Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2016 – 02:04 PM EDT

PDB ID	:	5SZY
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	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

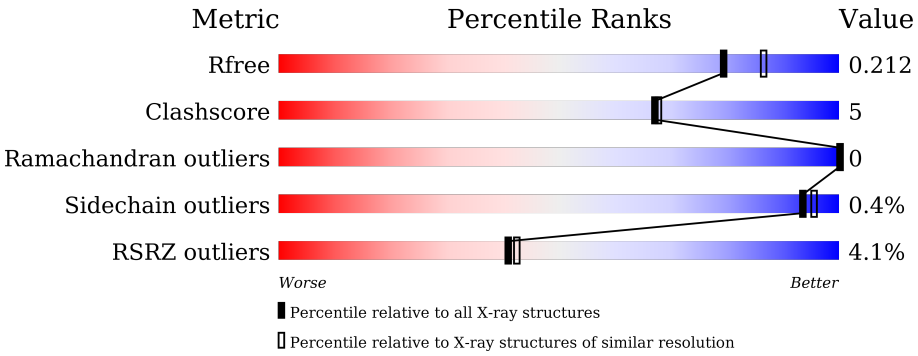
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	5% 87% 6% 7%
1	B	160	3% 84% 8% · 8%
1	C	160	4% 79% 14% 8%
1	D	160	3% 88% 5% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5301 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.

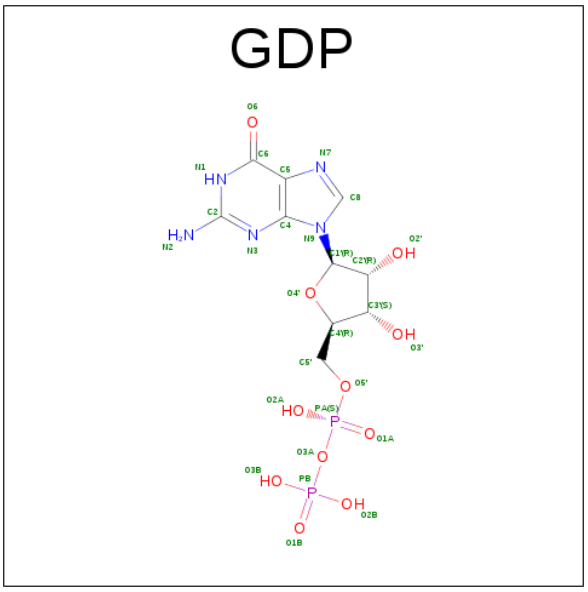
- Molecule 1 is a protein called Acyl-CoA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1170	736	207	218	9			
1	B	147	Total	C	N	O	S	0	0	0
			1159	730	205	215	9			
1	C	148	Total	C	N	O	S	0	1	0
			1167	735	206	216	10			
1	D	148	Total	C	N	O	S	0	1	0
			1167	735	206	216	10			

There are 16 discrepancies between the modelled and reference sequences:

