WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 10:23 am BST

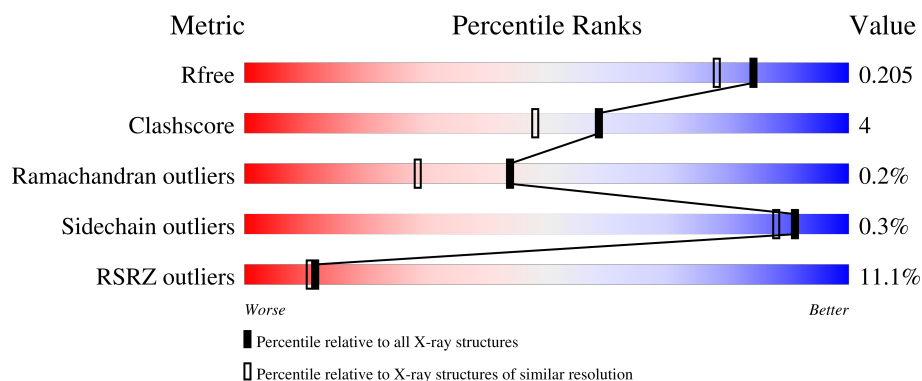|		
PDB ID	:	9HRH / pdb_00009hrh
Title	:	Human holo aromatic L-amino acid decarboxylase (AADC) R347Q variant native structure
Authors	:	Perduca, M.; Bisello, G.; Bertoldi, M.
Deposited on	:	2024-12-18
Resolution	:	1.70 Å(reported)

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 1.70 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	Percentile Ranks	Value
Rfree		0.205
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		0.3%
RSRZ outliers		11.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	480	11% / 86% / 10% / •

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4049 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 Aromatic-L-amino-acid decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total 3670	C 2352	N 632	O 657	P 1	S 28	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLN	ARG	engineered mutation	UNP Q53Y41

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

PG4
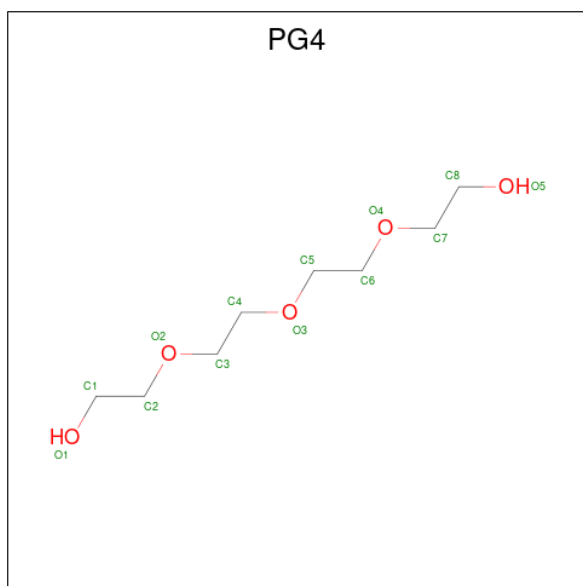
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 8	O 5	0	0
2	A	1	Total 13	C 8	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	353	Total 353	O 353	0	0

3 Residue-property plots ⓘ

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: Aromatic-L-amino-acid decarboxylase
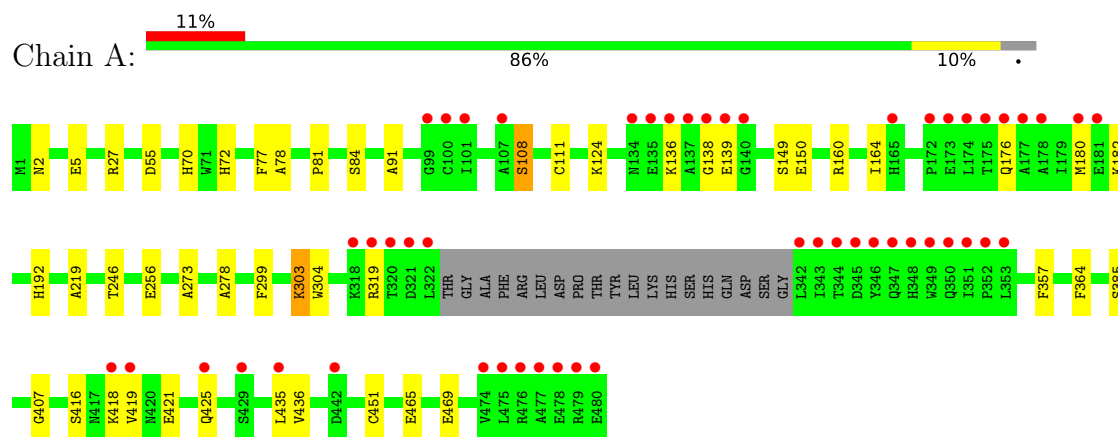
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.27Å 107.27Å 218.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.64 – 1.70 53.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.64-1.70) 100.0 (53.64-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.206 0.199 , 0.205	Depositor DCC
R_{free} test set	4127 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4049	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, LLP

