



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:33 AM GMT

PDB ID : 2WL5  
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE  
H348N MUTANT WITH COENZYME A.  
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.  
Deposited on : 2009-06-22  
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

---

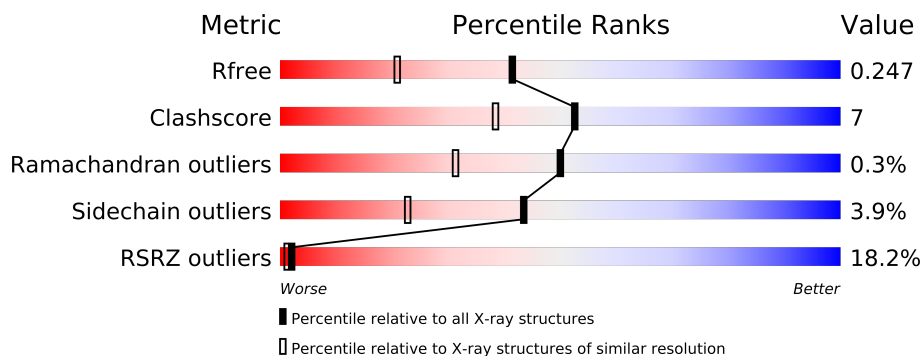
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
2	C	392	
2	D	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1395	-	X
3	SO4	A	1397	-	X
3	SO4	B	1396	-	X
3	SO4	B	1397	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
4	DNO	A	1398	-	X
4	DNO	C	1397	-	X
6	NA	B	1398	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12780 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	8	0
			2856	1783	513	539	21			
1	B	389	Total	C	N	O	S	0	7	0
			2850	1775	511	541	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 2 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	389	Total	C	N	O	S	0	1	0
			2815	1748	508	538	21			
2	D	389	Total	C	N	O	S	0	0	0
			2811	1744	508	538	21			

There are 4 discrepancies between the modelled and reference sequences:

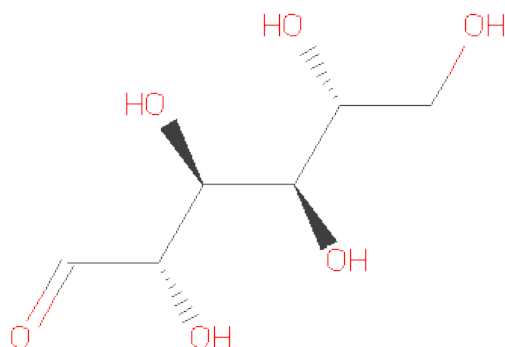
Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	348	ASN	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



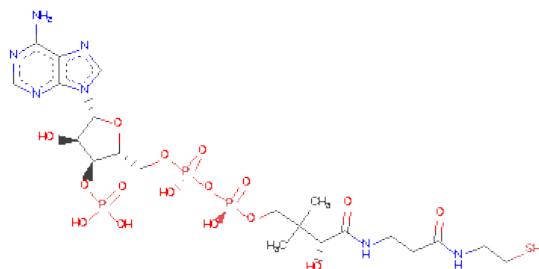
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SUGAR (D-MANNOSE) (three-letter code: DNO) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	
5	B	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na		
			1	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

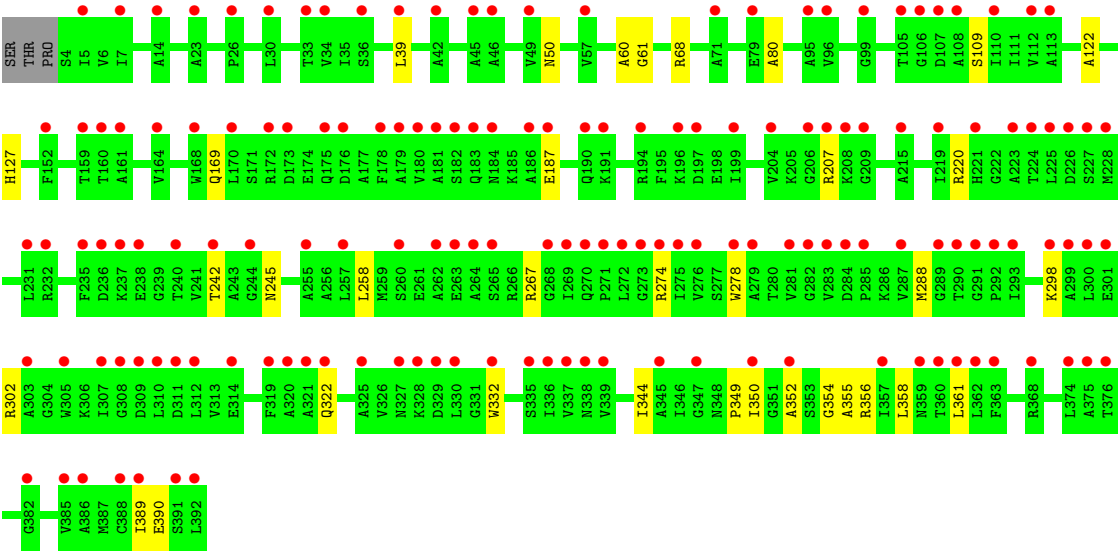
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl		
			1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	453	Total	O		
			453	453	0	0
8	B	479	Total	O		
			479	479	0	0
8	C	171	Total	O		
			171	171	0	0
8	D	129	Total	O		
			129	129	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.70Å 79.20Å 153.00Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	19.39 – 1.80 19.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.39-1.80) 86.6 (19.39-1.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.257 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	9225 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 74.0	EDS
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 184510 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, CL, NA, DNO, COA, SO4

