wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 01:27 PM EDT

PDB ID	:	1OAC
Title	:	CRYSTAL STRUCTURE OF A QUINOENZYME: COPPER AMINE OXIDASE OF ESCHERICHIA COLI AT 2 ANGSTROEMS RESOLUTION
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Deposited on	:	1995-09-27
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

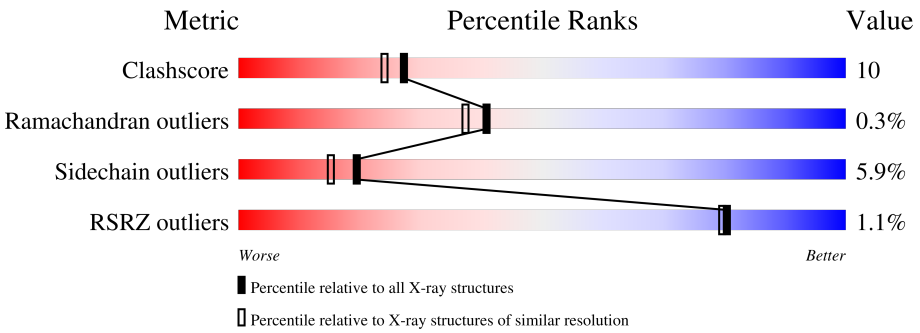
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

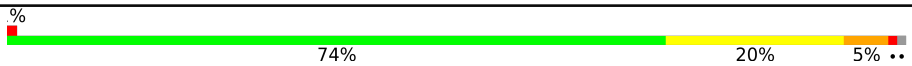
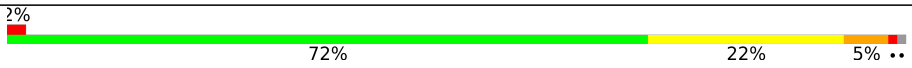
The reported resolution of this entry is 2.00 Å.

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	727	
1	B	727	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12358 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	720	5679	3611	968	1078	22	0	0	0
1	B	723	5705	3627	973	1083	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TPQ	TYR	CONFLICT	UNP P46883
B	466	TPQ	TYR	CONFLICT	UNP P46883

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	489	489	489	0	0

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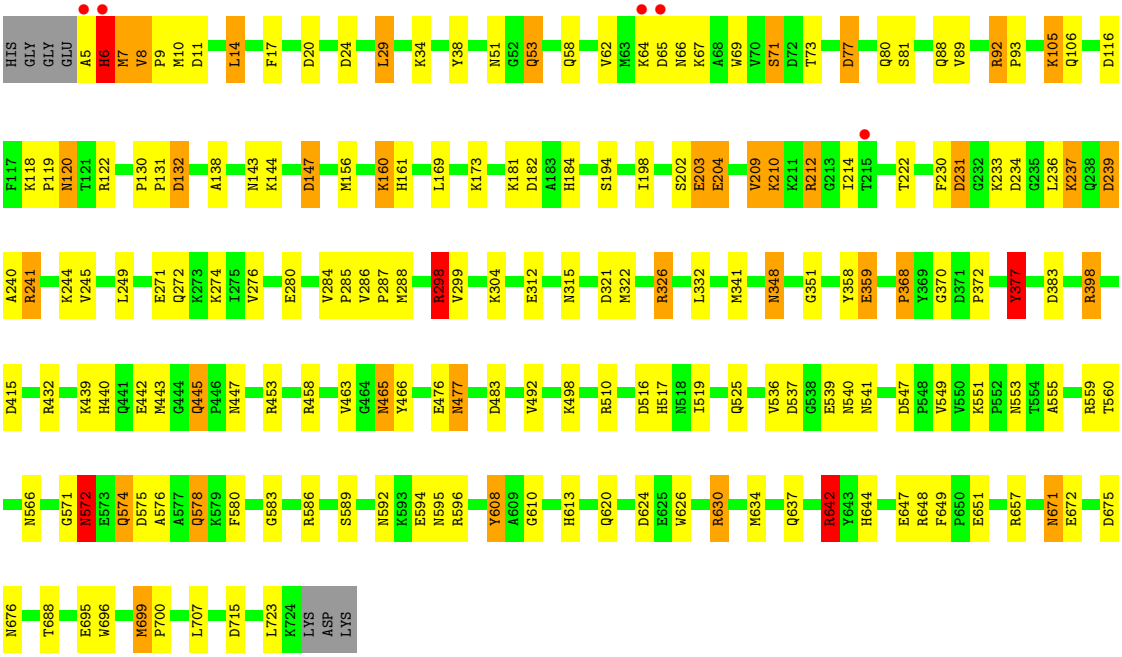
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	479	479	479	0	0

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.

