



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:34 am BST

PDB ID : 2WKU
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. THE N316H MUTANT.
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.
Deposited on : 2009-06-18
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

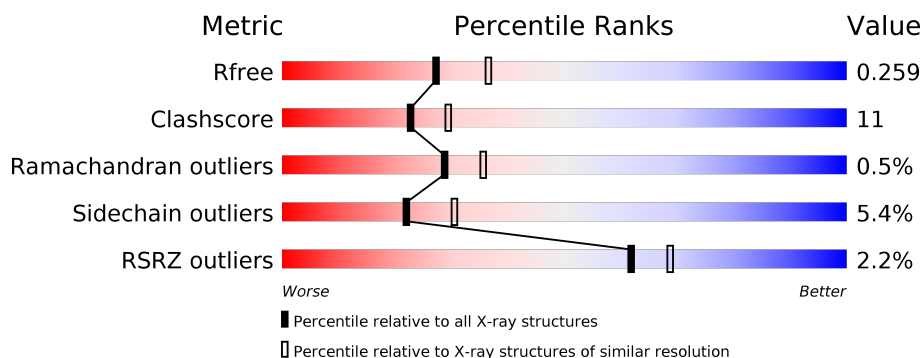
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 ≥ 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	392	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	392	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	392	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>
1	D	392	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DNO	A	1396	X	-	-	-
3	DNO	A	1397	X	-	X	-
3	DNO	A	1398	X	-	X	-
3	DNO	B	1397	X	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11989 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 ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2815	1748	510	536	21			
1	B	389	Total	C	N	O	S	0	1	0
			2821	1753	511	536	21			
1	C	389	Total	C	N	O	S	0	0	0
			2815	1748	510	536	21			
1	D	389	Total	C	N	O	S	0	0	0
			2815	1748	510	536	21			

There are 8 discrepancies between the modelled and reference sequences:

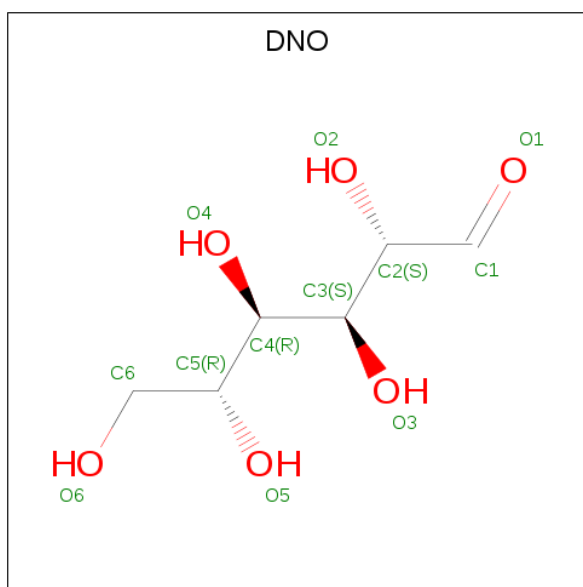
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	316	HIS	ASN	engineered mutation	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	316	HIS	ASN	engineered mutation	UNP P07097
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	316	HIS	ASN	engineered mutation	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	316	HIS	ASN	engineered mutation	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is D-mannose (three-letter code: DNO) (formula: C₆H₁₂O₆).



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

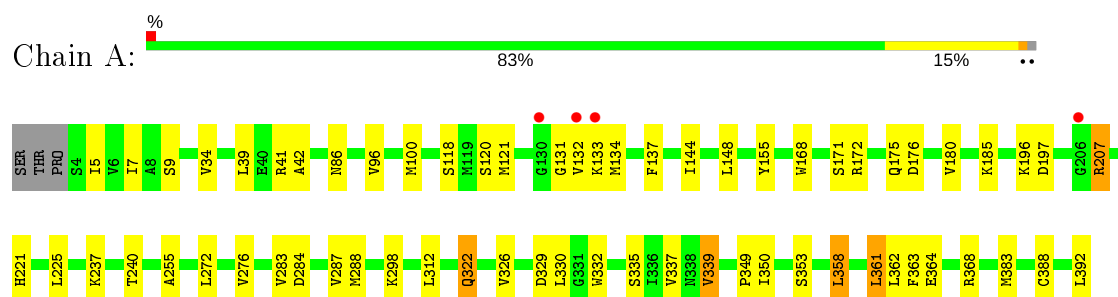
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	214	Total	O	0	0
			214	214		
4	C	115	Total	O	0	0
			115	115		
4	D	106	Total	O	0	0
			106	106		

