wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 02:54 am BST

PDB ID	:	4GXF
Title	:	Role of the biradical intermediate observed during the turnover of SLAC: A two-domain laccase from Streptomyces coelicolor
Authors	:	Nederlof, I.; Gupta, A.; Canters, G.W.
Deposited on	:	2012-09-04
Resolution	:	2.73 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 following versions of software and data (see references (1)) were used in the production of this report:

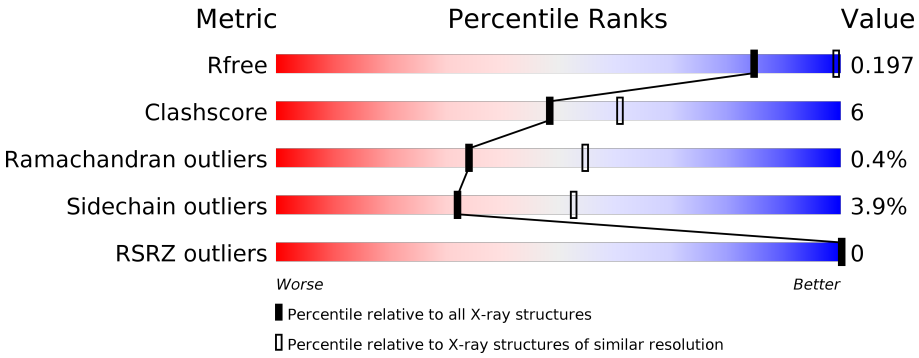
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	279	87% 11%
1	B	279	86% 13%
1	C	279	87% 11%

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
3	PG4	A	409	-	-	X	-
3	PG4	C	408	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6888 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 Putative copper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2157	1348	393	405	11			
1	B	279	Total	C	N	O	S	0	0	0
			2157	1348	393	405	11			
1	C	279	Total	C	N	O	S	0	0	0
			2157	1348	393	405	11			

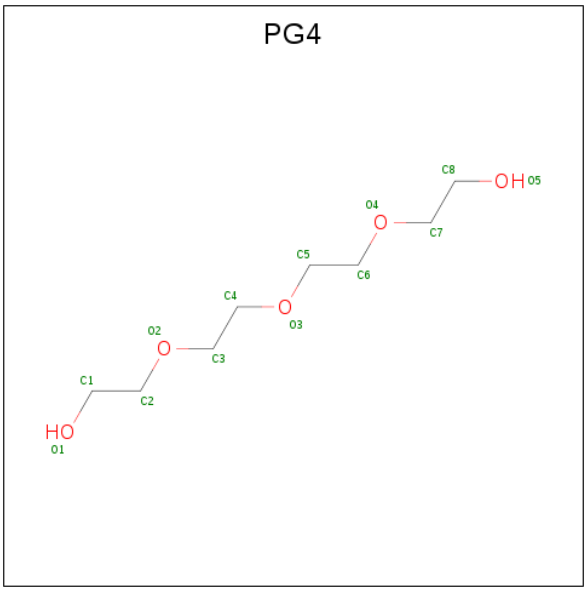
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	PHE	TYR	ENGINEERED MUTATION	UNP Q9XAL8
B	108	PHE	TYR	ENGINEERED MUTATION	UNP Q9XAL8
C	108	PHE	TYR	ENGINEERED MUTATION	UNP Q9XAL8

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cu	0	0
			3	3		
2	A	5	Total	Cu	0	0
			5	5		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 10 6 4	0	0
3	C	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	A	1	Total O 1 1	0	0

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

- Molecule 5 is water.

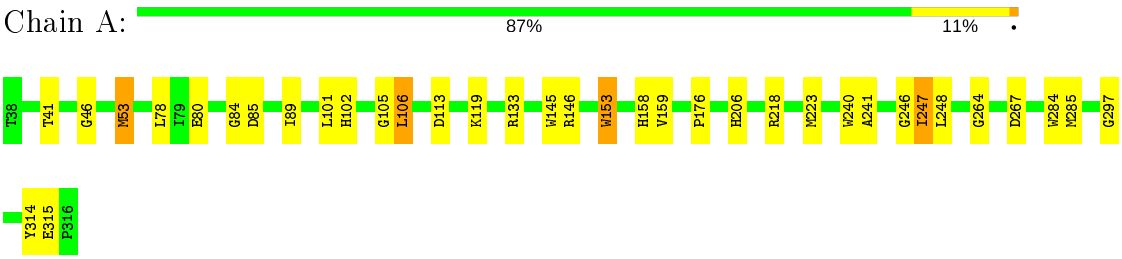
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	89	Total O 89 89	0	0
5	B	91	Total O 91 91	0	0
5	C	101	Total O 101 101	0	0

3 Residue-property plots (i)

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.

