



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:19 pm GMT

PDB ID : 5HSI
Title : Crystal structure of tyrosine decarboxylase at 1.73 Angstroms resolution
Authors : Ni, Y.; Zhou, J.; Zhu, H.; Zhang, K.
Deposited on : 2016-01-25
Resolution : 1.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

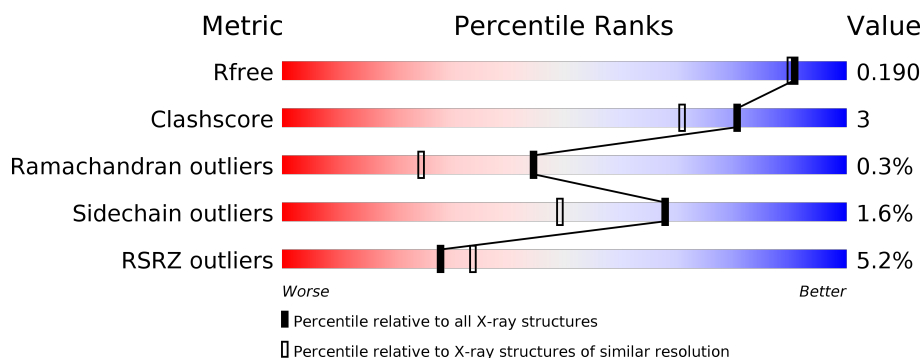
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	100719	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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. 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	634	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	634	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10743 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 decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	1	0
			4792	3071	801	902	18			
1	B	597	Total	C	N	O	S	0	0	0
			4749	3038	799	894	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	627	LEU	-	expression tag	UNP J7GQ11
A	628	GLU	-	expression tag	UNP J7GQ11
A	629	HIS	-	expression tag	UNP J7GQ11
A	630	HIS	-	expression tag	UNP J7GQ11
A	631	HIS	-	expression tag	UNP J7GQ11
A	632	HIS	-	expression tag	UNP J7GQ11
A	633	HIS	-	expression tag	UNP J7GQ11
A	634	HIS	-	expression tag	UNP J7GQ11
B	627	LEU	-	expression tag	UNP J7GQ11
B	628	GLU	-	expression tag	UNP J7GQ11
B	629	HIS	-	expression tag	UNP J7GQ11
B	630	HIS	-	expression tag	UNP J7GQ11
B	631	HIS	-	expression tag	UNP J7GQ11
B	632	HIS	-	expression tag	UNP J7GQ11
B	633	HIS	-	expression tag	UNP J7GQ11
B	634	HIS	-	expression tag	UNP J7GQ11

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

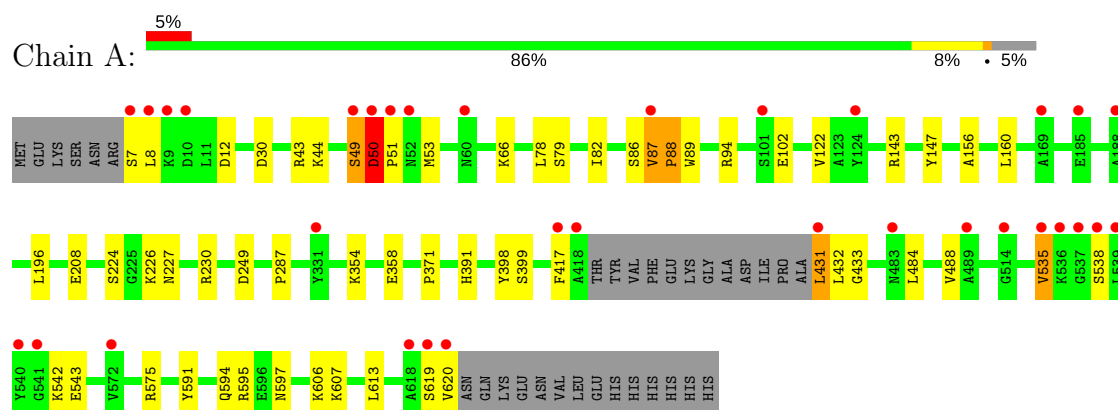
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	559	Total 559	O 559	0	0
3	B	642	Total 642	O 642	0	0

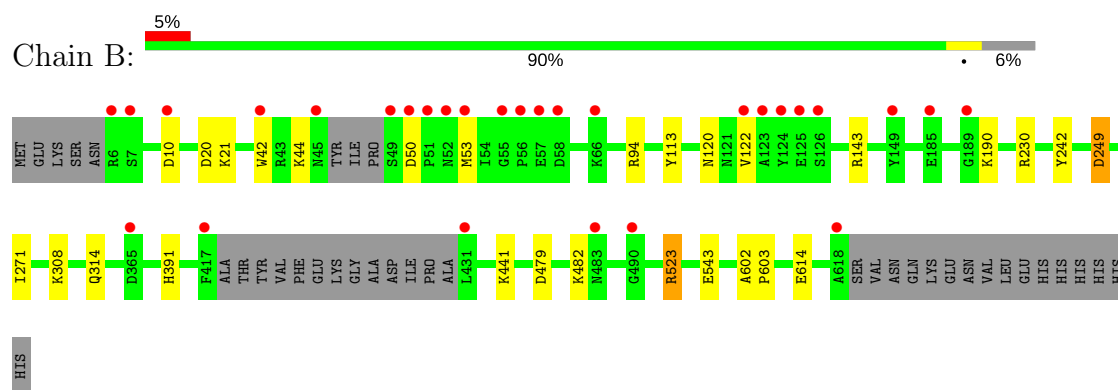
3 Residue-property plots [i](#)