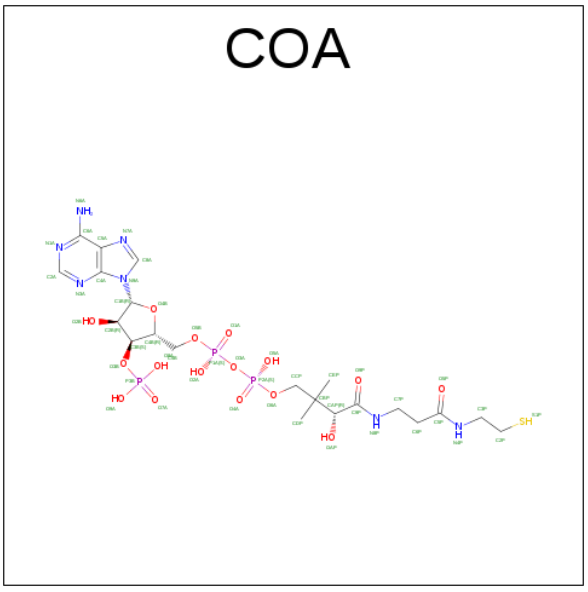
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0Y5D4F5
A	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
A	0	ALA	-	expression tag	UNP A0A0Y5D4F5
A	24	ALA	ASN	engineered mutation	UNP A0A0Y5D4F5
B	-2	SER	-	expression tag	UNP A0A0Y5D4F5
B	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
B	0	ALA	-	expression tag	UNP A0A0Y5D4F5
B	24	ALA	ASN	engineered mutation	UNP A0A0Y5D4F5
C	-2	SER	-	expression tag	UNP A0A0Y5D4F5
C	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
C	0	ALA	-	expression tag	UNP A0A0Y5D4F5
C	24	ALA	ASN	engineered mutation	UNP A0A0Y5D4F5
D	-2	SER	-	expression tag	UNP A0A0Y5D4F5
D	-1	ASN	-	expression tag	UNP A0A0Y5D4F5
D	0	ALA	-	expression tag	UNP A0A0Y5D4F5
D	24	ALA	ASN	engineered mutation	UNP A0A0Y5D4F5

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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		
2	C	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		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 5 is water.

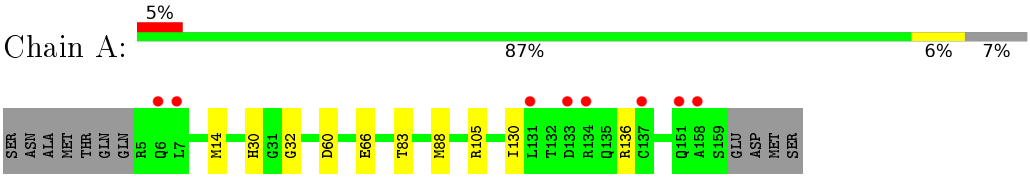
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	73	Total	O	0	0
			73	73		
5	C	87	Total	O	0	0
			87	87		
5	D	81	Total	O	0	0
			81	81		

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.

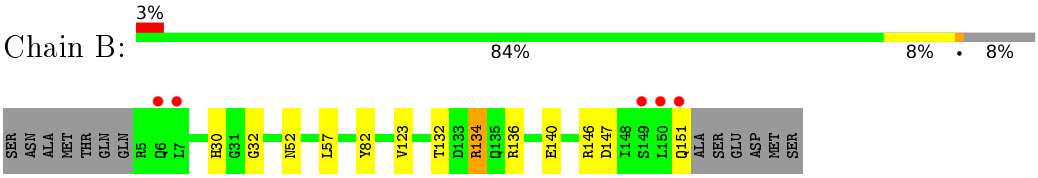
- Molecule 1: Acyl-CoA hydrolase

Chain A:



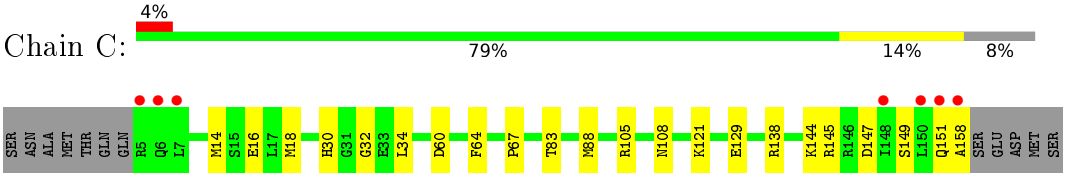
- Molecule 1: Acyl-CoA hydrolase

Chain B:



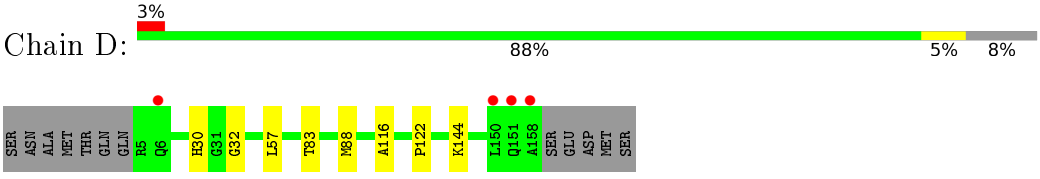
- Molecule 1: Acyl-CoA hydrolase

Chain C:



