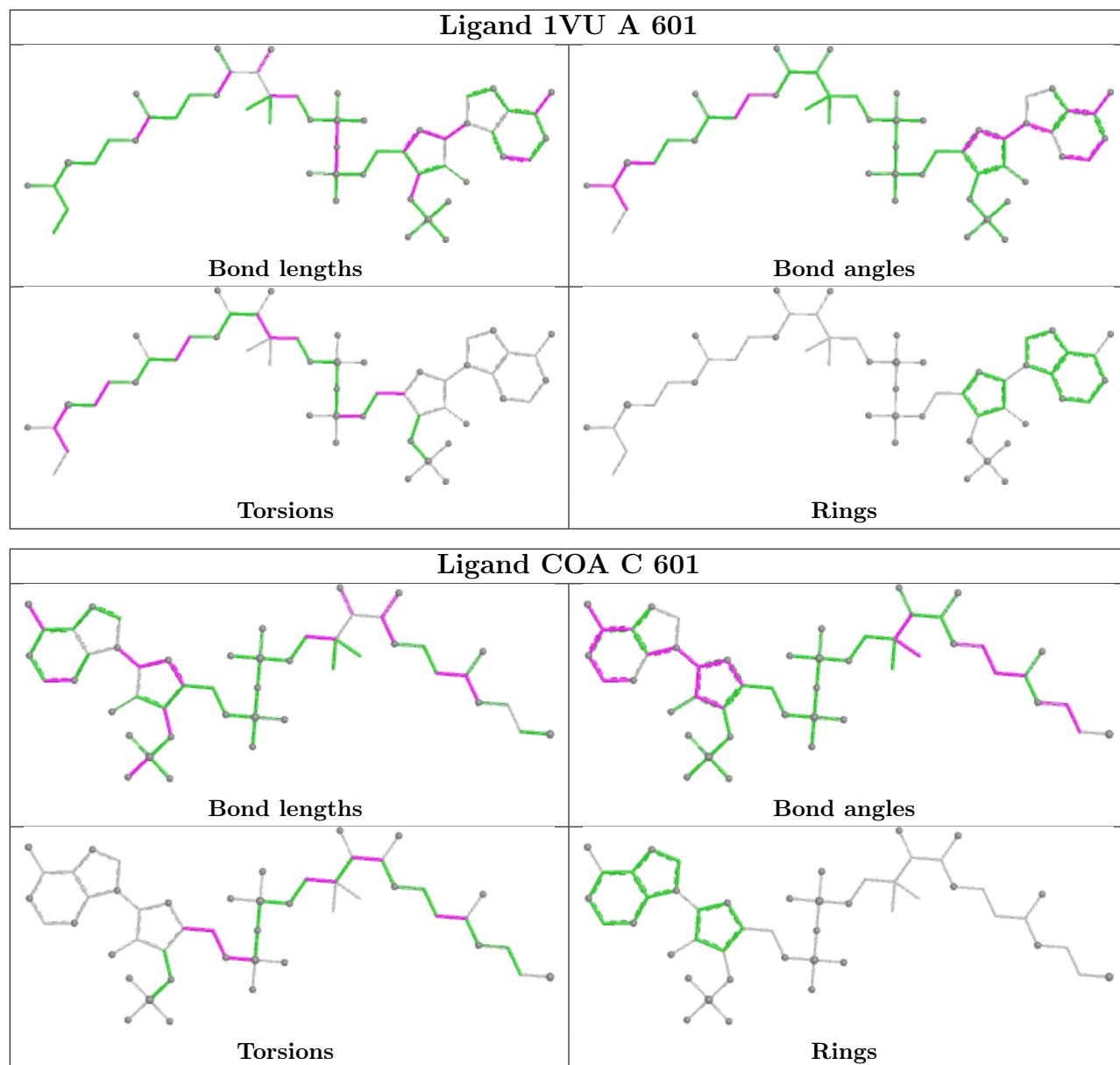
There are no ring outliers.

