



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:35 PM GMT

PDB ID : 5CSL
Title : Crystal structure of the 500 kD yeast acetyl-CoA carboxylase holoenzyme dimer
Authors : Wei, J.; Tong, L.
Deposited on : 2015-07-23
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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-20026982
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-20026982

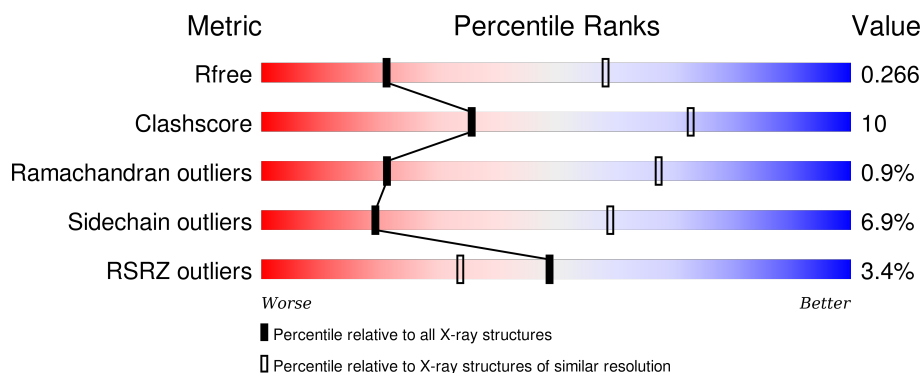
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. 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	2218	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 8%</div> </div> </div>
1	B	2218	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32777 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.

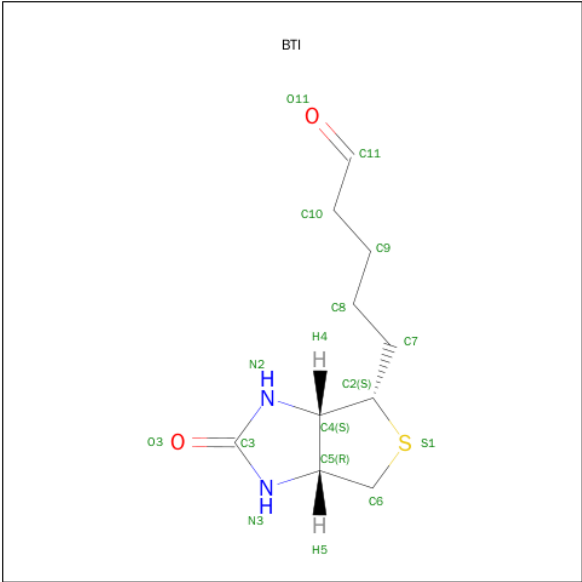
- Molecule 1 is a protein called Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2050	Total	C	N	O	S	0	0	0
			16249	10332	2798	3062	57			
1	B	2072	Total	C	N	O	S	0	0	0
			16402	10428	2835	3085	54			

There are 12 discrepancies between the modelled and reference sequences:

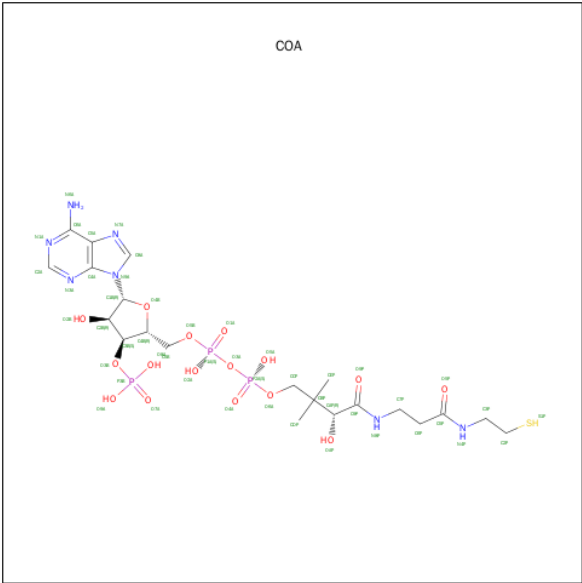
Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).