- Molecule 1: Acyl-CoA hydrolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	152.80Å 152.80Å 152.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.02 – 2.00 36.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.02-2.00) 98.8 (36.02-2.00)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.60 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.212 0.197 , 0.212	Depositor DCC
R_{free} test set	3978 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/1190	0.58	0/1607
1	B	0.39	0/1180	0.59	0/1595
1	C	0.41	0/1190	0.61	0/1607
1	D	0.42	0/1190	0.58	0/1607
All	All	0.40	0/4750	0.59	0/6416

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

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	1170	0	1181	7	0
1	B	1159	0	1172	13	0
1	C	1167	0	1181	18	0
1	D	1167	0	1181	7	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	1	0
2	D	28	0	12	0	0
3	A	48	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	32	2	0
3	C	48	0	32	1	0
3	D	48	0	32	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	89	0	0	1	0
5	B	73	0	0	0	0
5	C	87	0	0	4	0
5	D	81	0	0	0	0
All	All	5301	0	4891	47	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 5.

All (47) 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)
3:A:201:COA:C1B	3:A:201:COA:O4B	1.67	1.27
3:B:202:COA:C1B	3:B:202:COA:O4B	1.67	1.20
3:D:201:COA:O4B	3:D:201:COA:C1B	1.67	1.17
3:C:201:COA:O4B	3:C:201:COA:C1B	1.66	1.14
1:B:82:TYR:OH	1:B:146:ARG:NH1	2.18	0.77
1:D:83:THR:HG22	1:D:88:MET:HG2	1.69	0.74
1:B:52:ASN:HD22	1:B:123:VAL:HG21	1.56	0.70
1:B:30:HIS:CD2	1:B:32:GLY:H	2.11	0.68
1:A:66:GLU:HB3	1:A:105:ARG:NH2	2.09	0.68
1:A:14:MET:HG3	1:C:14:MET:HG3	1.76	0.68
1:B:52:ASN:ND2	1:B:123:VAL:HG21	2.11	0.65
1:A:83:THR:HG22	1:A:88:MET:HG2	1.79	0.64
1:C:121:LYS:HE3	1:C:121:LYS:HA	1.82	0.62
1:C:16:GLU:HG2	1:C:18:MET:CE	2.30	0.61
1:C:30:HIS:CD2	1:C:32:GLY:H	2.21	0.59
1:B:30:HIS:HD2	1:B:32:GLY:H	1.51	0.58
1:D:30:HIS:HD2	1:D:32:GLY:H	1.52	0.58
1:C:138:ARG:HD2	2:C:200:GDP:O1B	2.03	0.58
1:B:136:ARG:NH1	1:B:140:GLU:HG2	2.20	0.57
1:D:30:HIS:CD2	1:D:32:GLY:H	2.22	0.57
1:B:52:ASN:HD22	1:B:123:VAL:CG2	2.21	0.53
1:C:67:PRO:O	1:C:105:ARG:NH2	2.42	0.53
1:C:147:ASP:O	1:C:151:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:HD2	1:B:32:GLY:N	2.08	0.52
1:A:66:GLU:HB3	1:A:105:ARG:HH21	1.72	0.52
1:C:149:SER:O	1:C:158:ALA:N	2.44	0.51
1:C:60:ASP:OD2	1:C:145:ARG:HD3	2.11	0.50
1:C:16:GLU:HG2	1:C:18:MET:HE1	1.94	0.50
1:A:30:HIS:CD2	1:A:32:GLY:H	2.29	0.49
1:C:16:GLU:HB2	5:C:327:HOH:O	2.11	0.49
1:B:136:ARG:HH12	1:B:140:GLU:HG2	1.77	0.49
1:C:108:ASN:HB2	5:C:361:HOH:O	2.15	0.47
1:B:147:ASP:O	1:B:151:GLN:HG3	2.14	0.47
1:B:132:THR:OG1	1:B:134:ARG:HG2	2.15	0.46
1:D:30:HIS:HD2	1:D:32:GLY:N	2.14	0.46
1:D:57:LEU:HD21	3:D:201:COA:C4A	2.47	0.45
1:A:60:ASP:OD2	5:A:301:HOH:O	2.21	0.45
1:C:105:ARG:NH1	5:C:301:HOH:O	2.34	0.44
1:A:130:ILE:HG21	1:A:136:ARG:HG2	1.98	0.44
1:C:16:GLU:HG2	1:C:18:MET:HE2	2.00	0.44
1:D:144:LYS:HB3	1:D:144:LYS:HE2	1.79	0.44
1:D:116:ALA:O	1:D:122:PRO:HA	2.19	0.43
1:C:83:THR:HG22	1:C:88:MET:HG2	2.00	0.43
1:B:146:ARG:NH2	1:C:129:GLU:OE1	2.41	0.42
1:B:57:LEU:HD21	3:B:202:COA:C4A	2.51	0.41
1:C:34:LEU:HD23	1:C:64:PHE:CE1	2.55	0.41
1:C:151:GLN:CG	5:C:306:HOH:O	2.69	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	145/160 (91%)	144 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	145/160 (91%)	144 (99%)	1 (1%)	0	100	100
1	C	146/160 (91%)	145 (99%)	1 (1%)	0	100	100
1	D	146/160 (91%)	145 (99%)	1 (1%)	0	100	100
All	All	582/640 (91%)	578 (99%)	4 (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	130/140 (93%)	130 (100%)	0	100	100
1	B	129/140 (92%)	128 (99%)	1 (1%)	86	89
1	C	130/140 (93%)	129 (99%)	1 (1%)	86	89
1	D	130/140 (93%)	130 (100%)	0	100	100
All	All	519/560 (93%)	517 (100%)	2 (0%)	93	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	ARG
1	C	144	LYS

