



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 12:07 AM EDT

PDB ID : 1RU3
Title : Crystal Structure of the monomeric acetyl-CoA synthase from *Carboxydothermus hydrogenoformans*
Authors : Svetlitchnyi, V.; Dobbek, H.; Meyer-Klaucke, W.; Meins, T.; Thiele, B.; Rmer, P.; Huber, R.; Meyer, O.
Deposited on : 2003-12-11
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

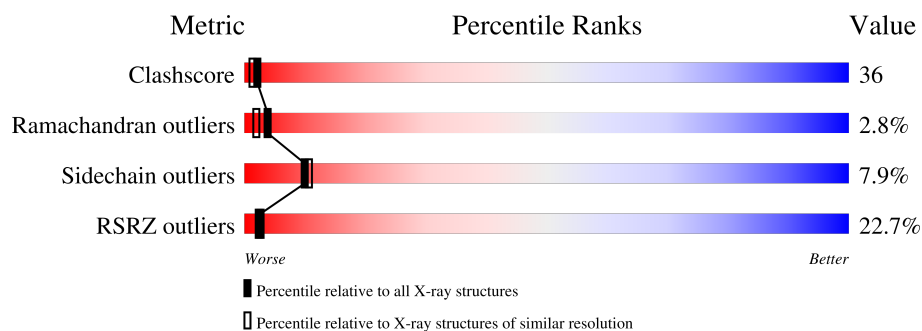
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.20 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))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 of 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	732	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	959	-	X	-	-
4	GOL	A	960	-	X	-	-
4	GOL	A	961	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	962	-	X	-	-
4	GOL	A	963	-	X	-	-
4	GOL	A	964	-	X	-	-
4	GOL	A	965	-	X	-	-
4	GOL	A	966	-	X	-	-
4	GOL	A	967	-	X	-	-
4	GOL	A	968	-	X	-	-
4	GOL	A	969	-	X	-	-
4	GOL	A	970	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6064 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.

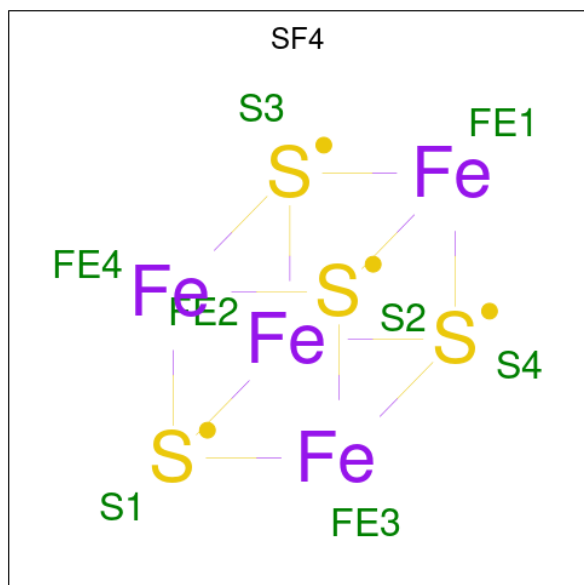
- Molecule 1 is a protein called Acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5759	3697	964	1069	29			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ni	0	0
			2	2		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