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 decarboxylase



- Molecule 1: Putative decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.79Å 126.17Å 82.73Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	25.93 – 1.73 25.93 – 1.73	Depositor EDS
% Data completeness (in resolution range)	93.3 (25.93-1.73) 93.3 (25.93-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.155 , 0.191 0.154 , 0.190	Depositor DCC
R_{free} test set	5773 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10743	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/4913	0.52	1/6656 (0.0%)
1	B	0.33	0/4863	0.53	1/6583 (0.0%)
All	All	0.33	0/9776	0.52	2/13239 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	249	ASP	CB-CG-OD1	5.48	123.23	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4792	0	4688	45	0
1	B	4749	0	4645	26	0
2	B	1	0	0	0	0
3	A	559	0	0	13	0
3	B	642	0	0	8	0
All	All	10743	0	9333	59	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 3.

All (59) 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:230:ARG:NH1	3:B:801:HOH:O	1.98	0.96
1:A:49:SER:HA	1:A:50:ASP:HB2	1.65	0.78
1:A:208:GLU:OE2	3:A:701:HOH:O	2.11	0.68
1:B:614:GLU:OE2	3:B:802:HOH:O	2.12	0.68
1:A:591:TYR:HB3	1:B:53:MET:HE2	1.74	0.68
1:B:479:ASP:HA	1:B:482:LYS:HE2	1.75	0.67
1:A:597:ASN:HB3	1:B:53:MET:HE1	1.77	0.67
1:B:314:GLN:OE1	3:B:803:HOH:O	2.14	0.65
1:A:226:LYS:O	3:A:702:HOH:O	2.14	0.64
1:A:49:SER:HA	1:A:50:ASP:CB	2.30	0.61
1:B:44:LYS:NZ	3:B:813:HOH:O	2.33	0.60
1:B:94:ARG:NH2	1:B:543:GLU:OE2	2.34	0.60
1:A:535:VAL:O	1:A:538:SER:OG	2.18	0.59
1:A:122:VAL:HG13	1:A:433:GLY:HA3	1.84	0.59
1:B:20:ASP:OD1	3:B:804:HOH:O	2.17	0.57
1:B:143:ARG:NH1	3:B:817:HOH:O	2.38	0.56
1:A:94:ARG:HD3	1:A:543:GLU:HA	1.88	0.56
1:A:371:PRO:HG3	3:A:1057:HOH:O	2.06	0.55
1:A:43:ARG:O	1:B:21:LYS:HE2	2.08	0.53
1:A:595:ARG:NH1	3:A:721:HOH:O	2.43	0.52
1:A:50:ASP:OD2	3:A:703:HOH:O	2.18	0.51
1:A:543:GLU:HG2	3:A:744:HOH:O	2.12	0.49
1:A:488:VAL:HG21	1:A:613:LEU:HB3	1.94	0.49
1:B:308:LYS:HE3	3:B:940:HOH:O	2.12	0.48
1:A:196:LEU:HD13	1:A:287:PRO:HG3	1.94	0.48
1:A:89:TRP:CE3	1:B:42:TRP:HZ3	2.31	0.47
1:A:354:LYS:HE2	1:A:358:GLU:OE2	2.14	0.47
1:A:66:LYS:NZ	1:B:10:ASP:HB2	2.30	0.47
1:A:94:ARG:NE	1:B:50:ASP:OD2	2.49	0.46
1:A:53:MET:HE2	1:A:53:MET:HB3	1.66	0.45
1:A:44:LYS:O	1:B:21:LYS:NZ	2.48	0.45
1:A:50:ASP:OD2	1:B:21:LYS:NZ	2.40	0.45
1:A:484:LEU:HD11	1:A:606:LYS:HE2	2.00	0.44
1:B:190:LYS:NZ	3:B:839:HOH:O	2.50	0.44
1:A:147:TYR:O	3:A:706:HOH:O	2.21	0.44
1:A:143:ARG:NH1	3:A:717:HOH:O	2.41	0.43
1:A:89:TRP:HE3	1:B:42:TRP:HZ3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PHE:N	1:B:242:TYR:OH	2.51	0.43
1:A:50:ASP:HB3	1:A:51:PRO:CA	2.48	0.43
1:A:66:LYS:HB3	1:A:66:LYS:HE2	1.81	0.43
1:A:79:SER:HA	1:B:113:TYR:CE2	2.52	0.43
1:A:607:LYS:HG3	3:A:809:HOH:O	2.18	0.42
1:A:30:ASP:OD2	3:A:705:HOH:O	2.21	0.42
1:A:12:ASP:OD2	3:A:704:HOH:O	2.21	0.42
1:A:398:TYR:HA	1:A:399:SER:HA	1.82	0.42
1:A:82:ILE:O	1:A:86:SER:HB2	2.20	0.42
1:A:156:ALA:HB3	1:A:160:LEU:HD12	2.01	0.42
1:A:224:SER:OG	1:A:226:LYS:HG2	2.20	0.42
1:A:431:LEU:HB3	1:A:432:LEU:H	1.73	0.42
1:A:575:ARG:NH1	3:A:732:HOH:O	2.48	0.42
1:B:271:ILE:HG13	1:B:308:LYS:HE2	2.02	0.41
1:A:102:GLU:HA	1:A:102:GLU:OE1	2.21	0.41
1:A:94:ARG:HD3	1:A:542:LYS:O	2.20	0.41
1:A:102:GLU:HG2	3:A:713:HOH:O	2.18	0.41
1:A:87:VAL:HA	1:A:88:PRO:HD2	1.88	0.41
1:B:120:ASN:OD1	1:B:122:VAL:HG22	2.20	0.41
1:B:602:ALA:HB3	1:B:603:PRO:HD3	2.03	0.41
1:B:523:ARG:CZ	1:B:523:ARG:HB3	2.50	0.41
1:A:50:ASP:CG	1:B:21:LYS:HZ2	2.21	0.40