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	0.54	0/2912	0.67	0/3928
1	B	0.54	0/2900	0.69	3/3910 (0.1%)
2	C	0.27	0/2858	0.46	0/3859
2	D	0.26	0/2851	0.46	0/3849
All	All	0.43	0/11521	0.58	3/15546 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	361	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	367	ARG	NE-CZ-NH1	5.27	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2856	0	0	25	0
1	B	2850	0	0	15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2815	0	0	21	0
2	D	2811	0	0	19	0
3	A	20	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
4	A	12	0	12	0	0
4	C	36	0	36	2	0
5	A	48	0	32	4	0
5	B	48	0	32	1	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	453	0	0	17	0
8	B	479	0	0	9	0
8	C	171	0	0	14	0
8	D	129	0	0	13	0
All	All	12780	0	112	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 83 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:125:CYS:SG	8:D:2021:HOH:O	2.30	0.89
1:B:125:CYS:SG	8:B:2183:HOH:O	2.48	0.72
2:C:136:ASP:N	4:C:1397:DNO:HO6	1.90	0.68
1:A:220[B]:ARG:NH1	8:A:2300:HOH:O	2.27	0.67
2:C:128:LEU:O	8:C:2065:HOH:O	2.14	0.65

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/392 (100%)	378 (96%)	16 (4%)	0	100	100
1	B	393/392 (100%)	380 (97%)	12 (3%)	1 (0%)	50	31
2	C	388/392 (99%)	365 (94%)	22 (6%)	1 (0%)	50	31
2	D	387/392 (99%)	359 (93%)	26 (7%)	2 (0%)	38	19
All	All	1562/1568 (100%)	1482 (95%)	76 (5%)	4 (0%)	50	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	350	ILE
2	D	350	ILE
2	D	169	GLN
1	B	350	ILE

### 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	283/278 (102%)	269 (95%)	14 (5%)	35	15
1	B	282/278 (101%)	268 (95%)	14 (5%)	34	14
2	C	277/279 (99%)	270 (98%)	7 (2%)	60	42
2	D	276/279 (99%)	265 (96%)	11 (4%)	42	22
All	All	1118/1114 (100%)	1072 (96%)	46 (4%)	43	21

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	263	GLU
1	B	358[A]	LEU
2	D	322	GLN
1	B	288	MET
1	B	322	GLN

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	CSO	A	89	1	6,6,7	7.62	2 (33%)	3,6,8	1.82	1 (33%)
1	CSO	B	89	1	6,6,7	7.28	3 (50%)	3,6,8	0.92	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
1	CSO	A	89	1	-	0/2/5/7	0/0/0/0
1	CSO	B	89	1	-	0/2/5/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	CSO	O-C	18.18	1.23	1.11
1	B	89	CSO	O-C	17.21	1.23	1.11
1	B	89	CSO	OD-SG	4.07	1.79	1.62
1	A	89	CSO	OD-SG	3.95	1.79	1.62
1	B	89	CSO	CA-C	2.10	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	CSO	CA-CB-SG	-3.08	107.54	113.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\# Z  > 2$
3	SO4	A	1394	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	A	1395	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	1396	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	1397	-	4,4,4	0.21	0	6,6,6	0.06	0
4	DNO	A	1398	-	11,11,11	1.95	3 (27%)	14,14,14	2.04	6 (42%)
5	COA	A	1399	-	50,50,50	2.42	17 (34%)	75,75,75	2.18	16 (21%)
3	SO4	B	1394	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	1395	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	1396	-	4,4,4	0.19	0	6,6,6	0.06	0
3	SO4	B	1397	-	4,4,4	0.24	0	6,6,6	0.08	0
5	COA	B	1399	-	50,50,50	2.42	15 (30%)	75,75,75	2.31	16 (21%)
3	SO4	B	1401	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	C	1393	-	4,4,4	0.20	0	6,6,6	0.06	0
3	SO4	C	1394	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	C	1395	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	C	1396	-	4,4,4	0.21	0	6,6,6	0.09	0
4	DNO	C	1397	-	11,11,11	1.81	2 (18%)	14,14,14	1.74	5 (35%)
4	DNO	C	1398	-	11,11,11	1.88	2 (18%)	14,14,14	1.99	7 (50%)
4	DNO	C	1399	-	11,11,11	1.94	3 (27%)	14,14,14	2.02	7 (50%)
3	SO4	D	1393	-	4,4,4	0.18	0	6,6,6	0.13	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	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1397	-	-	0/0/0/0	0/0/0/0
4	DNO	A	1398	-	2/2/4/5	0/15/16/16	0/0/0/0
5	COA	A	1399	-	-	0/48/64/64	0/1/3/3
3	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1396	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1397	-	-	0/0/0/0	0/0/0/0
5	COA	B	1399	-	-	0/48/64/64	0/1/3/3
3	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1393	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1396	-	-	0/0/0/0	0/0/0/0
4	DNO	C	1397	-	2/2/4/5	1/15/16/16	0/0/0/0
4	DNO	C	1398	-	2/2/4/5	0/15/16/16	0/0/0/0
4	DNO	C	1399	-	2/2/4/5	0/15/16/16	0/0/0/0
3	SO4	D	1393	-	-	0/0/0/0	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1399	COA	C9P-N8P	6.70	1.48	1.33
5	A	1399	COA	C9P-N8P	6.57	1.47	1.33
5	B	1399	COA	C5P-N4P	5.75	1.46	1.33
5	A	1399	COA	C5P-N4P	5.72	1.46	1.33
5	B	1399	COA	C4A-N9A	4.86	1.44	1.37