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

Mol	Chain	Res	Type
1	A	30	HIS
1	B	30	HIS
1	B	52	ASN
1	C	30	HIS
1	D	30	HIS

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	1.18	2 (8%)	26,47,47	1.79	5 (19%)
3	COA	A	201	-	41,50,50	4.20	14 (34%)	49,75,75	2.30	10 (20%)
2	GDP	B	201	-	24,30,30	1.15	2 (8%)	26,47,47	1.94	6 (23%)
3	COA	B	202	-	41,50,50	4.25	14 (34%)	49,75,75	2.33	11 (22%)
2	GDP	C	200	-	24,30,30	1.12	2 (8%)	26,47,47	1.92	5 (19%)
3	COA	C	201	-	41,50,50	4.13	14 (34%)	49,75,75	2.23	9 (18%)
2	GDP	D	200	-	24,30,30	1.07	2 (8%)	26,47,47	1.98	5 (19%)
3	COA	D	201	-	41,50,50	4.21	15 (36%)	49,75,75	2.35	10 (20%)

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	201	-	-	0/12/32/32	0/3/3/3
3	COA	B	202	-	-	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 (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	COA	C2B-C1B	-12.97	1.33	1.53
3	B	202	COA	C2B-C1B	-12.80	1.33	1.53
3	C	201	COA	C2B-C1B	-12.39	1.33	1.53
3	A	201	COA	C2B-C1B	-12.39	1.34	1.53
3	A	201	COA	O4B-C4B	-6.37	1.30	1.45
3	C	201	COA	O4B-C4B	-6.36	1.30	1.45
3	D	201	COA	O4B-C4B	-6.25	1.30	1.45
3	B	202	COA	O4B-C4B	-6.22	1.30	1.45
3	A	201	COA	O3B-C3B	-4.27	1.30	1.44
3	D	201	COA	O3B-C3B	-4.21	1.30	1.44
3	B	202	COA	O3B-C3B	-4.17	1.30	1.44
3	C	201	COA	O3B-C3B	-3.85	1.31	1.44
3	B	202	COA	C5A-C4A	-3.82	1.31	1.40
3	D	201	COA	C5A-C4A	-3.63	1.32	1.40
3	A	201	COA	C5A-C4A	-3.56	1.32	1.40
3	D	201	COA	P3B-O9A	-3.53	1.42	1.54
3	C	201	COA	C5A-C4A	-3.50	1.32	1.40
3	B	202	COA	P3B-O9A	-3.49	1.42	1.54
3	D	201	COA	P3B-O7A	-3.48	1.39	1.50
3	C	201	COA	P3B-O9A	-3.48	1.42	1.54
3	D	201	COA	C7P-N8P	-3.36	1.38	1.46