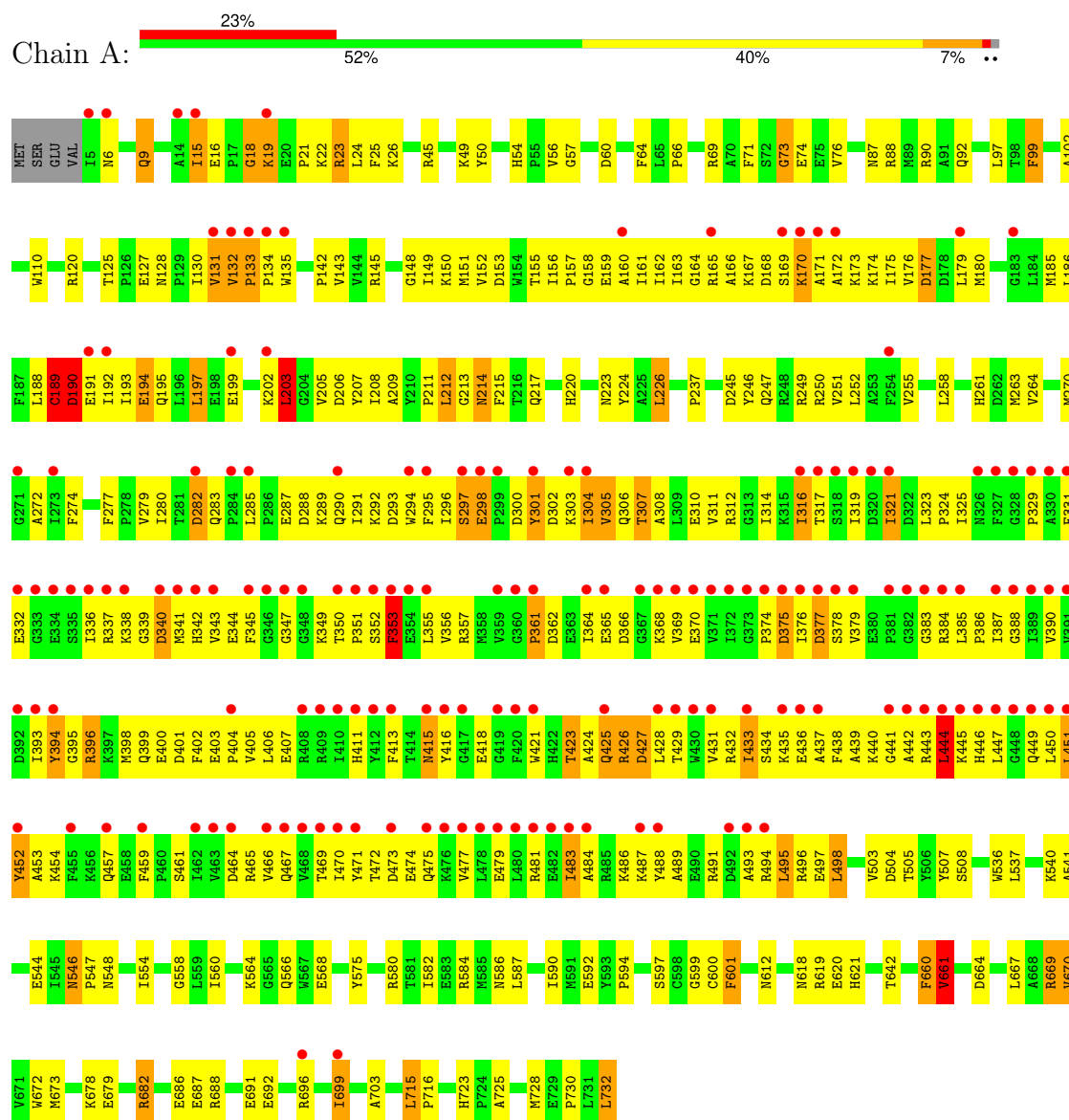
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total 223	O 223	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	200.31Å 200.31Å 169.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 98.7 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.274 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: NI, GOL, SF4

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	0.77	1/5893 (0.0%)	0.96	18/7978 (0.2%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	VAL	CB-CG1	-5.46	1.41	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	CYS	CA-C-N	-11.37	92.19	117.20
1	A	669	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	189	CYS	O-C-N	8.47	136.25	122.70
1	A	189	CYS	C-N-CA	8.16	142.11	121.70
1	A	600	CYS	CA-CB-SG	-6.15	102.93	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	CYS	Mainchain
1	A	394	TYR	Sidechain

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	5759	0	5735	419	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	72	0	48	8	0
5	A	223	0	0	6	0
All	All	6064	0	5783	422	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 36.

The worst 5 of 422 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)
4:A:966:GOL:C1	4:A:966:GOL:O1	1.65	1.42
1:A:351:PRO:HG2	1:A:386:PRO:HB3	1.23	1.19
1:A:22:LYS:HE2	1:A:97:LEU:HD12	1.34	1.09
1:A:163:ILE:HA	1:A:189:CYS:O	1.58	1.03
1:A:385:LEU:HD12	1:A:386:PRO:HD2	1.38	1.01

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	726/732 (99%)	639 (88%)	67 (9%)	20 (3%)	4 2

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	A	301	TYR
1	A	304	ILE
1	A	375	ASP
1	A	353	PHE

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	610/614 (99%)	562 (92%)	48 (8%)	10 11

