



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K8X  
Title : Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with tepraloxydim  
Authors : Xiang, S.; Callaghan, M.M.; Watson, K.G.; Tong, L.  
Deposited on : 2009-10-15  
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](mailto: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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

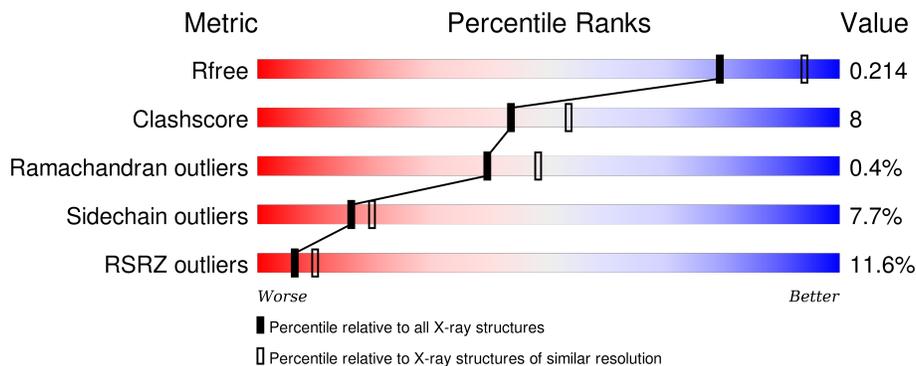
# 1 Overall quality at a glance i

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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  $\geq 3$ , 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	 9% 75% 13% • 9%
1	B	758	 11% 71% 15% • 10%
1	C	758	 11% 73% 14% •• 11%

## 2 Entry composition [i](#)

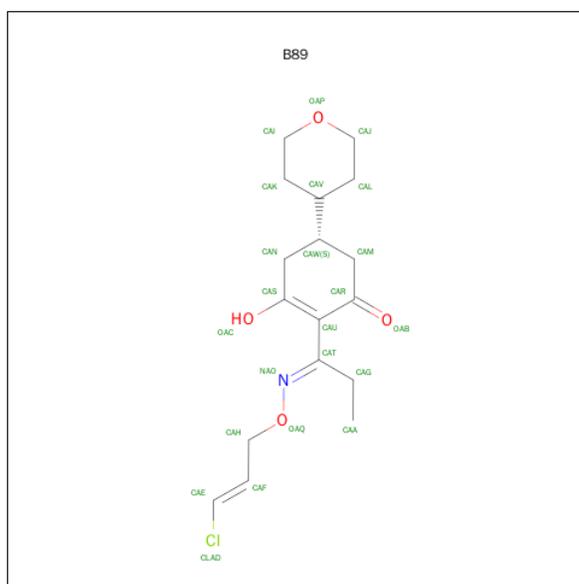
There are 3 unique types of molecules in this entry. The entry contains 17693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	688	Total	C	N	O	S	0	0	0
			5491	3500	944	1028	19			
1	B	682	Total	C	N	O	S	0	0	0
			5443	3468	937	1019	19			
1	C	675	Total	C	N	O	S	0	0	0
			5387	3428	927	1013	19			

- Molecule 2 is (5S)-2-[(1E)-N-[(2E)-3-CHLOROPROP-2-EN-1-YL]OXY}PROPANIMID OYL]-3-HYDROXY-5-(TETRAHYDRO-2H-PYRAN-4-YL)CYCLOHEX-2-EN-1-ONE (three-letter code: B89) (formula: C<sub>17</sub>H<sub>24</sub>ClNO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		
2	B	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		

*Continued on next page...*

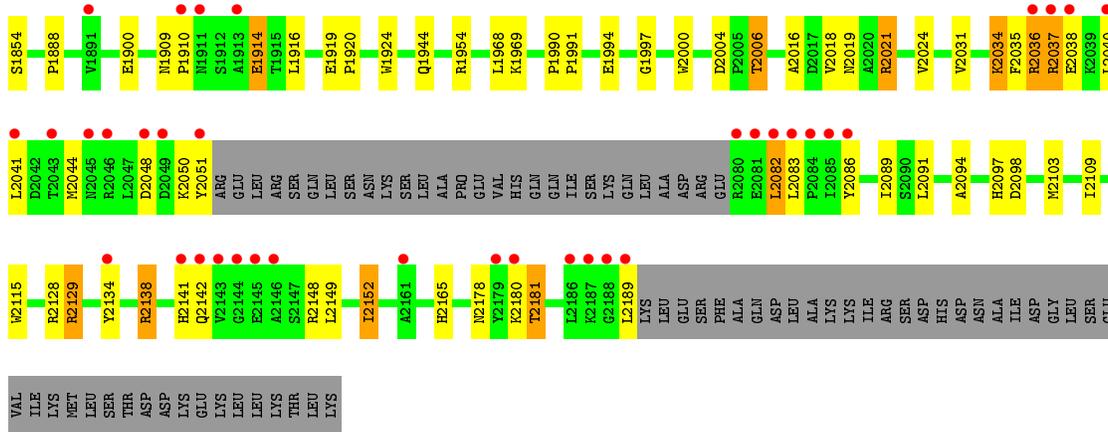
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	C	1	23	17	1	1	4	0	0