3	A	201	COA	P3B-O9A	-3.25	1.43	1.54
3	C	201	COA	P3B-O7A	-3.22	1.40	1.50
3	B	202	COA	C7P-N8P	-3.21	1.38	1.46
3	B	202	COA	P3B-O7A	-3.11	1.41	1.50
3	A	201	COA	P3B-O7A	-2.99	1.41	1.50
3	A	201	COA	C7P-N8P	-2.94	1.39	1.46
3	C	201	COA	C7P-N8P	-2.77	1.39	1.46
3	D	201	COA	C4A-N3A	2.01	1.38	1.35
3	D	201	COA	O5P-C5P	2.08	1.27	1.23
3	A	201	COA	O5P-C5P	2.12	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	COA	O5P-C5P	2.23	1.28	1.23
3	B	202	COA	O2B-C2B	2.26	1.48	1.43
3	C	201	COA	O2B-C2B	2.43	1.48	1.43
3	D	201	COA	O2B-C2B	2.43	1.48	1.43
3	A	201	COA	O2B-C2B	2.45	1.48	1.43
3	B	202	COA	O5P-C5P	2.51	1.28	1.23
2	D	200	GDP	C5-C4	2.72	1.46	1.40
3	C	201	COA	C3B-C4B	2.84	1.60	1.52
2	A	200	GDP	C5-C4	2.96	1.47	1.40
3	D	201	COA	C3B-C4B	2.98	1.61	1.52
3	A	201	COA	C3B-C4B	2.98	1.61	1.52
2	C	200	GDP	C5-C4	3.03	1.47	1.40
3	B	202	COA	C3B-C4B	3.06	1.61	1.52
2	B	201	GDP	C5-C4	3.09	1.47	1.40
2	D	200	GDP	C6-C5	3.18	1.47	1.41
2	B	201	GDP	C6-C5	3.40	1.48	1.41
3	B	202	COA	C6A-N6A	3.42	1.48	1.34
2	C	200	GDP	C6-C5	3.44	1.48	1.41
3	C	201	COA	C6A-N6A	3.52	1.48	1.34
3	A	201	COA	C6A-N6A	3.56	1.48	1.34
3	D	201	COA	C6A-N6A	3.58	1.48	1.34
2	A	200	GDP	C6-C5	3.68	1.48	1.41
3	A	201	COA	C5P-N4P	3.70	1.42	1.33
3	D	201	COA	C5P-N4P	3.88	1.42	1.33
3	C	201	COA	C5P-N4P	3.90	1.42	1.33
3	B	202	COA	C5P-N4P	4.09	1.43	1.33
3	D	201	COA	C9P-N8P	6.86	1.47	1.33
3	A	201	COA	C9P-N8P	7.27	1.48	1.33
3	C	201	COA	C9P-N8P	7.34	1.48	1.33
3	B	202	COA	C9P-N8P	7.36	1.48	1.33
3	C	201	COA	O4B-C1B	17.78	1.66	1.41
3	D	201	COA	O4B-C1B	18.07	1.67	1.41
3	A	201	COA	O4B-C1B	18.41	1.67	1.41
3	B	202	COA	O4B-C1B	18.42	1.67	1.41