8 monomers are involved in 34 short contacts:

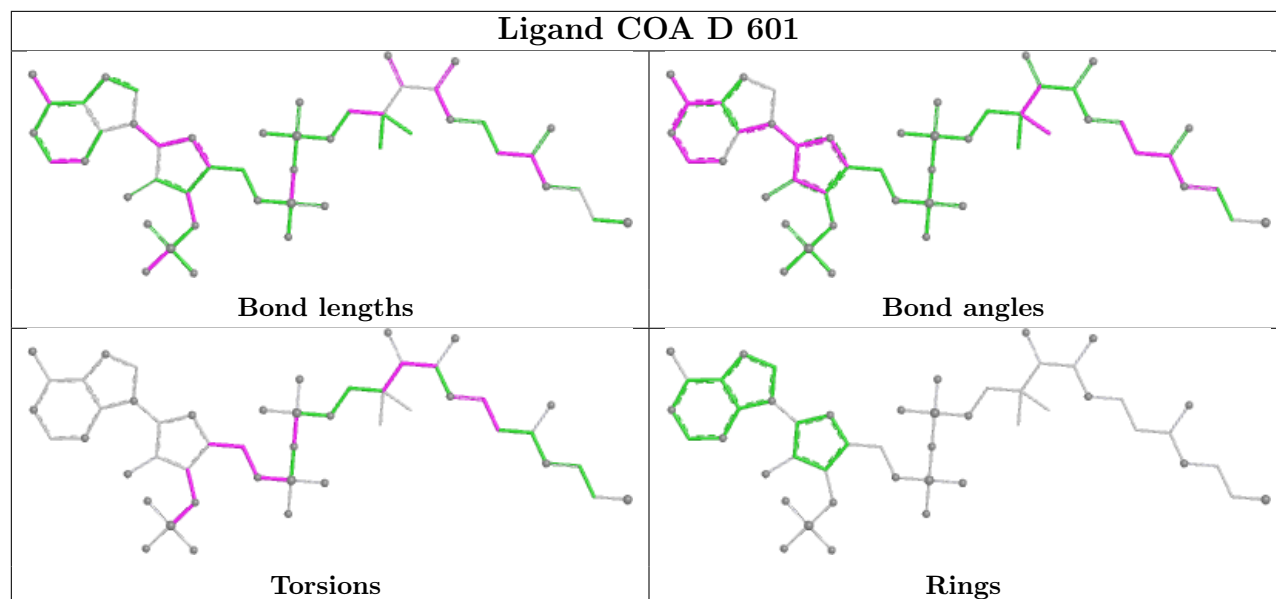
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	COA	6	0
3	B	603	1PE	2	0
3	A	602	1PE	1	0
3	D	602	1PE	2	0
3	C	602	1PE	1	0
2	A	601	1VU	7	0
4	C	601	COA	7	0
4	D	601	COA	8	0

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, 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	438/525 (83%)	-0.60	0 100 100	9, 16, 32, 48	1 (0%)
1	B	438/525 (83%)	-0.57	1 (0%) 92 92	10, 17, 34, 57	1 (0%)
1	C	445/525 (84%)	-0.55	2 (0%) 89 90	9, 16, 33, 50	1 (0%)
1	D	438/525 (83%)	-0.27	0 100 100	9, 23, 41, 56	2 (0%)
All	All	1759/2100 (83%)	-0.50	3 (0%) 92 92	9, 18, 35, 57	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	ALA	3.0
1	C	49	SER	2.7
1	C	43	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	6KM	A	330[A]	10/11	0.91	0.12	14,21,29,34	10
1	6KM	B	330[A]	10/11	0.92	0.10	17,21,31,34	10
1	6KM	D	330[A]	10/11	0.92	0.12	19,25,34,40	10
1	6KM	C	330[A]	10/11	0.95	0.09	13,17,28,33	10