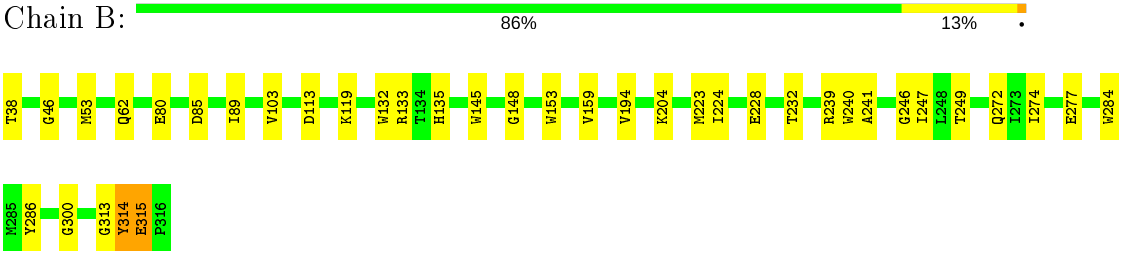
- Molecule 1: Putative copper oxidase

Chain A:



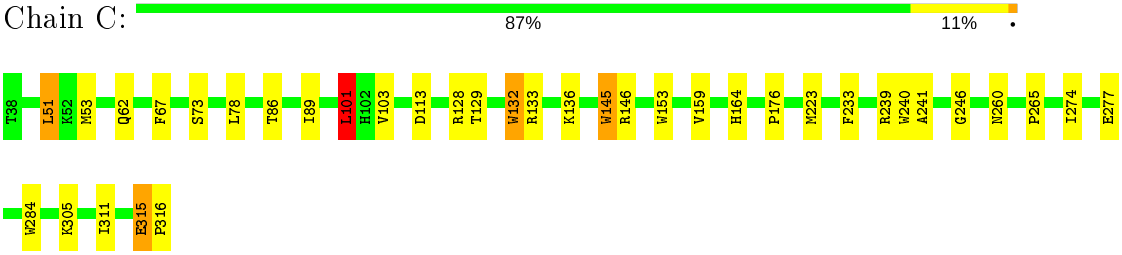
- Molecule 1: Putative copper oxidase

Chain B:



- Molecule 1: Putative copper oxidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	176.66Å 176.66Å 176.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.73 49.01 – 2.73	Depositor EDS
% Data completeness (in resolution range)	79.7 (49.01-2.73) 79.6 (49.01-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.182 , 0.199 0.181 , 0.197	Depositor DCC
R_{free} test set	1192 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.470 for -h,l,k 0.467 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6888	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, O, 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	0.68	4/2220 (0.2%)	0.76	1/3013 (0.0%)
1	B	0.68	4/2220 (0.2%)	0.76	1/3013 (0.0%)
1	C	0.68	5/2220 (0.2%)	0.75	2/3013 (0.1%)
All	All	0.68	13/6660 (0.2%)	0.76	4/9039 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	TRP	CD2-CE2	5.66	1.48	1.41
1	C	284	TRP	CD2-CE2	5.53	1.48	1.41
1	B	240	TRP	CD2-CE2	5.53	1.48	1.41
1	A	153	TRP	CD2-CE2	5.52	1.48	1.41
1	A	240	TRP	CD2-CE2	5.44	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	101	LEU	CA-CB-CG	5.56	128.10	115.30
1	C	51	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	313	GLY	N-CA-C	-5.33	99.78	113.10
1	A	106	LEU	CA-CB-CG	5.17	127.18	115.30

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	2157	0	2037	25	0
1	B	2157	0	2037	18	0
1	C	2157	0	2037	31	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
3	A	36	0	49	13	0
3	B	36	0	49	6	0
3	C	49	0	67	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	89	0	0	0	0
5	B	91	0	0	2	0
5	C	101	0	0	1	0
All	All	6888	0	6276	77	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 6.

The worst 5 of 77 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:C:315:GLU:HB2	1:C:316:PRO:HA	1.48	0.94
1:A:133:ARG:HB3	3:A:408:PG4:H42	1.57	0.87
3:B:407:PG4:H61	3:B:407:PG4:O5	1.74	0.86
1:C:73:SER:HA	3:C:407:PG4:H31	1.61	0.81
1:C:136:LYS:H	3:C:408:PG4:H22	1.48	0.78

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	277/279 (99%)	271 (98%)	4 (1%)	2 (1%)	22 40
1	B	277/279 (99%)	268 (97%)	9 (3%)	0	100 100
1	C	277/279 (99%)	267 (96%)	9 (3%)	1 (0%)	34 55
All	All	831/837 (99%)	806 (97%)	22 (3%)	3 (0%)	34 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	TYR
1	A	315	GLU
1	C	315	GLU

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	224/224 (100%)	215 (96%)	9 (4%)	31 52
1	B	224/224 (100%)	213 (95%)	11 (5%)	25 43
1	C	224/224 (100%)	218 (97%)	6 (3%)	44 65
All	All	672/672 (100%)	646 (96%)	26 (4%)	32 53