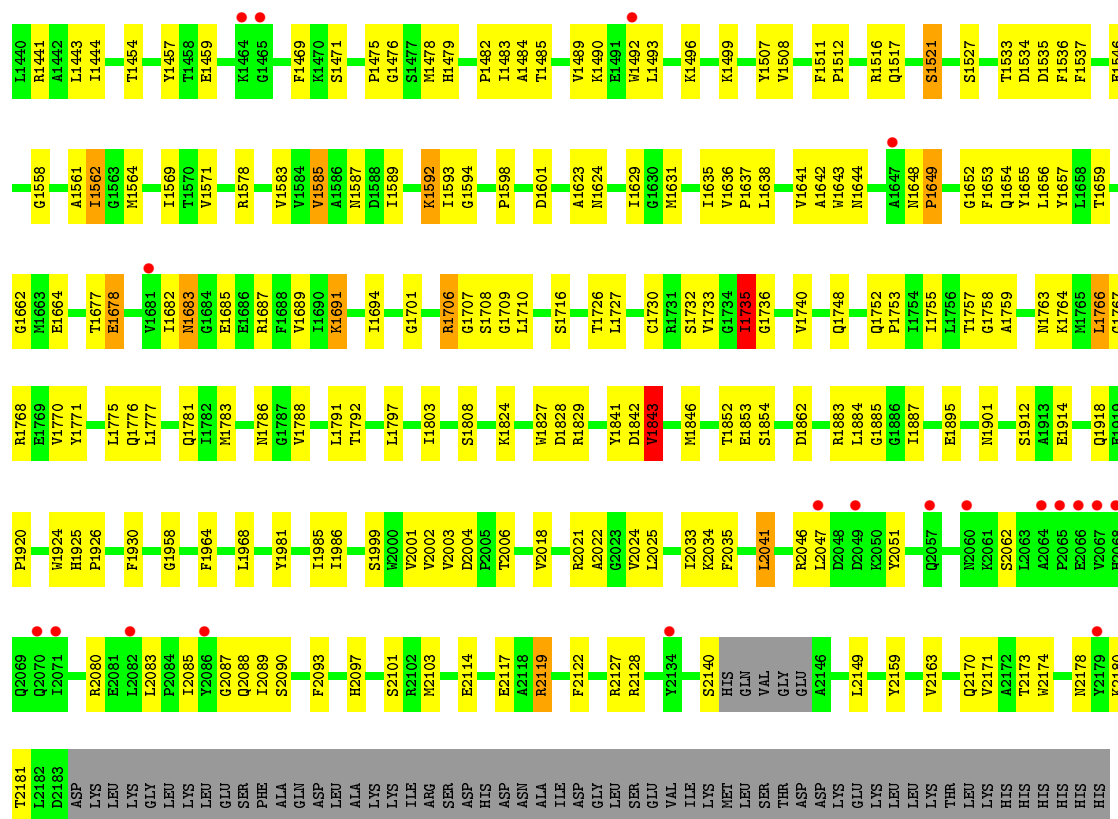


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

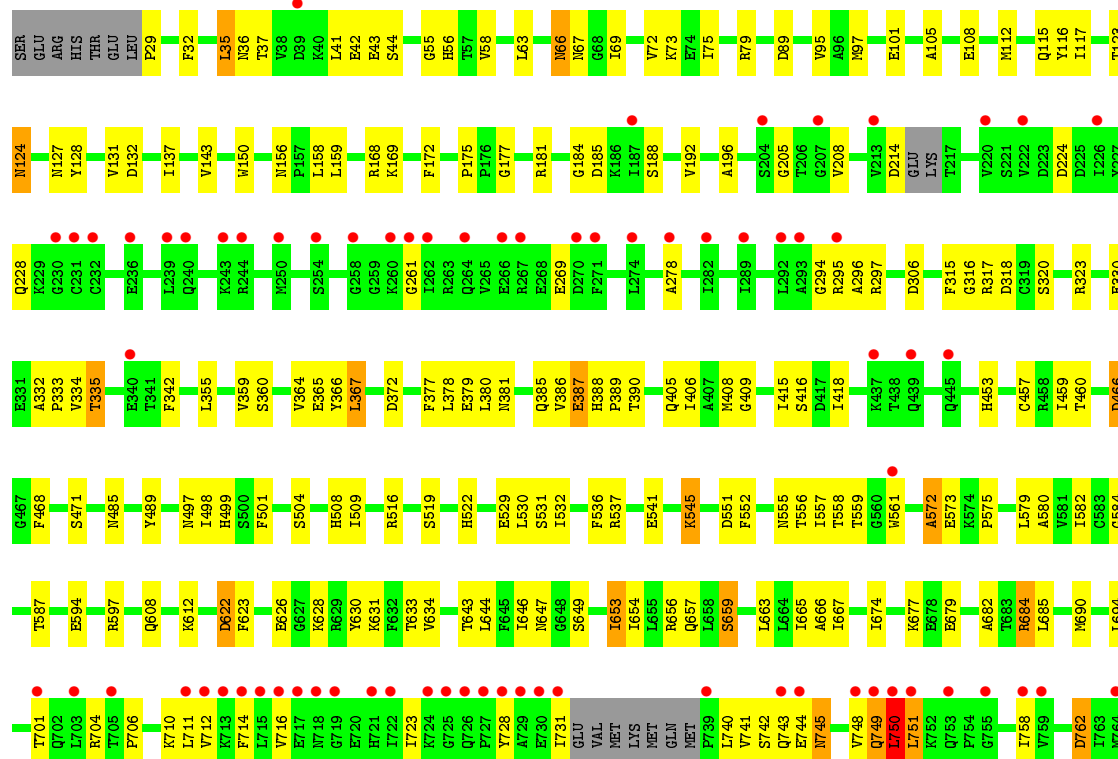
- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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		