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

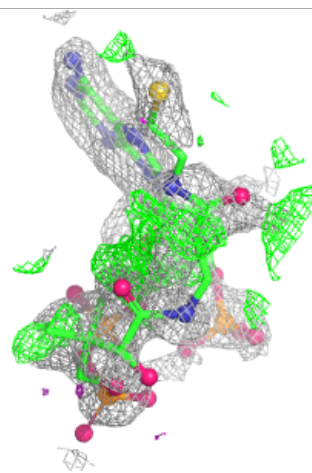
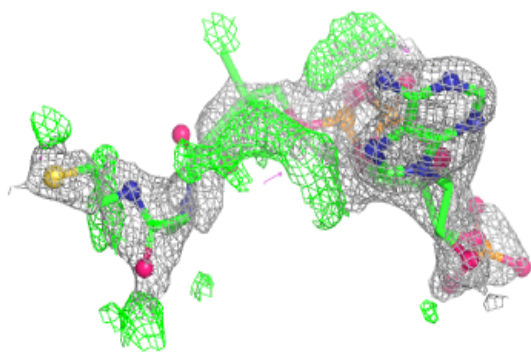
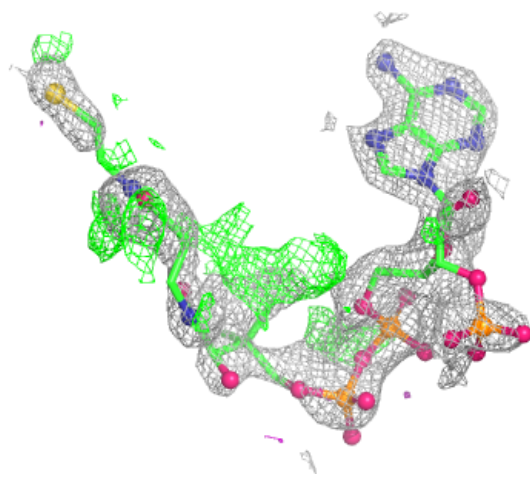
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	COA	D	601	48/48	0.66	0.20	28,56,74,83	48
4	COA	C	601	48/48	0.68	0.21	18,47,66,76	48
2	1VU	A	601	52/52	0.73	0.19	19,44,64,78	52
4	COA	B	601	48/48	0.76	0.17	23,49,65,79	48
3	1PE	D	602	16/16	0.81	0.14	27,44,58,62	0
3	1PE	B	602	16/16	0.83	0.13	31,45,58,58	0
3	1PE	B	603	16/16	0.85	0.13	26,41,48,51	0
3	1PE	C	602	16/16	0.87	0.11	30,37,47,49	0
3	1PE	C	603	16/16	0.87	0.12	30,40,44,49	0
3	1PE	A	602	16/16	0.87	0.11	25,35,43,47	0
3	1PE	D	603	16/16	0.88	0.12	36,45,54,55	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.

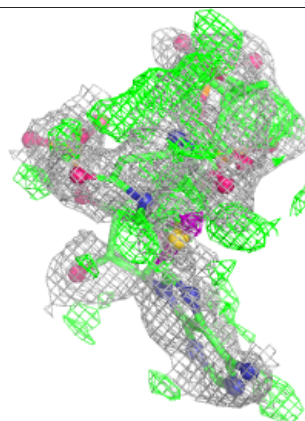
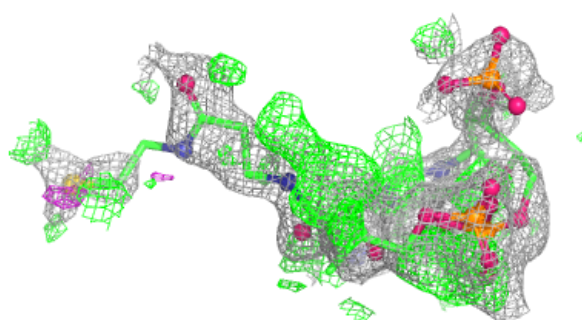
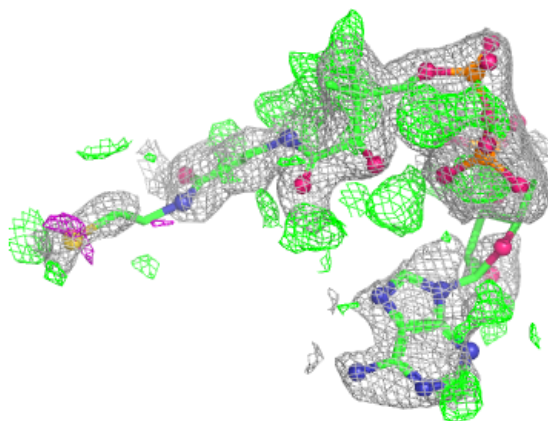
**Electron density around COA D 601:**