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1399	COA	N3A-C2A-N1A	-11.52	119.08	128.71
5	A	1399	COA	N3A-C2A-N1A	-10.59	119.86	128.71
5	B	1399	COA	O4B-C1B-N9A	7.57	115.48	108.44
5	A	1399	COA	C2B-C1B-N9A	6.33	129.51	113.27
5	B	1399	COA	P2A-O3A-P1A	-6.23	113.42	131.68



5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1399	DNO	C2
4	C	1399	DNO	C3
4	A	1398	DNO	C2
4	A	1398	DNO	C3
4	C	1398	DNO	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1397	DNO	O1-C1-C2-C3

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	389/392 (99%)	-0.13	5 (1%) 74 70	5, 13, 34, 96	0
1	B	389/392 (99%)	-0.17	3 (0%) 83 81	5, 13, 32, 88	0
2	C	389/392 (99%)	1.64	124 (31%) 1 1	18, 50, 79, 108	0
2	D	389/392 (99%)	1.98	154 (39%) 1 1	20, 57, 102, 131	0
All	All	1556/1568 (99%)	0.83	286 (18%) 2 1	5, 34, 81, 131	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	285	PRO	9.5
2	D	269	ILE	8.4
2	D	265	SER	8.2
2	D	207	ARG	8.2
2	D	307	ILE	8.1

### 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	A	89	7/8	0.08	-0.28	7,9,23,28	0
1	CSO	B	89	7/8	0.07	-1.76	2,6,26,28	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NA	B	1398	1/1	1.47	189.14	123,123,123,123	0
3	SO4	B	1397	5/5	0.28	17.33	71,71,73,77	0
3	SO4	B	1396	5/5	0.31	15.25	77,80,81,82	0
4	DNO	C	1397	12/12	0.23	13.18	44,55,91,93	0
4	DNO	A	1398	12/12	0.31	10.05	42,52,75,76	0
3	SO4	A	1395	5/5	0.15	4.11	43,50,53,57	0
3	SO4	A	1397	5/5	0.15	2.62	72,73,76,77	0
3	SO4	C	1394	5/5	0.33	1.20	129,131,131,131	0
3	SO4	C	1396	5/5	0.29	0.46	64,66,67,71	0
3	SO4	C	1395	5/5	0.31	0.34	81,83,86,87	0
4	DNO	C	1398	12/12	0.31	0.27	57,65,78,79	0
3	SO4	B	1394	5/5	0.10	0.17	30,39,41,43	0
5	COA	A	1399	48/48	0.12	0.17	15,28,76,107	0
5	COA	B	1399	48/48	0.10	0.15	12,27,61,75	0
3	SO4	B	1395	5/5	0.10	-0.64	41,44,47,48	0
4	DNO	C	1399	12/12	0.23	-0.78	42,55,72,72	0
3	SO4	C	1393	5/5	0.18	-1.39	75,77,78,79	0
3	SO4	A	1394	5/5	0.08	-1.81	40,44,50,56	0
3	SO4	D	1393	5/5	0.10	-2.48	61,62,65,67	0
7	CL	B	1400	1/1	0.13	-	68,68,68,68	0
3	SO4	A	1396	5/5	0.17	-	64,64,66,66	0
3	SO4	B	1401	5/5	0.27	-	89,90,91,92	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.