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	599/634 (94%)	577 (96%)	18 (3%)	4 (1%)	25	9
1	B	591/634 (93%)	579 (98%)	12 (2%)	0	100	100
All	All	1190/1268 (94%)	1156 (97%)	30 (2%)	4 (0%)	44	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	88	PRO
1	A	49	SER
1	A	619	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	502/530 (95%)	490 (98%)	12 (2%)	54	30
1	B	497/530 (94%)	493 (99%)	4 (1%)	85	75
All	All	999/1060 (94%)	983 (98%)	16 (2%)	68	49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	LEU
1	A	50	ASP
1	A	78	LEU
1	A	87	VAL
1	A	227	ASN
1	A	230	ARG
1	A	391	HIS
1	A	431	LEU
1	A	535	VAL
1	A	594	GLN
1	A	620	VAL
1	B	249	ASP
1	B	391	HIS
1	B	441	LYS
1	B	523	ARG

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

Mol	Chain	Res	Type
1	A	227	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](#)

Of 1 ligands modelled in this entry, 1 is 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

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	602/634 (94%)	0.21	33 (5%) 26 31	16, 24, 42, 75	0
1	B	597/634 (94%)	0.07	29 (4%) 30 36	15, 21, 38, 57	0
All	All	1199/1268 (94%)	0.14	62 (5%) 28 34	15, 22, 40, 75	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	VAL	14.2
1	A	540	TYR	12.3
1	A	539	LEU	10.8
1	A	620	VAL	9.6
1	A	537	GLY	8.5
1	B	6	ARG	7.5
1	B	49	SER	6.6
1	A	87	VAL	6.5
1	A	418	ALA	6.4
1	A	536	LYS	6.2
1	A	619	SER	5.9
1	A	618	ALA	5.6
1	A	51	PRO	5.3
1	A	417	PHE	5.1
1	B	417	PHE	5.0
1	A	7	SER	4.9
1	A	541	GLY	4.9
1	B	51	PRO	4.8
1	A	50	ASP	4.5
1	B	50	ASP	4.4
1	A	538	SER	4.3
1	B	7	SER	3.9
1	B	124	TYR	3.9
1	B	126	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	123	ALA	3.6
1	B	55	GLY	3.5
1	B	10	ASP	3.5
1	B	57	GLU	3.5
1	A	124	TYR	3.2
1	B	53	MET	3.2
1	B	45	ASN	3.2
1	B	149	TYR	3.2
1	B	483	ASN	3.1
1	B	56	PRO	3.1
1	A	9	LYS	3.1
1	A	489	ALA	3.1
1	B	125	GLU	3.0
1	A	572	VAL	3.0
1	B	58	ASP	2.9
1	B	189	GLY	2.8
1	A	185	GLU	2.7
1	A	10	ASP	2.7
1	B	52	ASN	2.7
1	B	185	GLU	2.6
1	A	8	LEU	2.5
1	A	431	LEU	2.4
1	B	42	TRP	2.4
1	A	52	ASN	2.4
1	B	431	LEU	2.4
1	B	490	GLY	2.3
1	A	331[A]	TYR	2.3
1	B	365	ASP	2.3
1	A	49	SER	2.3
1	A	60	ASN	2.2
1	A	101	SER	2.2
1	A	514	GLY	2.1
1	A	169	ALA	2.1
1	B	66	LYS	2.0
1	B	618	ALA	2.0
1	A	483	ASN	2.0
1	B	122	VAL	2.0
1	A	188	ALA	2.0

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 [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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	701	1/1	0.99	0.06	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.