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

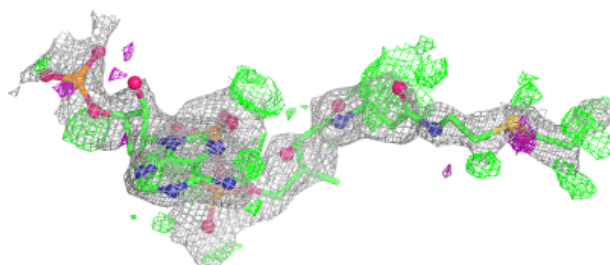
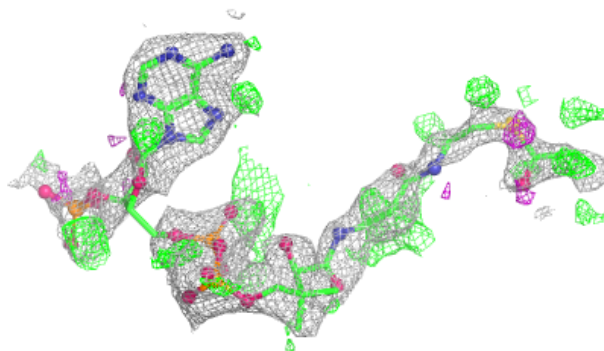


**Electron density around COA C 601:**

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

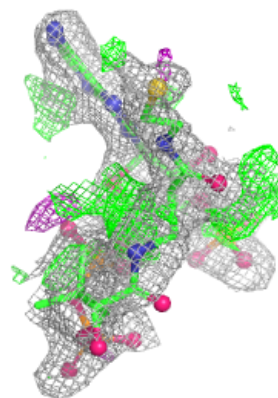
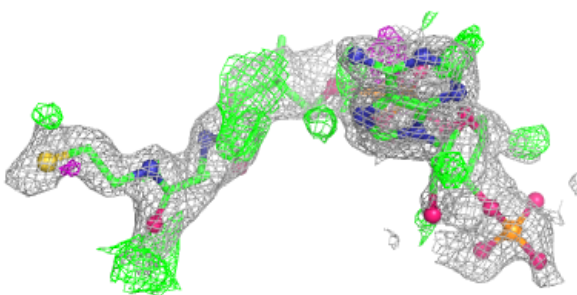
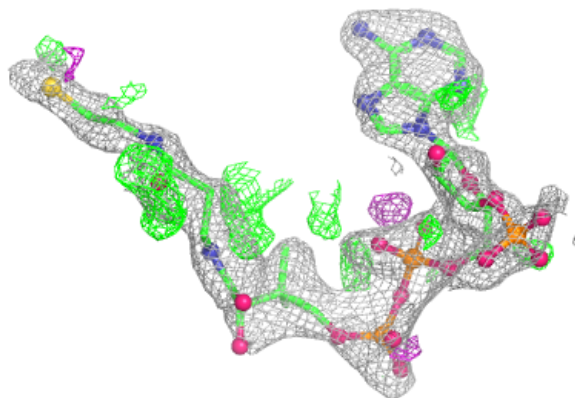
**Electron density around 1VU A 601:**

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



**Electron density around COA B 601:**

$2mF_o-DF_c$  (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.