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	0.13	0/3739	0.35	0/5059

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	3670	0	3649	31	0
2	A	26	0	36	3	0
3	A	353	0	0	4	1
All	All	4049	0	3685	32	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 4.

All (32) 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:149:SER:OG	3:A:701:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HD11	1:A:180[A]:MET:HE3	1.77	0.66
1:A:182:LYS:HZ3	2:A:602:PG4:H41	1.60	0.65
1:A:303:LLP:NZ	1:A:303:LLP:O3	2.27	0.63
1:A:421:GLU:O	1:A:425:GLN:HG3	2.00	0.60
1:A:124:LYS:NZ	3:A:705:HOH:O	2.35	0.60
1:A:160:ARG:HD2	1:A:180[B]:MET:HE1	1.83	0.59
1:A:418:LYS:HD3	1:A:418:LYS:C	2.28	0.59
1:A:2:ASN:OD1	1:A:5[B]:GLU:HG3	2.07	0.54
1:A:176:GLN:O	1:A:180[B]:MET:HG2	2.08	0.53
1:A:55:ASP:OD1	3:A:702:HOH:O	2.19	0.53
1:A:27:ARG:HD2	1:A:70:HIS:CE1	2.44	0.52
1:A:192:HIS:HD2	1:A:246:THR:HG21	1.76	0.51
1:A:219:ALA:HB2	1:A:256:GLU:HB3	1.92	0.51
1:A:150:GLU:HA	3:A:1028:HOH:O	2.12	0.50
1:A:81:PRO:HB3	1:A:451:CYS:HA	1.94	0.49
1:A:78:ALA:HB1	1:A:436:VAL:HG13	1.95	0.49
1:A:72:HIS:CE1	1:A:84:SER:HB2	2.49	0.47
1:A:192:HIS:CD2	1:A:246:THR:HG21	2.51	0.46
1:A:416:SER:O	1:A:419:VAL:HG12	2.15	0.46
1:A:91:ALA:HB2	1:A:364:PHE:CG	2.53	0.44
1:A:136:LYS:HD3	1:A:136:LYS:HA	1.66	0.44
1:A:278:ALA:HB2	1:A:304:TRP:CZ3	2.52	0.44
1:A:465:GLU:O	1:A:469:GLU:HG3	2.18	0.43
2:A:602:PG4:H41	2:A:602:PG4:H22	1.68	0.43
1:A:385:SER:HB2	1:A:407:GLY:HA2	2.01	0.42
1:A:111:CYS:HA	1:A:357:PHE:CE1	2.55	0.42
1:A:138:GLY:O	1:A:319:ARG:NH1	2.53	0.42
1:A:139:GLU:O	1:A:319:ARG:HG3	2.20	0.41
1:A:273:ALA:HA	1:A:299:PHE:HA	2.01	0.41
1:A:77:PHE:HB2	1:A:435:LEU:HD23	2.03	0.41
1:A:182:LYS:NZ	2:A:602:PG4:H41	2.33	0.41

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:902:HOH:O	3:A:902:HOH:O[10_554]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	459/480 (96%)	449 (98%)	9 (2%)	1 (0%)	44	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER

