



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2016 – 03:14 PM EDT

PDB ID : 5SZZ  
Title : Novel Structural Insights into GDP-Mediated Regulation of Acyl-CoA Thioesterases  
Authors : Khandokar, Y.B.; Srivastava, P.; Forwood, J.K.  
Deposited on : 2016-08-15  
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

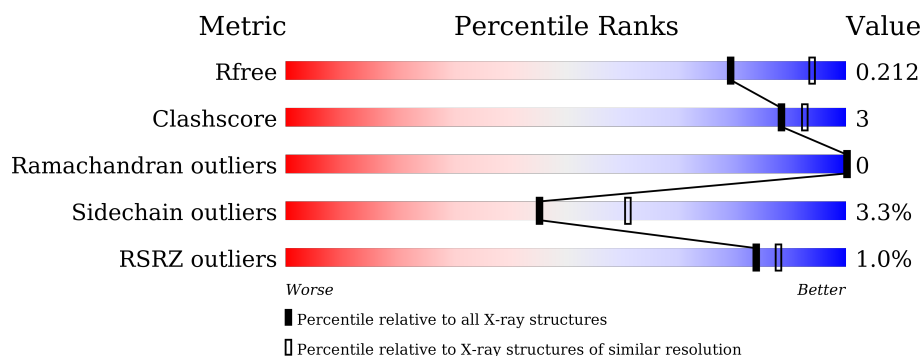
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	160	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>8%</span> <span>•</span> <span>8%</span> </div> </div>
1	B	160	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 82%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>10%</span> <span>•</span> <span>8%</span> </div> </div>
1	C	160	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>88%</span> <span>•</span> <span>•</span> <span>8%</span> </div> </div>
1	D	160	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>8%</span> <span>•</span> <span>8%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5363 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.

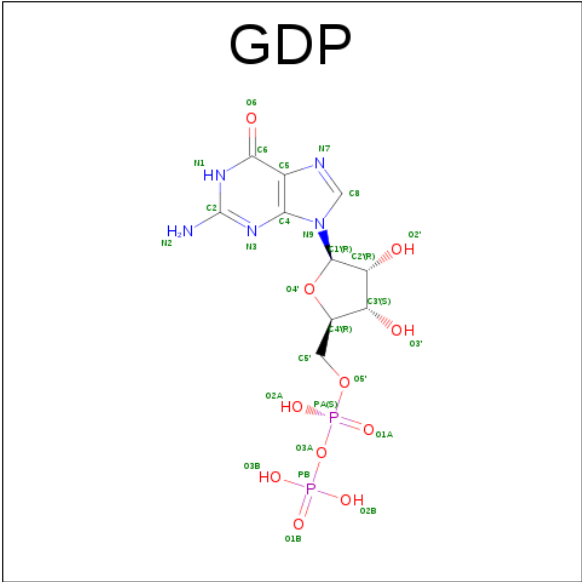
- Molecule 1 is a protein called Acyl-CoA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1167	734	207	217	9			
1	D	148	Total	C	N	O	S	0	0	0
			1167	734	207	217	9			
1	C	148	Total	C	N	O	S	0	1	0
			1170	736	207	217	10			
1	B	148	Total	C	N	O	S	0	0	0
			1167	734	207	217	9			

There are 12 discrepancies between the modelled and reference sequences:

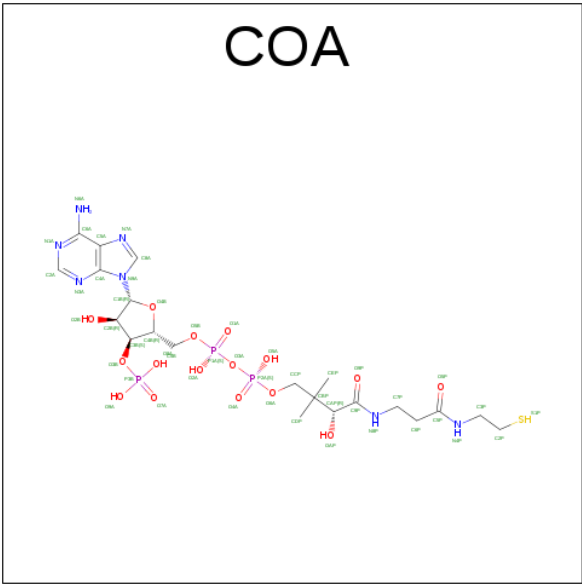
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0Y5D4F5
A	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
A	0	ALA	-	expression tag	UNP A0A0Y5D4F5
D	-2	SER	-	expression tag	UNP A0A0Y5D4F5
D	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
D	0	ALA	-	expression tag	UNP A0A0Y5D4F5
C	-2	SER	-	expression tag	UNP A0A0Y5D4F5
C	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
C	0	ALA	-	expression tag	UNP A0A0Y5D4F5
B	-2	SER	-	expression tag	UNP A0A0Y5D4F5
B	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
B	0	ALA	-	expression tag	UNP A0A0Y5D4F5

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	1	0
4	A	1	Total	Cl		
			1	1	1	0
4	D	1	Total	Cl		
			1	1	1	0
4	C	1	Total	Cl		
			1	1	1	0

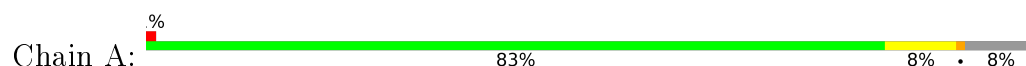
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O		
			87	87	0	0
5	D	101	Total	O		
			101	101	0	0
5	C	100	Total	O		
			100	100	0	0
5	B	96	Total	O		
			96	96	0	0

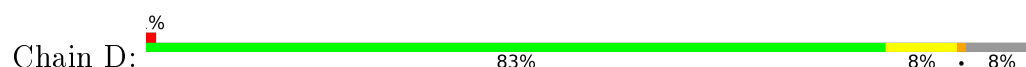
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

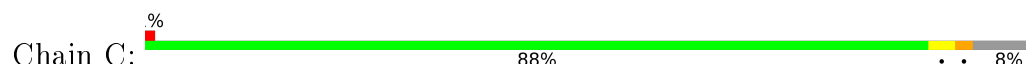
- Molecule 1: Acyl-CoA hydrolase



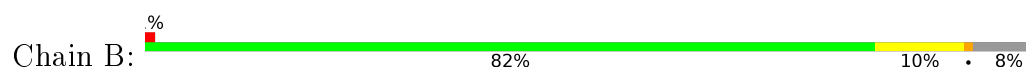
- Molecule 1: Acyl-CoA hydrolase



- Molecule 1: Acyl-CoA hydrolase



- Molecule 1: Acyl-CoA hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.62Å 152.62Å 152.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.12 – 2.30 33.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.12-2.30) 100.0 (33.30-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.09 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.190 , 0.212 0.190 , 0.212	Depositor DCC
$R_{free}$ test set	2627 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: GDP, COA, CL

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	0.87	1/1188 (0.1%)	0.83	2/1606 (0.1%)
1	B	0.65	0/1188	0.74	2/1606 (0.1%)
1	C	0.87	1/1194 (0.1%)	0.78	2/1614 (0.1%)
1	D	0.91	1/1188 (0.1%)	0.79	1/1606 (0.1%)
All	All	0.83	3/4758 (0.1%)	0.78	7/6432 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	CYS	CB-SG	-10.83	1.63	1.82
1	A	33	GLU	CD-OE1	-5.50	1.19	1.25
1	D	110	CYS	CB-SG	-5.22	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	D	61	LYS	CA-CB-CG	7.11	129.04	113.40
1	C	48	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	B	85	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	60	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	105	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	138	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.



