



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 01:36 am GMT

PDB ID : 1W2X
Title : Crystal structure of the carboxyltransferase domain of acetyl- coenzyme A
carboxylase in complex with CP-640186
Authors : Zhang, H.; Tweel, B.; Li, J.; Tong, L.
Deposited on : 2004-07-09
Resolution : 2.80 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

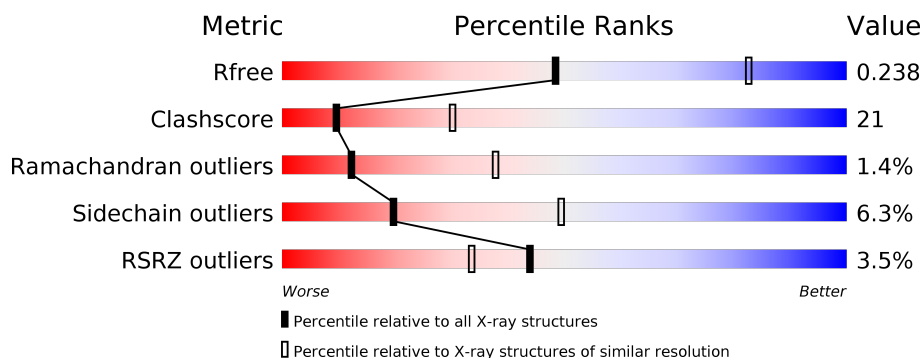
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 ≥ 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	758	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	758	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>35%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	758	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition [i](#)

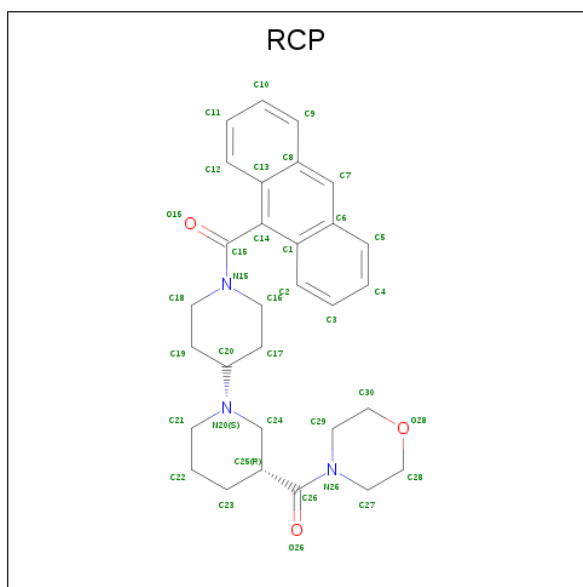
There are 3 unique types of molecules in this entry. The entry contains 16588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	682	Total	C	N	O	S	0	0	1
			5425	3459	931	1016	19			
1	B	676	Total	C	N	O	S	0	0	1
			5377	3427	924	1007	19			
1	C	666	Total	C	N	O	S	0	0	1
			5299	3374	913	993	19			

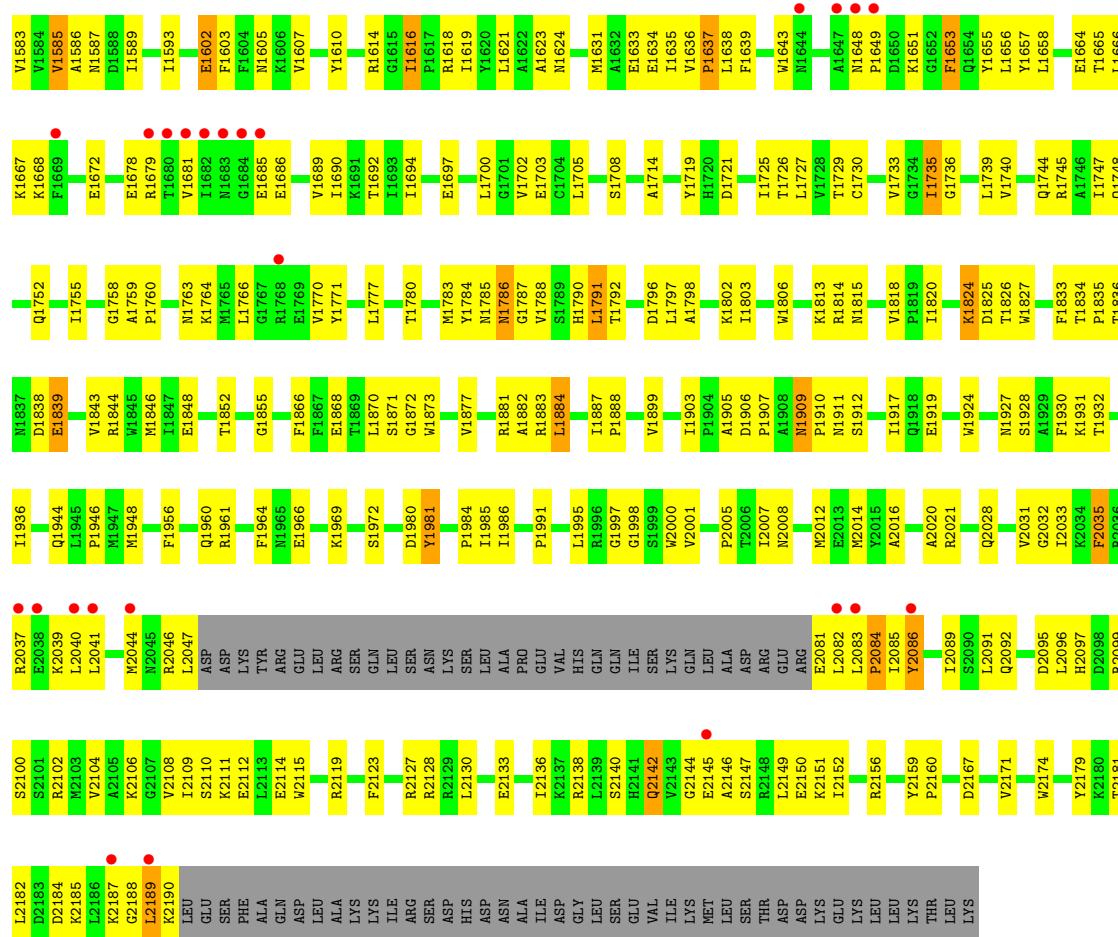
- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1, 4'-BIPIPERIDINE (three-letter code: RCP) (formula: C₃₀H₃₅N₃O₃).