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	385/398 (97%)	384 (100%)	1 (0%)	91	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	LLP	A	303	1	23,24,25	2.34	7 (30%)	25,32,34	1.72	6 (24%)

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	LLP	A	303	1	-	5/16/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	LLP	C2'-C2	-6.32	1.39	1.50
1	A	303	LLP	C4'-NZ	4.79	1.43	1.27
1	A	303	LLP	C5'-C5	-4.25	1.39	1.50
1	A	303	LLP	C4-C4'	-3.77	1.39	1.46
1	A	303	LLP	C6-N1	3.23	1.41	1.34
1	A	303	LLP	C4-C5	-2.48	1.38	1.42
1	A	303	LLP	C3-C2	-2.01	1.38	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	LLP	C4-C4'-NZ	-4.35	104.34	124.31
1	A	303	LLP	C4-C3-C2	3.80	122.54	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	LLP	CE-NZ-C4'	-2.98	109.75	118.90
1	A	303	LLP	OP2-P-OP4	-2.57	99.89	106.73
1	A	303	LLP	C5-C6-N1	-2.29	120.00	123.82
1	A	303	LLP	OP3-P-OP1	2.25	119.50	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	303	LLP	C4-C4'-NZ-CE
1	A	303	LLP	C4-C5-C5'-OP4
1	A	303	LLP	C6-C5-C5'-OP4
1	A	303	LLP	CE-CD-CG-CB
1	A	303	LLP	C5'-OP4-P-OP3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	303	LLP	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	PG4	A	601	-	12,12,12	0.54	0	11,11,11	0.50	0
2	PG4	A	602	-	12,12,12	0.51	0	11,11,11	0.80	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
2	PG4	A	601	-	-	0/10/10/10	-
2	PG4	A	602	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	PG4	C5-C6-O4-C7
2	A	602	PG4	C3-C4-O3-C5
2	A	602	PG4	O2-C3-C4-O3
2	A	602	PG4	O3-C5-C6-O4
2	A	602	PG4	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	PG4	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 ⓘ

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, 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	460/480 (95%)	0.44	51 (11%)	12	11	7, 19, 46, 81	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	LYS	8.0
1	A	344	THR	7.1
1	A	342	LEU	7.0
1	A	349	TRP	7.0
1	A	137	ALA	6.1
1	A	177	ALA	6.0
1	A	343	ILE	5.8
1	A	477	ALA	5.6
1	A	174	LEU	5.5
1	A	347	GLN	5.5
1	A	346	TYR	5.3
1	A	345	ASP	5.2
1	A	138	GLY	5.2
1	A	320	THR	4.6
1	A	322	LEU	4.5
1	A	479	ARG	4.3
1	A	348	HIS	4.2
1	A	480	GLU	4.0
1	A	173	GLU	3.8
1	A	178	ALA	3.8
1	A	351	ILE	3.6
1	A	134	ASN	3.5
1	A	135	GLU	3.3
1	A	353	LEU	3.3
1	A	175	THR	3.2
1	A	350	GLN	3.1
1	A	318	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLN	2.9
1	A	180[A]	MET	2.9
1	A	99	GLY	2.8
1	A	321	ASP	2.8
1	A	418	LYS	2.8
1	A	476	ARG	2.8
1	A	419	VAL	2.8
1	A	139	GLU	2.8
1	A	140	GLY	2.8
1	A	478	GLU	2.7
1	A	425	GLN	2.7
1	A	181	GLU	2.7
1	A	172	PRO	2.6
1	A	429	SER	2.6
1	A	475	LEU	2.5
1	A	101	ILE	2.4
1	A	319	ARG	2.4
1	A	100	CYS	2.3
1	A	435	LEU	2.3
1	A	474	VAL	2.3
1	A	352	PRO	2.1
1	A	165	HIS	2.0
1	A	107	ALA	2.0
1	A	442	ASP	2.0

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

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	LLP	A	303	24/25	0.95	0.08	10,16,20,21	0

6.3 Carbohydrates ⓘ

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
2	PG4	A	602	13/13	0.80	0.21	35,48,57,58	0
2	PG4	A	601	13/13	0.90	0.12	26,30,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.