## 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	1167	0	1178	6	0
1	B	1167	0	1178	10	0
1	C	1170	0	1183	6	0
1	D	1167	0	1178	9	0
2	A	28	0	12	0	0
2	B	28	0	12	2	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
3	A	48	0	32	2	0
3	B	48	0	32	0	0
3	C	48	0	32	0	0
3	D	48	0	32	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	87	0	0	1	0
5	B	96	0	0	0	0
5	C	100	0	0	1	0
5	D	101	0	0	1	0
All	All	5363	0	4893	25	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 3.

All (25) 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:D:60:ASP:OD2	5:D:301:HOH:O	2.00	0.79
1:A:61:LYS:NZ	1:B:149:SER:OG	2.17	0.78
1:A:67:PRO:O	1:A:105:ARG:NH2	2.18	0.74
3:A:201:COA:H62A	1:B:65:LYS:HE3	1.57	0.68
1:D:138:ARG:NH1	2:D:200:GDP:O3B	2.30	0.65
1:C:134:ARG:NH1	1:C:138:ARG:HH22	1.98	0.61
1:C:85:ARG:NH1	5:C:301:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:COA:H62A	1:B:65:LYS:CE	2.15	0.60
1:D:73:LEU:HD22	1:C:48:ARG:HD2	1.87	0.56
1:B:109:SER:OG	2:B:202:GDP:O1A	2.21	0.50
1:D:34:LEU:HD23	1:D:64:PHE:CE1	2.50	0.47
1:D:133:ASP:OD1	1:D:136:ARG:NH1	2.48	0.46
1:D:73:LEU:CD2	1:C:48:ARG:HD2	2.44	0.46
1:D:120:GLY:C	1:D:121:LYS:HD3	2.36	0.46
1:A:105:ARG:HD3	5:A:350:HOH:O	2.16	0.46
1:B:34:LEU:HD23	1:B:64:PHE:CE1	2.50	0.46
1:A:88:MET:CE	1:A:125:VAL:HG11	2.48	0.44
1:A:60:ASP:HA	1:B:61:LYS:HG3	2.01	0.43
1:D:99:ILE:HD12	1:C:48:ARG:HA	2.00	0.42
1:B:147:ASP:O	1:B:151:GLN:HG2	2.18	0.42
1:D:43:TYR:CE2	1:C:17:LEU:HD23	2.55	0.42
1:A:116:ALA:O	1:A:122:PRO:HA	2.21	0.41
1:B:138:ARG:HD2	2:B:202:GDP:O3B	2.20	0.41
1:B:18:MET:HE3	1:B:74:VAL:HB	2.02	0.41
1:B:66:GLU:OE1	1:B:105:ARG:NH1	2.48	0.40

There are no symmetry-related clashes.

## 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	146/160 (91%)	142 (97%)	4 (3%)	0	100	100
1	B	146/160 (91%)	143 (98%)	3 (2%)	0	100	100
1	C	147/160 (92%)	143 (97%)	4 (3%)	0	100	100
1	D	146/160 (91%)	144 (99%)	2 (1%)	0	100	100
All	All	585/640 (91%)	572 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	130/141 (92%)	123 (95%)	7 (5%)	27	36
1	B	130/141 (92%)	127 (98%)	3 (2%)	58	75
1	C	131/141 (93%)	128 (98%)	3 (2%)	58	75
1	D	130/141 (92%)	126 (97%)	4 (3%)	47	64
All	All	521/564 (92%)	504 (97%)	17 (3%)	45	61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	100	ARG
1	A	121	LYS
1	A	130	ILE
1	A	138	ARG
1	A	140	GLU
1	A	146	ARG
1	D	61	LYS
1	D	88	MET
1	D	110	CYS
1	D	134	ARG
1	C	6	GLN
1	C	61	LYS
1	C	134	ARG
1	B	6	GLN
1	B	65	LYS
1	B	134	ARG