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	COA	N3A-C2A-N1A	-11.93	119.50	128.87
3	D	201	COA	N3A-C2A-N1A	-11.51	119.83	128.87
3	C	201	COA	N3A-C2A-N1A	-11.34	119.97	128.87
3	A	201	COA	N3A-C2A-N1A	-11.05	120.19	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	COA	N6A-C6A-N1A	-6.50	107.61	118.52
3	C	201	COA	N6A-C6A-N1A	-6.20	108.11	118.52
3	D	201	COA	N6A-C6A-N1A	-6.11	108.26	118.52
3	A	201	COA	N6A-C6A-N1A	-6.11	108.27	118.52
2	B	201	GDP	C5-C6-N1	-4.55	117.58	123.52
2	D	200	GDP	C5-C6-N1	-4.37	117.81	123.52
3	D	201	COA	C7P-C6P-C5P	-4.36	104.73	112.22
2	A	200	GDP	C5-C6-N1	-4.26	117.95	123.52
3	A	201	COA	C7P-C6P-C5P	-4.26	104.92	112.22
2	C	200	GDP	C5-C6-N1	-4.16	118.08	123.52
2	C	200	GDP	C6-C5-C4	-3.98	116.31	120.86
2	D	200	GDP	C6-C5-C4	-3.64	116.70	120.86
2	B	201	GDP	C6-C5-C4	-3.63	116.72	120.86
2	D	200	GDP	N3-C2-N1	-3.60	122.66	127.56
2	C	200	GDP	N3-C2-N1	-3.50	122.80	127.56
2	A	200	GDP	N3-C2-N1	-3.35	123.00	127.56
2	A	200	GDP	C6-C5-C4	-3.27	117.12	120.86
3	B	202	COA	C7P-C6P-C5P	-3.14	106.83	112.22
3	D	201	COA	C6P-C7P-N8P	-3.13	104.92	111.94
3	D	201	COA	C7P-N8P-C9P	-2.98	116.65	122.62
3	A	201	COA	C1B-N9A-C4A	-2.96	123.50	126.81
2	B	201	GDP	N3-C2-N1	-2.94	123.56	127.56
3	B	202	COA	C6P-C7P-N8P	-2.93	105.38	111.94
2	D	200	GDP	C1'-N9-C4	-2.92	123.55	126.81
3	A	201	COA	C6P-C7P-N8P	-2.86	105.55	111.94
3	A	201	COA	C3P-N4P-C5P	-2.83	117.18	122.79
3	C	201	COA	C1B-N9A-C4A	-2.82	123.66	126.81
2	B	201	GDP	C1'-N9-C4	-2.71	123.78	126.81
3	A	201	COA	C7P-N8P-C9P	-2.70	117.20	122.62
3	A	201	COA	CDP-CBP-CCP	-2.58	105.16	108.50
3	D	201	COA	C3P-N4P-C5P	-2.57	117.70	122.79
2	C	200	GDP	C1'-N9-C4	-2.55	123.95	126.81
3	D	201	COA	C1B-N9A-C4A	-2.54	123.97	126.81
3	C	201	COA	C6P-C7P-N8P	-2.46	106.43	111.94
3	C	201	COA	C7P-C6P-C5P	-2.44	108.03	112.22
3	C	201	COA	C3P-N4P-C5P	-2.35	118.14	122.79
3	D	201	COA	O5P-C5P-C6P	-2.29	117.99	121.97
3	C	201	COA	C4B-O4B-C1B	-2.23	107.28	109.64
3	B	202	COA	C7P-N8P-C9P	-2.22	118.17	122.62
3	C	201	COA	C2P-C3P-N4P	-2.21	108.05	112.44
3	B	202	COA	C1B-N9A-C4A	-2.12	124.44	126.81
3	B	202	COA	C2P-C3P-N4P	-2.11	108.26	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	COA	O5P-C5P-C6P	-2.06	118.39	121.97
3	A	201	COA	O5P-C5P-C6P	-2.01	118.49	121.97
3	B	202	COA	CDP-CBP-CAP	2.00	112.82	109.17
3	B	202	COA	C6P-C5P-N4P	2.01	119.95	116.46
3	C	201	COA	CEP-CBP-CCP	2.07	111.19	108.50
3	D	201	COA	C6P-C5P-N4P	2.24	120.35	116.46
3	D	201	COA	CDP-CBP-CAP	2.33	113.43	109.17
3	A	201	COA	C6P-C5P-N4P	2.35	120.54	116.46
3	B	202	COA	O5A-P2A-O3A	2.42	115.63	105.27
2	B	201	GDP	O2A-PA-O3A	2.44	115.70	105.27
2	A	200	GDP	N2-C2-N1	2.56	121.43	117.20
2	A	200	GDP	C6-N1-C2	4.84	121.55	115.88
2	B	201	GDP	C6-N1-C2	5.43	122.25	115.88
2	C	200	GDP	C6-N1-C2	5.69	122.55	115.88
2	D	200	GDP	C6-N1-C2	5.82	122.70	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	151:GLN	C	158:ALA	N	3.30
1	C	151:GLN	C	158:ALA	N	3.23
1	A	151:GLN	C	158:ALA	N	3.18