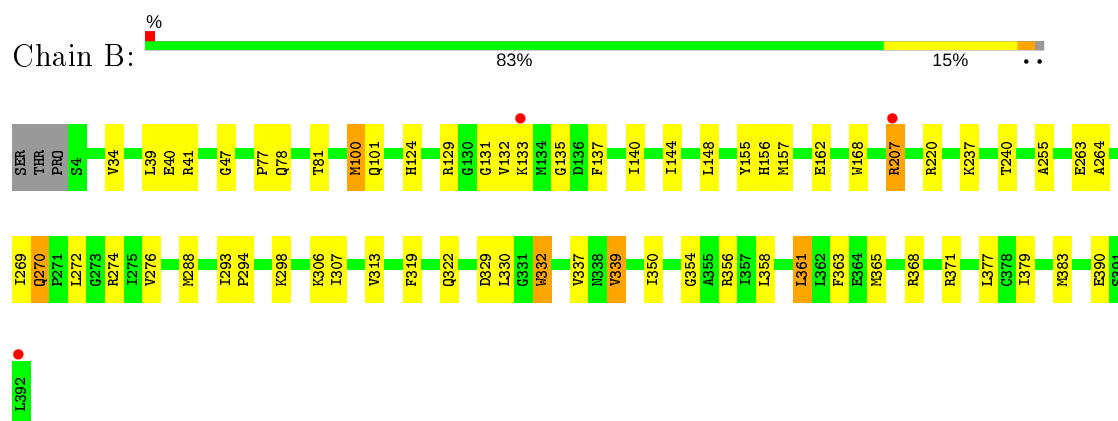
3 Residue-property plots

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

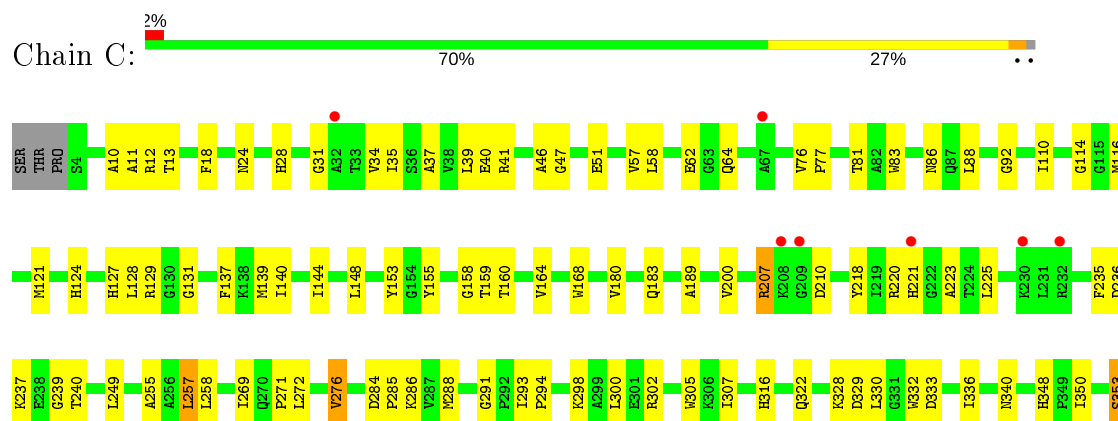
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE



• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

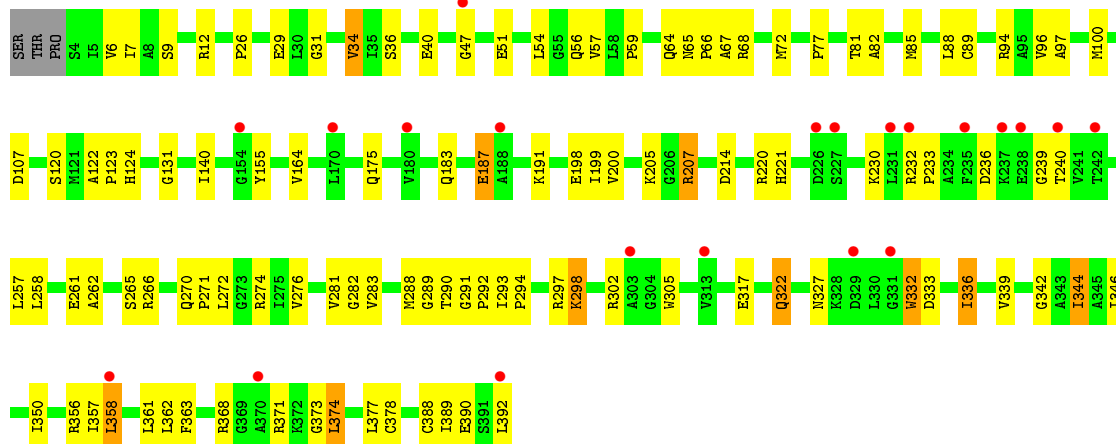


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE





• Molecule 1: ACETYL-COA ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.50 Å 79.50 Å 147.70 Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-2.30) 92.4 (19.99-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 2.30 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.258 0.203 , 0.259	Depositor DCC
R_{free} test set	4345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.209 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11989	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.333 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: DNO, 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	0.34	0/2857	0.52	0/3857
1	B	0.33	0/2866	0.53	0/3868
1	C	0.26	0/2857	0.46	0/3857
1	D	0.25	0/2857	0.46	0/3857
All	All	0.30	0/11437	0.49	0/15439

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	2815	0	2820	50	0
1	B	2821	0	2833	50	0
1	C	2815	0	2820	88	0
1	D	2815	0	2820	82	0
2	A	15	0	0	0	0
2	B	25	0	0	1	0
2	C	5	0	0	0	0
3	A	36	0	36	17	0
3	B	12	0	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	195	0	0	3	0
4	B	214	0	0	6	0
4	C	115	0	0	7	0
4	D	106	0	0	10	0
All	All	11989	0	11341	260	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 11.

The worst 5 of 260 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:269:ILE:HB	4:B:2164:HOH:O	1.41	1.18
1:B:41:ARG:HG2	3:B:1397:DNO:H6	1.37	1.05
1:B:41:ARG:HB3	3:B:1397:DNO:H3	1.41	1.01
1:D:120:SER:HA	4:D:2004:HOH:O	1.67	0.94
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.33	0.92

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	387/392 (99%)	373 (96%)	12 (3%)	2 (0%)	29	35
1	B	388/392 (99%)	372 (96%)	15 (4%)	1 (0%)	41	50
1	C	387/392 (99%)	364 (94%)	21 (5%)	2 (0%)	29	35
1	D	387/392 (99%)	358 (92%)	27 (7%)	2 (0%)	29	35
All	All	1549/1568 (99%)	1467 (95%)	75 (5%)	7 (0%)	29	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	A	134	MET
1	A	350	ILE
1	C	210	ASP

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	276/279 (99%)	263 (95%)	13 (5%)	26	37
1	B	277/279 (99%)	262 (95%)	15 (5%)	22	30
1	C	276/279 (99%)	260 (94%)	16 (6%)	20	27
1	D	276/279 (99%)	260 (94%)	16 (6%)	20	27
All	All	1105/1116 (99%)	1045 (95%)	60 (5%)	22	30

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	LEU
1	C	257	LEU
1	D	336	ILE
1	C	200	VAL
1	C	272	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	GLN
1	C	175	GLN
1	D	184	ASN
1	B	322	GLN
1	D	316	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 ⓘ