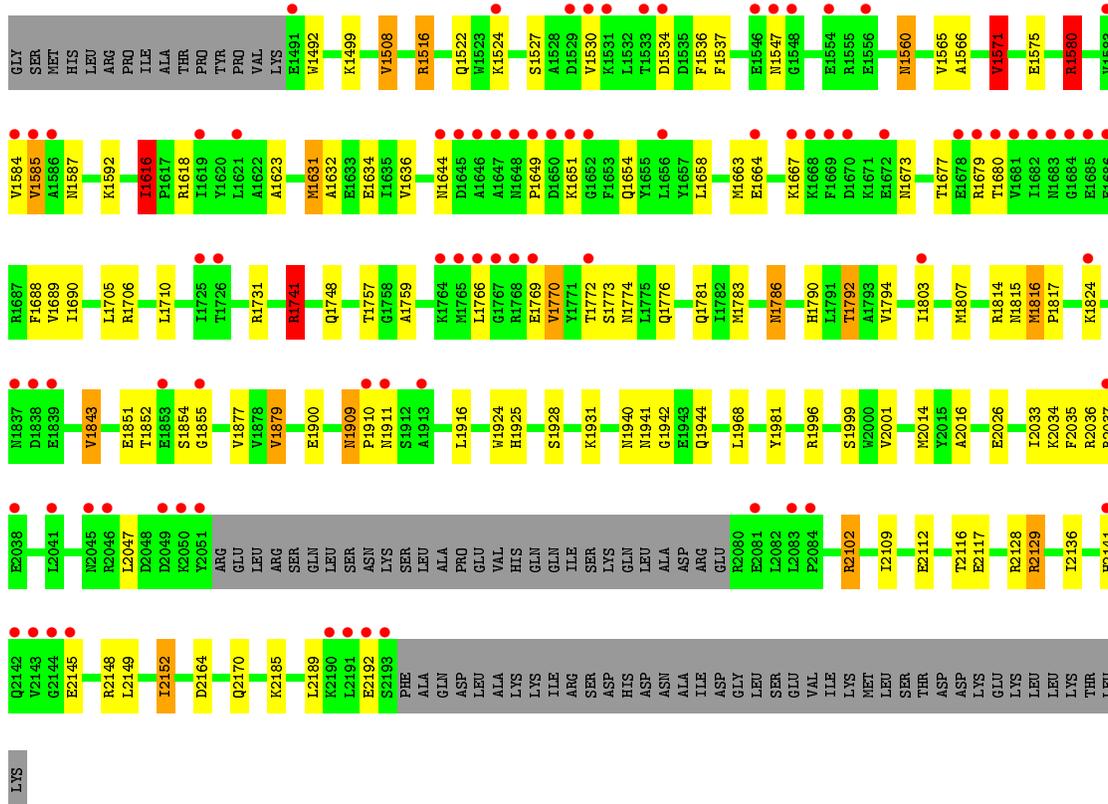
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	483	Total 483	O 483	0	0
3	B	415	Total 415	O 415	0	0
3	C	405	Total 405	O 405	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, $\alpha$ , $\beta$ , $\gamma$	247.30Å 124.80Å 145.37Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.30) 98.7 (29.93-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.187 , 0.221 0.181 , 0.214	Depositor DCC
$R_{free}$ test set	9659 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtrriage
Anisotropy	0.418	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 192187 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: B89

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	0.73	2/5614 (0.0%)	0.82	16/7605 (0.2%)
1	B	0.70	0/5565	0.79	15/7540 (0.2%)
1	C	0.70	1/5505 (0.0%)	0.78	14/7454 (0.2%)
All	All	0.71	3/16684 (0.0%)	0.80	45/22599 (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	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1942	GLY	N-CA	7.12	1.56	1.46
1	A	1786	ASN	CB-CG	-6.26	1.36	1.51
1	C	1942	GLY	N-CA	6.21	1.55	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1745	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	A	1717	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	A	1745	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	1941	ASN	C-N-CA	-10.64	99.95	122.30
1	C	1741	ARG	NE-CZ-NH1	10.34	125.47	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1482	PRO	Peptide
1	B	1481	ARG	Peptide