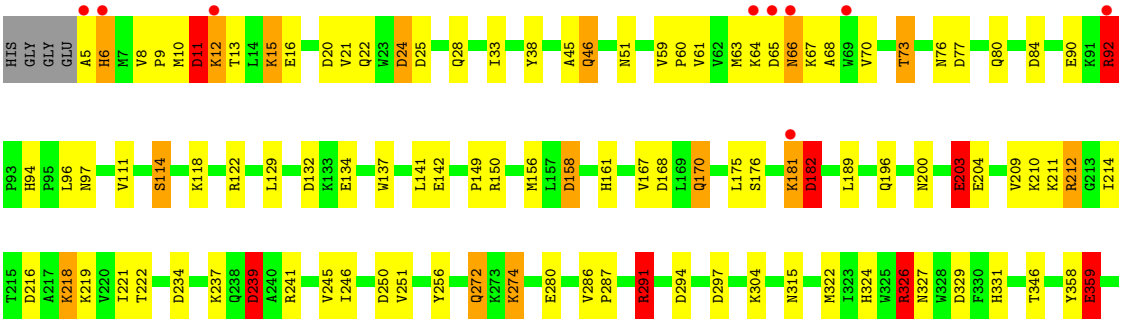
• Molecule 1: COPPER AMINE OXIDASE

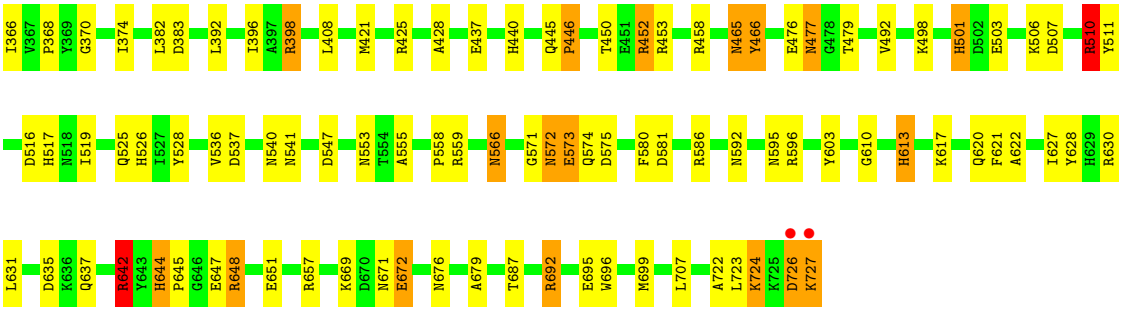
Chain A:



• Molecule 1: COPPER AMINE OXIDASE

Chain B:




I366 V367 P368 Y369 G370 I374 L382 D383 L392 I396 A397 R398 L408 M421 R425 A428 E437 H440 Q445 P446 T450 E451 R452 R453 R458 N465 Y466 E476 M477 G478 T479 V492 K498 H501 D502 E503 K506 D507 R510 Y511
D516 H517 N518 I519 Q525 H526 I527 Y528 V536 D537 N540 N541 D547 N553 T554 A555 P558 R559 N566 G571 N572 E573 Q574 D575 F580 D581 R586 N592 N595 R596 Y603 G610 H613 K617 Q620 F621 A622 I627 Y628 H629 R630
L631 D635 K636 Q637 R642 Y643 H644 P645 G646 E647 R648 E651 R657 K669 D670 N671 E672 N676 A679 T687 R692 E695 W696 M699 L707 A722 L723 K724 K725 D726 K727

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.73Å 167.78Å 81.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 18.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 87.4 (18.89-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.43 (at 2.00Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12358	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, TPQ, CU

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	0.86	0/5809	1.68	90/7908 (1.1%)
1	B	0.87	0/5835	1.68	82/7941 (1.0%)
All	All	0.87	0/11644	1.68	172/15849 (1.1%)

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	8
1	B	0	5
All	All	0	13

There are no bond length outliers.