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^{th} 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	149/160 (93%)	0.12	8 (5%) 29 31	12, 22, 47, 69	0
1	B	147/160 (91%)	-0.04	5 (3%) 49 50	12, 21, 47, 71	0
1	C	148/160 (92%)	0.05	7 (4%) 35 37	13, 22, 46, 70	0
1	D	148/160 (92%)	-0.09	4 (2%) 58 58	11, 21, 46, 68	0
All	All	592/640 (92%)	0.01	24 (4%) 41 42	11, 22, 47, 71	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	GLN	6.0
1	C	158	ALA	5.7
1	B	150	LEU	5.3
1	C	151	GLN	5.0
1	C	7	LEU	4.8
1	A	158	ALA	4.6
1	A	7	LEU	4.5
1	B	151	GLN	4.3
1	B	149	SER	4.3
1	A	6	GLN	3.8
1	D	158	ALA	3.6
1	D	6	GLN	3.5
1	A	134	ARG	3.5
1	D	151	GLN	3.2
1	D	150	LEU	3.2
1	C	5	ARG	3.2
1	A	151	GLN	3.1
1	A	133	ASP	3.1
1	B	6	GLN	2.8
1	A	137	CYS	2.7
1	B	7	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	150	LEU	2.2
1	C	148	ILE	2.1
1	A	131	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no 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^{th} 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^2)	Q<0.9
3	COA	B	202	48/48	0.94	0.12	-0.16	12,22,36,48	0
3	COA	A	201	48/48	0.95	0.11	-0.23	12,22,31,40	0
2	GDP	A	200	28/28	0.96	0.12	-0.24	18,28,40,52	0
2	GDP	B	201	28/28	0.97	0.11	-0.25	17,24,43,46	0
3	COA	C	201	48/48	0.95	0.10	-0.29	15,24,36,42	0
3	COA	D	201	48/48	0.96	0.10	-0.33	13,23,36,40	0
2	GDP	C	200	28/28	0.98	0.09	-0.82	15,21,30,33	0
2	GDP	D	200	28/28	0.98	0.08	-1.00	14,21,28,33	0
4	CL	B	204	1/1	-	-	-	16,16,16,16	1
4	CL	C	202	1/1	-	-	-	17,17,17,17	1
4	CL	A	202	1/1	-	-	-	17,17,17,17	1
4	CL	B	203	1/1	-	-	-	16,16,16,16	1

6.5 Other polymers (i)

There are no such residues in this entry.