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

Mol	Chain	Res	Type
1	A	40	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	GDP	A	200	-	24,30,30	1.09	2 (8%)	26,47,47	1.97	5 (19%)
3	COA	A	201	-	41,50,50	3.40	9 (21%)	49,75,75	2.56	7 (14%)
2	GDP	B	202	-	24,30,30	0.96	2 (8%)	26,47,47	2.25	8 (30%)
3	COA	B	203	-	41,50,50	3.49	12 (29%)	49,75,75	2.25	9 (18%)
2	GDP	C	200	-	24,30,30	1.13	3 (12%)	26,47,47	2.12	6 (23%)
3	COA	C	201	-	41,50,50	3.44	13 (31%)	49,75,75	2.30	8 (16%)
2	GDP	D	200	-	24,30,30	1.19	3 (12%)	26,47,47	2.04	6 (23%)
3	COA	D	201	-	41,50,50	3.50	9 (21%)	49,75,75	2.31	9 (18%)

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	GDP	A	200	-	-	0/12/32/32	0/3/3/3
3	COA	A	201	-	-	0/44/64/64	0/3/3/3
2	GDP	B	202	-	-	0/12/32/32	0/3/3/3
3	COA	B	203	-	-	0/44/64/64	0/3/3/3
2	GDP	C	200	-	-	0/12/32/32	0/3/3/3
3	COA	C	201	-	-	0/44/64/64	0/3/3/3
2	GDP	D	200	-	-	0/12/32/32	0/3/3/3
3	COA	D	201	-	-	0/44/64/64	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	COA	C2B-C1B	-11.73	1.35	1.53
3	A	201	COA	C2B-C1B	-11.37	1.35	1.53
3	D	201	COA	C2B-C1B	-11.33	1.35	1.53
3	C	201	COA	C2B-C1B	-11.03	1.36	1.53
3	C	201	COA	O4B-C4B	-6.63	1.29	1.45
3	A	201	COA	O4B-C4B	-6.13	1.31	1.45
3	B	203	COA	O4B-C4B	-5.92	1.31	1.45
3	D	201	COA	O4B-C4B	-5.87	1.31	1.45
3	B	203	COA	O3B-C3B	-3.32	1.33	1.44
3	A	201	COA	O3B-C3B	-3.05	1.34	1.44
3	C	201	COA	O3B-C3B	-2.96	1.34	1.44
3	D	201	COA	O3B-C3B	-2.81	1.35	1.44
3	A	201	COA	OAP-CAP	-2.53	1.37	1.42
3	A	201	COA	C5A-C4A	-2.44	1.35	1.40
3	C	201	COA	OAP-CAP	-2.32	1.37	1.42
3	B	203	COA	C5A-C4A	-2.24	1.35	1.40
2	D	200	GDP	PB-O3B	-2.15	1.47	1.54
3	C	201	COA	C5A-C4A	-2.14	1.35	1.40
2	C	200	GDP	PB-O3B	-2.01	1.47	1.54
3	B	203	COA	OAP-CAP	-2.00	1.38	1.42
3	D	201	COA	O2B-C2B	2.01	1.47	1.43
3	B	203	COA	C2A-N1A	2.06	1.37	1.33
3	C	201	COA	C2A-N1A	2.07	1.37	1.33
3	C	201	COA	C3B-C4B	2.10	1.58	1.52
3	B	203	COA	C6A-N6A	2.10	1.42	1.34
3	B	203	COA	C3B-C4B	2.16	1.59	1.52
2	B	202	GDP	C6-C5	2.20	1.45	1.41
2	C	200	GDP	C6-C5	2.30	1.45	1.41
3	A	201	COA	C3B-C4B	2.30	1.59	1.52
3	D	201	COA	C3B-C4B	2.32	1.59	1.52
3	C	201	COA	O2B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	COA	C2A-N3A	2.43	1.36	1.32
3	C	201	COA	C6A-N6A	2.47	1.44	1.34
3	B	203	COA	C2A-N3A	2.51	1.36	1.32
2	B	202	GDP	C5-C4	2.79	1.46	1.40
3	C	201	COA	C2A-N3A	2.93	1.37	1.32
2	A	200	GDP	C6-C5	3.06	1.47	1.41
2	C	200	GDP	C5-C4	3.15	1.47	1.40
2	D	200	GDP	C5-C4	3.22	1.47	1.40
2	A	200	GDP	C5-C4	3.33	1.48	1.40
2	D	200	GDP	C6-C5	3.53	1.48	1.41
3	A	201	COA	C5P-N4P	4.58	1.44	1.33
3	B	203	COA	C5P-N4P	4.80	1.45	1.33
3	A	201	COA	C9P-N8P	4.84	1.43	1.33
3	C	201	COA	C5P-N4P	5.31	1.46	1.33
3	C	201	COA	C9P-N8P	5.47	1.45	1.33
3	D	201	COA	C5P-N4P	5.51	1.46	1.33
3	B	203	COA	C9P-N8P	5.65	1.45	1.33
3	D	201	COA	C9P-N8P	6.36	1.46	1.33
3	C	201	COA	O4B-C1B	14.01	1.61	1.41