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	119	LYS
1	B	223	MET
1	C	239	ARG
1	B	159	VAL
1	B	204	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	HIS

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)

Of 25 ligands modelled in this entry, 15 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
3	PG4	A	404	-	9,9,12	0.54	0	8,8,11	0.26	0
3	PG4	B	403	-	9,9,12	0.55	0	8,8,11	0.21	0
3	PG4	B	407	-	12,12,12	0.70	0	11,11,11	0.95	0
3	PG4	C	408	-	12,12,12	0.69	0	11,11,11	0.52	0
3	PG4	C	406	-	9,9,12	0.42	0	8,8,11	0.42	0
3	PG4	C	407	-	12,12,12	0.57	0	11,11,11	0.34	0
3	PG4	A	408	-	12,12,12	0.63	0	11,11,11	0.69	0
3	PG4	A	409	-	12,12,12	0.61	0	11,11,11	1.04	1 (9%)
3	PG4	C	409	-	12,12,12	0.64	0	11,11,11	0.50	0
3	PG4	B	404	-	12,12,12	0.62	0	11,11,11	0.22	0

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	PG4	A	404	-	-	6/7/7/10	-
3	PG4	B	403	-	-	2/7/7/10	-
3	PG4	B	407	-	-	6/10/10/10	-
3	PG4	C	408	-	-	7/10/10/10	-
3	PG4	C	406	-	-	4/7/7/10	-
3	PG4	C	407	-	-	5/10/10/10	-
3	PG4	A	408	-	-	8/10/10/10	-
3	PG4	A	409	-	-	7/10/10/10	-
3	PG4	C	409	-	-	6/10/10/10	-
3	PG4	B	404	-	-	5/10/10/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	409	PG4	C5-O3-C4	2.19	122.77	113.29

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	409	PG4	C3-C4-O3-C5
3	C	407	PG4	O2-C3-C4-O3
3	A	409	PG4	O2-C3-C4-O3
3	B	404	PG4	O3-C5-C6-O4
3	A	409	PG4	O3-C5-C6-O4

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	PG4	1	0
3	B	407	PG4	4	0
3	C	408	PG4	3	0
3	C	406	PG4	2	0
3	C	407	PG4	2	0
3	A	408	PG4	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	PG4	7	0
3	C	409	PG4	1	0
3	B	404	PG4	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

6.1 Protein, DNA and RNA chains

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^{th} 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	279/279 (100%)	-0.15	0	100	100	23, 34, 53, 105	15 (5%)
1	B	279/279 (100%)	-0.16	0	100	100	24, 33, 54, 99	14 (5%)
1	C	279/279 (100%)	-0.16	0	100	100	23, 33, 54, 95	14 (5%)
All	All	837/837 (100%)	-0.16	0	100	100	23, 33, 54, 105	43 (5%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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	PG4	C	408	13/13	0.79	0.43	70,76,93,99	0
3	PG4	A	408	13/13	0.85	0.37	62,76,90,94	0
3	PG4	C	407	13/13	0.89	0.37	78,89,103,104	0
3	PG4	B	404	13/13	0.89	0.42	80,94,108,109	0
3	PG4	C	409	13/13	0.91	0.17	60,64,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PG4	B	403	10/13	0.91	0.27	50,61,68,70	0
2	CU	A	406	1/1	0.94	0.15	53,53,53,53	1
3	PG4	B	407	13/13	0.94	0.18	49,51,64,64	0
3	PG4	A	404	10/13	0.95	0.24	56,64,66,67	0
3	PG4	A	409	13/13	0.96	0.17	41,44,55,59	0
2	CU	C	405	1/1	0.97	0.13	40,40,40,40	1
3	PG4	C	406	10/13	0.97	0.17	45,54,57,58	0
2	CU	A	403	1/1	0.97	0.10	46,46,46,46	1
4	O	C	402	1/1	0.98	0.22	13,13,13,13	1
2	CU	A	402	1/1	0.98	0.10	58,58,58,58	0
2	CU	C	404	1/1	0.98	0.12	56,56,56,56	0
2	CU	C	401	1/1	0.99	0.14	42,42,42,42	0
4	O	A	407	1/1	0.99	0.18	9,9,9,9	1
2	CU	B	405	1/1	0.99	0.14	40,40,40,40	0
4	O	B	406	1/1	0.99	0.20	9,9,9,9	1
2	CU	B	402	1/1	1.00	0.13	52,52,52,52	0
2	CU	C	403	1/1	1.00	0.15	32,32,32,32	0
2	CU	B	401	1/1	1.00	0.15	33,33,33,33	0
2	CU	A	405	1/1	1.00	0.14	41,41,41,41	0
2	CU	A	401	1/1	1.00	0.15	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.