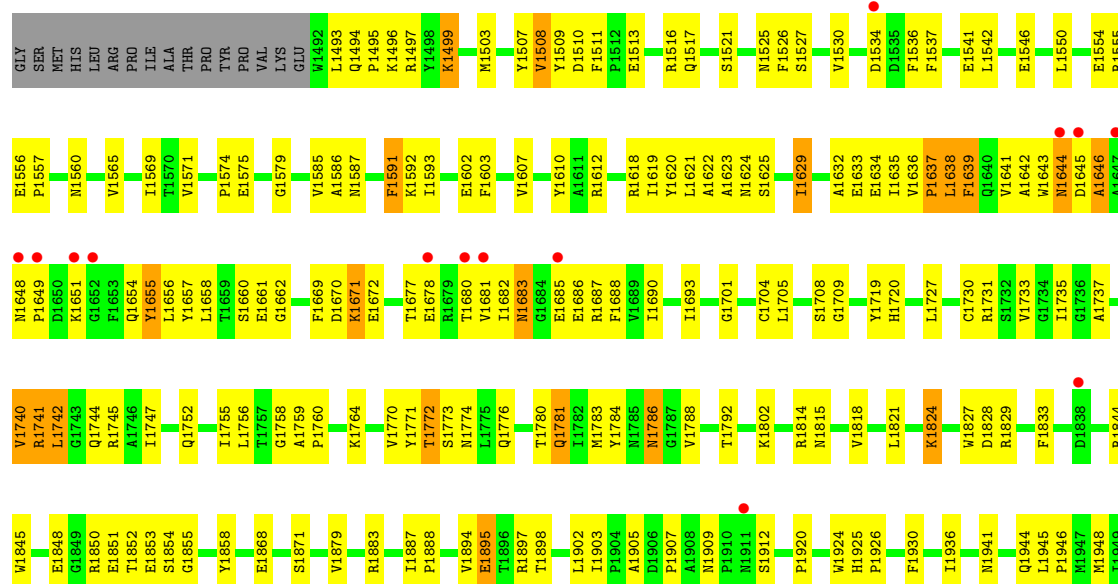
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		

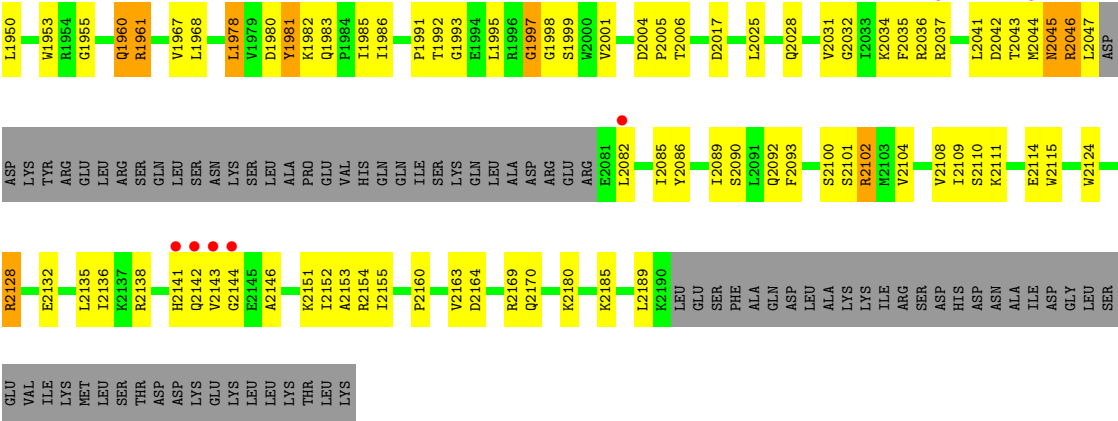
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total 147	O 147	0	0
3	B	128	Total 128	O 128	0	0
3	C	104	Total 104	O 104	0	0



• Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.59Å 124.60Å 145.60Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.66 – 2.80 29.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.66-2.80) 88.7 (29.66-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.234 0.200 , 0.238	Depositor DCC
R_{free} test set	10186 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

5.1 Standard geometry

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

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	0/5547	0.61	0/7516
1	B	0.39	0/5498	0.62	0/7451
1	C	0.39	0/5416	0.60	0/7337
All	All	0.39	0/16461	0.61	0/22304

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	5425	0	5365	209	0
1	B	5377	0	5316	236	0
1	C	5299	0	5234	248	0
2	A	36	0	35	4	0
2	B	36	0	35	2	0
2	C	36	0	35	3	0
3	A	147	0	0	4	0
3	B	128	0	0	7	0
3	C	104	0	0	1	0
All	All	16588	0	16020	669	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 21.

The worst 5 of 669 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:1730:CYS:HA	1:B:1752:GLN:HE21	1.21	1.05
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.41	1.02
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.59	1.01
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.09	1.00
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.98	0.98

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	678/758 (89%)	618 (91%)	52 (8%)	8 (1%)	14	42
1	B	672/758 (89%)	611 (91%)	51 (8%)	10 (2%)	11	36
1	C	662/758 (87%)	588 (89%)	64 (10%)	10 (2%)	11	36
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	12	38

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2189	LEU
1	C	1644	ASN
1	A	1684	GLY
1	A	1997	GLY

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	577/648 (89%)	548 (95%)	29 (5%)	27	60
1	B	572/648 (88%)	534 (93%)	38 (7%)	18	47
1	C	563/648 (87%)	522 (93%)	41 (7%)	15	41
All	All	1712/1944 (88%)	1604 (94%)	108 (6%)	20	49

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1791	LEU
1	B	2035	PHE
1	C	1980	ASP
1	B	1797	LEU
1	B	1909	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1748	GLN
1	B	2028	GLN
1	C	2011	GLN
1	B	1752	GLN
1	B	1909	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](#)

3 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	RCP	A	3000	-	41,41,41	1.03	1 (2%)	58,58,58	1.29	7 (12%)
2	RCP	B	3000	-	41,41,41	1.02	1 (2%)	58,58,58	1.28	6 (10%)
2	RCP	C	3000	-	41,41,41	1.02	1 (2%)	58,58,58	1.31	7 (12%)

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	RCP	A	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	B	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	C	3000	-	-	0/20/48/48	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	RCP	C14-C15	3.67	1.53	1.50
2	B	3000	RCP	C14-C15	3.70	1.53	1.50
2	C	3000	RCP	C14-C15	3.78	1.53	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3000	RCP	O26-C26-N26	-2.33	118.94	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	RCP	O26-C26-N26	-2.28	118.99	121.68
2	A	3000	RCP	O26-C26-N26	-2.27	119.00	121.68
2	C	3000	RCP	C12-C13-C14	-2.22	120.71	122.94
2	B	3000	RCP	C12-C13-C14	-2.19	120.73	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	RCP	4	0
2	B	3000	RCP	2	0
2	C	3000	RCP	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	682/758 (89%)	-0.24	21 (3%)	49 38	22, 47, 98, 99	0
1	B	676/758 (89%)	-0.20	28 (4%)	37 27	24, 49, 99, 99	0
1	C	666/758 (87%)	-0.27	21 (3%)	47 37	22, 49, 99, 99	0
All	All	2024/2274 (89%)	-0.23	70 (3%)	44 33	22, 48, 99, 99	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	6.2
1	C	1644	ASN	5.8
1	B	1492	TRP	5.2
1	B	1680	THR	5.2
1	B	1683	ASN	4.7

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 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
2	RCP	C	3000	36/36	0.90	0.24	73,87,94,95	0
2	RCP	B	3000	36/36	0.94	0.20	58,63,71,71	0
2	RCP	A	3000	36/36	0.94	0.17	60,68,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.