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ARG	NE-CZ-NH1	17.98	129.29	120.30
1	A	630	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	A	458	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	A	122	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	B	425	ARG	NE-CZ-NH2	14.75	127.67	120.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	326	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	596	ARG	Sidechain
1	A	92	ARG	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	5679	0	5550	112	0
1	B	5705	0	5580	128	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	489	0	0	8	0
4	B	479	0	0	23	0
All	All	12358	0	11130	228	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 10.

The worst 5 of 228 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:93:PRO:HG2	4:A:1172:HOH:O	1.49	1.11
1:A:315:ASN:HD21	1:B:304:LYS:H	1.08	0.97
1:B:216:ASP:HB3	1:B:219:LYS:HD2	1.46	0.97
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.92
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.52	0.91

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	717/727 (99%)	696 (97%)	20 (3%)	1 (0%)	51	49
1	B	720/727 (99%)	697 (97%)	19 (3%)	4 (1%)	25	19
All	All	1437/1454 (99%)	1393 (97%)	39 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	HIS
1	A	6	HIS
1	B	726	ASP
1	B	182	ASP
1	B	66	ASN

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	610/615 (99%)	578 (95%)	32 (5%)	23	19
1	B	613/615 (100%)	573 (94%)	40 (6%)	17	12
All	All	1223/1230 (99%)	1151 (94%)	72 (6%)	19	15

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	326	ARG

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Mol	Chain	Res	Type
1	B	727	LYS
1	B	374	ILE
1	B	572	ASN
1	A	445	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	567	GLN
1	B	595	ASN
1	A	572	ASN
1	A	566	ASN
1	B	599	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)

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	TPQ	A	466	2,1	13,14,15	2.01	4 (30%)	15,19,21	1.15	1 (6%)
1	TPQ	B	466	2,1	13,14,15	1.86	3 (23%)	15,19,21	1.53	2 (13%)

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	TPQ	A	466	2,1	-	4/5/22/24	0/1/1/1
1	TPQ	B	466	2,1	-	3/5/22/24	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TPQ	C1-C2	-4.67	1.42	1.49
1	A	466	TPQ	C1-C2	-4.65	1.42	1.49
1	A	466	TPQ	C3-C4	2.74	1.39	1.35
1	B	466	TPQ	C3-C4	2.36	1.39	1.35
1	B	466	TPQ	C4-C5	-2.31	1.40	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	466	TPQ	O2-C2-C3	-3.40	114.00	121.78
1	A	466	TPQ	O2-C2-C3	-2.54	115.97	121.78
1	B	466	TPQ	C6-C1-C2	-2.43	116.77	118.64

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	C-CA-CB-C1
1	A	466	TPQ	C2-C1-CB-CA
1	B	466	TPQ	C-CA-CB-C1
1	A	466	TPQ	N-CA-CB-C1
1	B	466	TPQ	N-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	TPQ	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	719/727 (98%)	-0.76	5 (0%)	87	87	11, 22, 56, 100	0
1	B	722/727 (99%)	-0.63	11 (1%)	73	72	10, 25, 61, 100	0
All	All	1441/1454 (99%)	-0.70	16 (1%)	80	79	10, 24, 59, 100	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	9.7
1	B	727	LYS	6.5
1	B	65	ASP	5.0
1	B	726	ASP	4.5
1	A	6	HIS	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPQ	B	466	14/15	0.95	0.11	15,37,48,58	0
1	TPQ	A	466	14/15	0.96	0.09	16,41,47,60	0

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
3	CA	B	803	1/1	0.98	0.05	22,22,22,22	0
3	CA	B	802	1/1	0.99	0.04	18,18,18,18	0
3	CA	A	803	1/1	0.99	0.04	20,20,20,20	0
2	CU	A	801	1/1	1.00	0.02	19,19,19,19	0
2	CU	B	801	1/1	1.00	0.02	19,19,19,19	0
3	CA	A	802	1/1	1.00	0.05	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.