3	A	201	COA	O4B-C1B	14.39	1.61	1.41
3	B	203	COA	O4B-C1B	14.59	1.62	1.41
3	D	201	COA	O4B-C1B	14.63	1.62	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	COA	N3A-C2A-N1A	-12.44	119.10	128.87
3	C	201	COA	N3A-C2A-N1A	-10.80	120.39	128.87
3	B	203	COA	N3A-C2A-N1A	-10.52	120.61	128.87
3	D	201	COA	N3A-C2A-N1A	-9.76	121.20	128.87
3	A	201	COA	N6A-C6A-N1A	-9.16	103.15	118.52
3	D	201	COA	N6A-C6A-N1A	-8.22	104.72	118.52
3	B	203	COA	N6A-C6A-N1A	-7.58	105.80	118.52
3	C	201	COA	N6A-C6A-N1A	-6.84	107.03	118.52
2	B	202	GDP	C5-C6-N1	-5.27	116.63	123.52
2	C	200	GDP	C5-C6-N1	-5.18	116.75	123.52
3	C	201	COA	C7P-C6P-C5P	-5.12	103.44	112.22
3	A	201	COA	C7P-C6P-C5P	-4.76	104.05	112.22
3	D	201	COA	C7P-C6P-C5P	-4.70	104.16	112.22
2	A	200	GDP	C5-C6-N1	-4.62	117.49	123.52
2	D	200	GDP	C5-C6-N1	-4.55	117.58	123.52
2	B	202	GDP	C1'-N9-C4	-3.78	122.59	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	COA	C7P-C6P-C5P	-3.77	105.75	112.22
3	C	201	COA	C6P-C7P-N8P	-3.37	104.40	111.94
2	C	200	GDP	C1'-N9-C4	-3.22	123.22	126.81
2	D	200	GDP	C6-C5-C4	-3.18	117.22	120.86
2	A	200	GDP	C6-C5-C4	-3.15	117.26	120.86
3	B	203	COA	C6P-C7P-N8P	-3.12	104.94	111.94
2	A	200	GDP	C1'-N9-C4	-3.07	123.38	126.81
2	C	200	GDP	C6-C5-C4	-3.05	117.38	120.86
2	D	200	GDP	C1'-N9-C4	-2.95	123.52	126.81
2	D	200	GDP	N3-C2-N1	-2.87	123.65	127.56
3	A	201	COA	C1B-N9A-C4A	-2.82	123.66	126.81
3	A	201	COA	C6P-C7P-N8P	-2.76	105.76	111.94
2	B	202	GDP	N3-C2-N1	-2.74	123.83	127.56
2	C	200	GDP	N3-C2-N1	-2.72	123.86	127.56
2	A	200	GDP	N3-C2-N1	-2.63	123.98	127.56
3	D	201	COA	C2P-C3P-N4P	-2.57	107.35	112.44
3	C	201	COA	C2P-C3P-N4P	-2.49	107.51	112.44
3	B	203	COA	C2P-C3P-N4P	-2.46	107.57	112.44
3	D	201	COA	C3P-N4P-C5P	-2.40	118.04	122.79
3	D	201	COA	C6P-C7P-N8P	-2.36	106.65	111.94
2	B	202	GDP	C6-C5-C4	-2.31	118.22	120.86
3	B	203	COA	C3P-N4P-C5P	-2.25	118.34	122.79
2	B	202	GDP	O2'-C2'-C1'	-2.22	104.67	111.61
3	C	201	COA	C4B-O4B-C1B	-2.22	107.29	109.64
3	D	201	COA	C4B-O4B-C1B	-2.13	107.38	109.64
3	B	203	COA	C7P-N8P-C9P	-2.08	118.46	122.62
2	C	200	GDP	O2A-PA-O3A	-2.06	96.43	105.27
2	B	202	GDP	C2'-C1'-N9	-2.05	107.97	113.47
3	A	201	COA	C2P-C3P-N4P	-2.02	108.44	112.44
3	C	201	COA	C6P-C5P-N4P	2.06	120.04	116.46
3	B	203	COA	C6P-C5P-N4P	2.14	120.18	116.46
3	A	201	COA	CDP-CBP-CAP	2.24	113.25	109.17
3	D	201	COA	CEP-CBP-CAP	2.32	113.41	109.17
3	B	203	COA	CDP-CBP-CAP	2.33	113.43	109.17
3	D	201	COA	O5A-P2A-O3A	3.34	119.60	105.27
3	C	201	COA	O5A-P2A-O3A	3.49	120.24	105.27
2	D	200	GDP	O2A-PA-O3A	3.53	120.41	105.27
2	B	202	GDP	O2A-PA-O3A	3.56	120.54	105.27
2	D	200	GDP	C6-N1-C2	5.39	122.20	115.88
2	A	200	GDP	C6-N1-C2	5.76	122.63	115.88
2	C	200	GDP	C6-N1-C2	6.45	123.44	115.88
2	B	202	GDP	C6-N1-C2	6.48	123.47	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	COA	2	0
2	B	202	GDP	2	0
2	D	200	GDP	1	0