## 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	5491	0	5431	72	0
1	B	5443	0	5382	127	0
1	C	5387	0	5318	77	0
2	A	23	0	24	1	0
2	B	23	0	24	3	0
2	C	23	0	24	2	0
3	A	483	0	0	9	1
3	B	415	0	0	16	0
3	C	405	0	0	20	0
All	All	17693	0	16203	264	1

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 8.

The worst 5 of 264 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:A:1482:PRO:HB2	3:A:1267:HOH:O	1.40	1.15
1:B:2024:VAL:HG13	3:C:266:HOH:O	1.54	1.06
1:B:2016:ALA:HB2	1:B:2103:MET:HE3	1.46	0.97
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.06	0.94
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.09	0.93

All (1) 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)
3:A:241:HOH:O	3:A:1113:HOH:O[2_555]	2.19	0.01

## 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	684/758 (90%)	656 (96%)	24 (4%)	4 (1%)	30	36
1	B	678/758 (89%)	639 (94%)	36 (5%)	3 (0%)	39	48
1	C	671/758 (88%)	645 (96%)	24 (4%)	2 (0%)	46	57
All	All	2033/2274 (89%)	1940 (95%)	84 (4%)	9 (0%)	39	48

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	1764	LYS
1	B	2037	ARG
1	C	1492	TRP
1	C	2141	HIS

### 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	584/648 (90%)	547 (94%)	37 (6%)	22	29
1	B	579/648 (89%)	531 (92%)	48 (8%)	14	17

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	573/648 (88%)	524 (91%)	49 (9%)	13	15
All	All	1736/1944 (89%)	1602 (92%)	134 (8%)	16	20

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1824	LYS
1	B	2083	LEU
1	C	1924	TRP
1	B	1843	VAL
1	B	2006	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1644	ASN
1	B	1815	ASN
1	C	1911	ASN
1	B	1648	ASN
1	B	1763	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	B89	A	1	-	22,24,24	1.59	6 (27%)	20,31,31	1.94	5 (25%)
2	B89	B	2	-	22,24,24	1.68	7 (31%)	20,31,31	1.99	5 (25%)
2	B89	C	3	-	22,24,24	1.85	7 (31%)	20,31,31	1.88	4 (20%)

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	B89	A	1	-	-	0/11/40/40	0/2/2/2
2	B89	B	2	-	-	0/11/40/40	0/2/2/2
2	B89	C	3	-	-	0/11/40/40	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B89	OAQ-NAO	-2.98	1.36	1.42
2	C	3	B89	OAQ-NAO	-2.91	1.36	1.42
2	C	3	B89	CAH-CAF	-2.86	1.39	1.49
2	B	2	B89	CAH-CAF	-2.85	1.39	1.49
2	A	1	B89	CAH-CAF	-2.50	1.40	1.49

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	B89	OAC-CAS-CAU	-3.07	116.61	121.62
2	A	1	B89	CAJ-CAL-CAV	-2.34	106.90	110.46
2	A	1	B89	OAP-CAJ-CAL	-2.28	104.17	111.92
2	B	2	B89	OAB-CAR-CAU	-2.12	118.82	122.72
2	B	2	B89	CAG-CAT-CAU	2.06	124.23	121.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	B89	1	0
2	B	2	B89	3	0
2	C	3	B89	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, 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	688/758 (90%)	0.25	69 (10%) 9 14	17, 29, 75, 99	0
1	B	682/758 (89%)	0.40	86 (12%) 5 8	16, 33, 85, 103	0
1	C	675/758 (89%)	0.31	82 (12%) 6 9	17, 33, 83, 101	0
All	All	2045/2274 (89%)	0.32	237 (11%) 6 10	16, 31, 81, 103	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	10.9
1	A	2143	VAL	10.4
1	B	2143	VAL	9.7
1	B	2144	GLY	8.4
1	A	2194	PHE	8.2

### 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	B89	C	3	23/23	0.91	0.17	1.76	43,52,59,64	0
2	B89	A	1	23/23	0.90	0.15	0.94	29,38,49,52	0
2	B89	B	2	23/23	0.93	0.15	0.34	28,37,46,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.