13 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	SO4	B	1395	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	1393	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	A	1394	-	4,4,4	0.18	0	6,6,6	0.24	0
2	SO4	C	1393	-	4,4,4	0.16	0	6,6,6	0.04	0
2	SO4	B	1396	-	4,4,4	0.14	0	6,6,6	0.08	0
3	DNO	A	1396	-	10,11,11	2.00	1 (10%)	13,14,14	2.05	5 (38%)
2	SO4	B	1393	-	4,4,4	0.19	0	6,6,6	0.06	0
2	SO4	A	1395	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	B	1398	-	4,4,4	0.15	0	6,6,6	0.12	0
3	DNO	A	1398	-	10,11,11	1.99	2 (20%)	13,14,14	1.95	4 (30%)
3	DNO	A	1397	-	10,11,11	2.18	2 (20%)	13,14,14	2.00	4 (30%)
2	SO4	B	1394	-	4,4,4	0.14	0	6,6,6	0.13	0
3	DNO	B	1397	-	10,11,11	1.94	1 (10%)	13,14,14	2.67	9 (69%)

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	DNO	B	1397	-	2/2/4/5	8/14/16/16	-
3	DNO	A	1396	-	2/2/4/5	10/14/16/16	-
3	DNO	A	1398	-	2/2/4/5	9/14/16/16	-
3	DNO	A	1397	-	2/2/4/5	10/14/16/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1397	DNO	O1-C1	5.58	1.42	1.19
3	A	1396	DNO	O1-C1	5.46	1.41	1.19
3	B	1397	DNO	O1-C1	5.45	1.41	1.19
3	A	1398	DNO	O1-C1	5.42	1.41	1.19
3	A	1397	DNO	O2-C2	-2.09	1.39	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1397	DNO	C5-C4-C3	4.68	119.79	112.47
3	B	1397	DNO	O3-C3-C2	4.18	116.83	109.17
3	A	1397	DNO	C4-C3-C2	3.91	120.36	113.54
3	A	1396	DNO	O3-C3-C2	3.81	116.16	109.17
3	A	1398	DNO	O6-C6-C5	3.64	119.00	111.07

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1396	DNO	C2
3	A	1396	DNO	C3
3	A	1398	DNO	C2
3	A	1398	DNO	C3
3	A	1397	DNO	C2

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1396	DNO	C1-C2-C3-O3
3	A	1396	DNO	C2-C3-C4-C5
3	A	1396	DNO	C2-C3-C4-O4
3	A	1396	DNO	O3-C3-C4-C5
3	A	1396	DNO	O3-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1396	SO4	1	0
3	A	1396	DNO	4	0
3	A	1398	DNO	7	0
3	A	1397	DNO	6	0
3	B	1397	DNO	7	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	389/392 (99%)	-0.65	4 (1%) 82 86	11, 21, 49, 99	0
1	B	389/392 (99%)	-0.68	3 (0%) 86 89	9, 22, 47, 101	0
1	C	389/392 (99%)	0.01	7 (1%) 68 74	29, 45, 67, 98	0
1	D	389/392 (99%)	0.25	21 (5%) 25 32	30, 49, 78, 120	0
All	All	1556/1568 (99%)	-0.27	35 (2%) 62 69	9, 38, 69, 120	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	4.6
1	B	207	ARG	3.9
1	D	238	GLU	3.2
1	A	133	LYS	3.2
1	D	231	LEU	3.1

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. 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	B-factors(\AA^2)	Q<0.9
3	DNO	A	1398	12/12	0.76	0.36	39,93,112,116	0
2	SO4	B	1395	5/5	0.83	0.30	115,116,120,120	0
2	SO4	B	1396	5/5	0.84	0.20	96,98,101,107	0
3	DNO	A	1396	12/12	0.87	0.24	18,48,61,65	0
3	DNO	A	1397	12/12	0.89	0.28	11,53,77,83	0
3	DNO	B	1397	12/12	0.90	0.30	20,39,57,57	0
2	SO4	A	1395	5/5	0.94	0.17	69,69,82,83	0
2	SO4	B	1394	5/5	0.96	0.12	50,51,60,71	0
2	SO4	B	1393	5/5	0.97	0.13	37,56,61,68	0
2	SO4	A	1393	5/5	0.97	0.12	42,51,57,58	0
2	SO4	C	1393	5/5	0.97	0.12	63,66,68,77	0
2	SO4	A	1394	5/5	0.98	0.10	34,49,53,53	0
2	SO4	B	1398	5/5	0.98	0.13	47,57,61,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.