## 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 [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	148/160 (92%)	-0.46	1 (0%) 89 92	13, 21, 39, 67	0
1	B	148/160 (92%)	-0.40	1 (0%) 89 92	13, 21, 43, 69	0
1	C	148/160 (92%)	-0.36	2 (1%) 78 83	15, 21, 43, 68	0
1	D	148/160 (92%)	-0.36	2 (1%) 78 83	14, 23, 39, 61	0
All	All	592/640 (92%)	-0.39	6 (1%) 84 88	13, 21, 43, 69	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	GLN	4.6
1	C	151	GLN	3.7
1	C	6	GLN	3.3
1	A	134	ARG	2.7
1	D	134	ARG	2.5
1	D	6	GLN	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	COA	C	201	48/48	0.96	0.10	-0.30	13,24,34,48	0
3	COA	D	201	48/48	0.96	0.10	-0.40	14,22,32,53	0
2	GDP	A	200	28/28	0.97	0.11	-0.42	16,22,39,49	0
2	GDP	D	200	28/28	0.96	0.10	-0.42	19,26,31,44	0
3	COA	A	201	48/48	0.97	0.09	-0.43	13,21,32,39	0
3	COA	B	203	48/48	0.96	0.09	-0.45	9,22,34,45	0
2	GDP	C	200	28/28	0.97	0.09	-0.89	14,19,28,38	0
2	GDP	B	202	28/28	0.97	0.09	-0.89	13,18,33,38	0
4	CL	D	202	1/1	-	-	-	16,16,16,16	1
4	CL	A	202	1/1	-	-	-	16,16,16,16	1
4	CL	B	201	1/1	-	-	-	17,17,17,17	1
4	CL	C	202	1/1	-	-	-	17,17,17,17	1

## 6.5 Other polymers

There are no such residues in this entry.