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ASP
1	A	483	ILE
1	A	415	ASN
1	A	433	ILE
1	A	546	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	A	579	GLN
1	A	571	ASN
1	A	586	ASN
1	A	399	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
4	GOL	A	968	-	5,5,5	4.59	5 (100%)	5,5,5	6.08	3 (60%)
4	GOL	A	961	-	5,5,5	4.77	5 (100%)	5,5,5	6.07	3 (60%)
4	GOL	A	960	-	5,5,5	4.89	5 (100%)	5,5,5	6.16	3 (60%)
4	GOL	A	966	-	5,5,5	4.75	5 (100%)	5,5,5	6.26	3 (60%)
4	GOL	A	969	-	5,5,5	4.42	5 (100%)	5,5,5	5.82	3 (60%)
4	GOL	A	964	-	5,5,5	4.69	5 (100%)	5,5,5	6.23	3 (60%)
4	GOL	A	962	-	5,5,5	5.27	5 (100%)	5,5,5	5.92	3 (60%)
4	GOL	A	970	-	5,5,5	4.76	5 (100%)	5,5,5	6.14	3 (60%)
4	GOL	A	959	-	5,5,5	4.87	5 (100%)	5,5,5	6.07	3 (60%)
4	GOL	A	967	-	5,5,5	4.88	5 (100%)	5,5,5	5.91	3 (60%)
4	GOL	A	963	-	5,5,5	4.68	5 (100%)	5,5,5	6.06	3 (60%)
3	SF4	A	733	1	0,12,12	-	-	-	-	-
4	GOL	A	965	-	5,5,5	4.69	5 (100%)	5,5,5	6.11	3 (60%)

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
4	GOL	A	968	-	-	3/4/4/4	-
4	GOL	A	961	-	-	3/4/4/4	-
4	GOL	A	960	-	-	3/4/4/4	-
4	GOL	A	969	-	-	2/4/4/4	-
4	GOL	A	964	-	-	2/4/4/4	-
4	GOL	A	962	-	-	2/4/4/4	-
4	GOL	A	970	-	-	2/4/4/4	-
3	SF4	A	733	1	-	-	0/6/5/5
4	GOL	A	959	-	-	3/4/4/4	-
4	GOL	A	967	-	-	2/4/4/4	-
4	GOL	A	963	-	-	3/4/4/4	-
4	GOL	A	966	-	-	2/4/4/4	-
4	GOL	A	965	-	-	2/4/4/4	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	962	GOL	C3-C2	-8.73	1.18	1.51
4	A	959	GOL	C3-C2	-8.46	1.19	1.51
4	A	967	GOL	C3-C2	-8.28	1.20	1.51
4	A	960	GOL	C3-C2	-8.10	1.20	1.51
4	A	963	GOL	C3-C2	-7.98	1.21	1.51

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	966	GOL	O3-C3-C2	11.35	161.47	110.38
4	A	964	GOL	O3-C3-C2	11.32	161.33	110.38
4	A	960	GOL	O3-C3-C2	11.24	160.98	110.38
4	A	961	GOL	O3-C3-C2	11.09	160.30	110.38
4	A	970	GOL	O3-C3-C2	11.03	160.01	110.38

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	959	GOL	C1-C2-C3-O3
4	A	960	GOL	C1-C2-C3-O3
4	A	961	GOL	O1-C1-C2-C3
4	A	961	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	962	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	966	GOL	3	0
4	A	962	GOL	3	0
4	A	967	GOL	1	0
4	A	965	GOL	2	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	728/732 (99%)	0.94	165 (22%) 3 2	31, 62, 134, 162	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	TRP	10.4
1	A	364	ILE	6.3
1	A	433	ILE	6.1
1	A	477	VAL	6.0
1	A	298	GLU	5.7

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 monosaccharides 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(Å ²)	Q<0.9
4	GOL	A	964	6/6	0.58	0.18	90,106,110,114	0
4	GOL	A	968	6/6	0.62	0.13	79,83,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	961	6/6	0.69	0.18	94,104,108,113	0
4	GOL	A	963	6/6	0.70	0.14	108,119,123,125	0
4	GOL	A	966	6/6	0.76	0.18	63,84,90,92	0
4	GOL	A	960	6/6	0.77	0.14	88,101,102,103	0
4	GOL	A	970	6/6	0.79	0.12	95,107,113,115	0
4	GOL	A	969	6/6	0.83	0.13	63,70,84,87	0
4	GOL	A	965	6/6	0.87	0.13	74,96,108,109	0
4	GOL	A	962	6/6	0.87	0.25	48,59,66,71	0
4	GOL	A	967	6/6	0.87	0.11	85,95,101,101	0
4	GOL	A	959	6/6	0.89	0.16	85,98,102,107	0
3	SF4	A	733	8/8	0.96	0.10	44,47,48,48	0
2	NI	A	734	1/1	0.99	0.04	53,53,53,53	0
2	NI	A	735	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.