• Molecule 1: Acetyl-CoA carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.87Å 159.87Å 614.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.20 49.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.93-3.20) 97.2 (49.88-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.219 , 0.266 0.220 , 0.266	Depositor DCC
R_{free} test set	6460 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	84.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 128555 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32777	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/16580	0.76	1/22444 (0.0%)
1	B	0.56	1/16738 (0.0%)	0.77	10/22654 (0.0%)
All	All	0.56	1/33318 (0.0%)	0.77	11/45098 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2187	LYS	C-O	6.45	1.35	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1419	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	1108	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	1084	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	1580	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	1638	LEU	CA-CB-CG	5.86	128.77	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	768	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16249	0	16225	309	1
1	B	16402	0	16387	359	1
2	A	30	0	31	6	0
3	A	48	0	32	5	0
3	B	48	0	32	3	0
All	All	32777	0	32707	634	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 10.

The worst 5 of 634 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:B:297:ARG:NH2	1:B:555:ASN:O	1.71	1.22
1:B:723:ILE:HA	1:B:745:ASN:HB3	1.37	1.05
1:B:466:ASP:OD1	1:B:466:ASP:O	1.82	0.98
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.00	0.93
1:A:1493:LEU:HD11	1:A:1507:TYR:CE1	2.03	0.93

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:OD1	1:A:440:ASP:OD1[7_555]	2.14	0.06
1:B:1170:SER:O	1:B:2180:LYS:NZ[7_645]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2030/2218 (92%)	1810 (89%)	201 (10%)	19 (1%)	21	67
1	B	2050/2218 (92%)	1836 (90%)	197 (10%)	17 (1%)	24	69
All	All	4080/4436 (92%)	3646 (89%)	398 (10%)	36 (1%)	21	67

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1316	ASP
1	B	712	VAL
1	A	573	GLU
1	A	820	VAL
1	B	572	ALA

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	1769/1912 (92%)	1652 (93%)	117 (7%)	21	61
1	B	1782/1912 (93%)	1654 (93%)	128 (7%)	18	57
All	All	3551/3824 (93%)	3306 (93%)	245 (7%)	19	59

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2117	GLU

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Mol	Chain	Res	Type
1	B	545	LYS
1	B	1802	LYS
1	A	2140	SER
1	B	269	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2097	HIS
1	B	370	HIS
1	B	1925	HIS
1	A	2170	GLN
1	B	280	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BTI	A	2301	1	14,16,16	1.01	1 (7%)	14,21,21	1.99	4 (28%)
2	BTI	A	2302	-	14,16,16	0.93	0	14,21,21	2.15	3 (21%)
3	COA	A	2303	-	41,50,50	0.97	2 (4%)	49,75,75	1.77	8 (16%)
3	COA	B	2301	-	41,50,50	1.11	3 (7%)	49,75,75	2.21	11 (22%)

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	BTI	A	2301	1	-	0/5/27/27	0/2/2/2
2	BTI	A	2302	-	-	0/5/27/27	0/2/2/2
3	COA	A	2303	-	-	0/44/64/64	0/3/3/3
3	COA	B	2301	-	-	0/44/64/64	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2301	BTI	C3-N2	-2.71	1.31	1.35
3	B	2301	COA	C4A-N3A	2.35	1.39	1.35
3	A	2303	COA	O4B-C1B	2.45	1.44	1.41
3	B	2301	COA	O4B-C1B	2.56	1.44	1.41
3	B	2301	COA	C5A-C4A	3.18	1.47	1.40

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2301	COA	N3A-C2A-N1A	-10.84	120.35	128.87
3	A	2303	COA	N3A-C2A-N1A	-7.30	123.14	128.87
3	B	2301	COA	C1B-N9A-C4A	-3.90	122.45	126.81
2	A	2302	BTI	N2-C3-N3	-3.71	106.29	108.85
2	A	2301	BTI	O3-C3-N2	-3.58	121.72	125.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2301	BTI	4	0
2	A	2302	BTI	2	0
3	A	2303	COA	5	0
3	B	2301	COA	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2050/2218 (92%)	-0.05	51 (2%) 61 47	46, 89, 147, 228	0
1	B	2072/2218 (93%)	0.01	90 (4%) 39 25	43, 88, 170, 239	0
All	All	4122/4436 (92%)	-0.02	141 (3%) 49 34	43, 89, 159, 239	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	ALA	5.7
1	B	292	LEU	5.4
1	B	2182	LEU	5.2
1	B	748	VAL	5.2
1	B	226	ILE	5.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BTI	A	2302	15/15	0.86	0.28	1.68	70,80,93,100	0
2	BTI	A	2301	15/15	0.91	0.25	0.93	66,74,78,82	0
3	COA	B	2301	48/48	0.87	0.22	0.40	71,128,148,158	0
3	COA	A	2303	48/48	0.92	0.21	-0.07	74,104,123,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.