



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:59 PM GMT

PDB ID : 1ZD1
Title : Human Sulfortransferase SULT4A1
Authors : Dong, A.; Dombrowski, L.; Loppnau, P.; Edwards, A.M.; Arrowsmith, C.H.; Sundstrom, M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2005-04-13
Resolution : 2.24 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

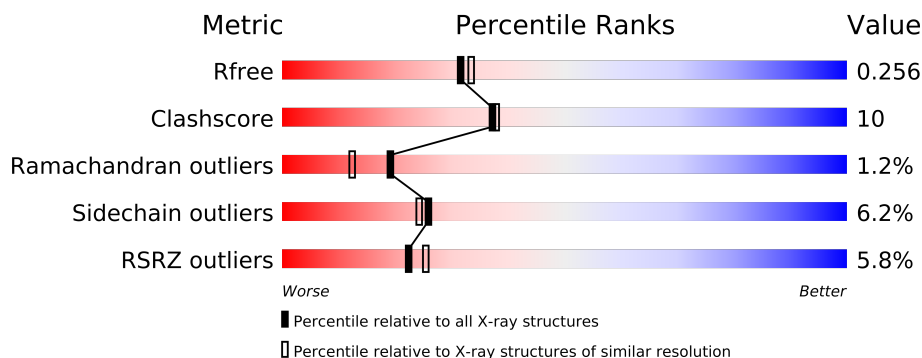
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.24 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}	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	3000	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4326 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sulfotransferase 4A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2073	1339	346	373	15			
1	B	245	Total	C	N	O	S	0	0	0
			2025	1310	340	360	15			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	76	Total	O	0	0
			76	76		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.94Å 74.19Å 85.83Å 90.00° 105.52° 90.00°	Depositor
Resolution (Å)	82.76 – 2.24 37.21 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.9 (82.76-2.24) 98.9 (37.21-2.24)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	0.87	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.262 0.186 , 0.256	Depositor DCC
R_{free} test set	1462 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28727 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	1.29	10/2130 (0.5%)	1.12	11/2875 (0.4%)
1	B	1.08	2/2081 (0.1%)	0.99	3/2810 (0.1%)
All	All	1.19	12/4211 (0.3%)	1.05	14/5685 (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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLU	CG-CD	7.38	1.63	1.51
1	A	161	PHE	CB-CG	-6.87	1.39	1.51
1	A	13	GLY	N-CA	6.85	1.56	1.46
1	B	264	LYS	CG-CD	5.73	1.72	1.52
1	A	37	GLU	CB-CG	5.55	1.62	1.52
1	A	250	VAL	CB-CG1	5.45	1.64	1.52
1	A	184	GLU	CG-CD	5.32	1.59	1.51
1	A	197	GLU	CD-OE1	5.13	1.31	1.25
1	A	36	GLU	CB-CG	5.10	1.61	1.52
1	A	181	GLU	CG-CD	5.07	1.59	1.51
1	B	36	GLU	CG-CD	5.07	1.59	1.51
1	A	165	PHE	CD2-CE2	5.05	1.49	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH1	15.77	128.18	120.30
1	A	47	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	157	THR	N-CA-C	8.15	133.01	111.00
1	A	247	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	47	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	B	266	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	186	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	109	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	A	247	ARG	CD-NE-CZ	5.70	131.57	123.60
1	A	219	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	210	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	264	LYS	CA-CB-CG	5.27	124.99	113.40
1	A	139	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	A	187	MET	CG-SD-CE	5.04	108.27	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2073	0	2013	33	0
1	B	2025	0	1978	49	0
2	B	6	0	8	0	0
3	A	146	0	0	4	0
3	B	76	0	0	8	1
All	All	4326	0	3999	82	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:TYR:CD2	1:A:161:PHE:HZ	1.72	1.08
1:A:142:TYR:CD2	1:A:161:PHE:CZ	2.47	1.02
1:B:19:TYR:CD2	1:B:26:ARG:HD3	2.08	0.89
1:B:238:CYS:HB3	1:B:242:ALA:HA	1.52	0.88
1:B:89:LEU:O	1:B:96:LEU:HD12	1.75	0.84
1:B:202:ASP:OD2	1:B:205:THR:OG1	1.95	0.84
1:B:220:LYS:O	1:B:224:GLU:HG3	1.84	0.78
1:B:31:CYS:HB3	1:B:35:MET:HE3	1.64	0.78
1:B:36:GLU:HB3	3:B:3062:HOH:O	1.87	0.74
1:A:186:ARG:HG3	1:A:187:MET:HE3	1.68	0.74
1:A:186:ARG:HG3	1:A:187:MET:CE	2.18	0.73
1:B:65:VAL:HG22	1:B:210:LEU:HD11	1.71	0.71
1:B:198:ASP:OD1	1:B:201:ARG:NH1	2.23	0.71
1:A:217:SER:HB3	3:A:428:HOH:O	1.89	0.70
1:A:142:TYR:CE2	1:A:161:PHE:HZ	2.09	0.69
1:B:89:LEU:O	1:B:96:LEU:CD1	2.40	0.69
1:B:62:GLN:HE22	1:B:109:LYS:HZ3	1.44	0.66
1:B:19:TYR:HB2	3:B:3051:HOH:O	1.96	0.65
1:B:187:MET:HB2	3:B:3011:HOH:O	1.96	0.65
1:A:146:HIS:HB2	3:A:349:HOH:O	1.96	0.65
1:B:171:GLY:HA3	3:B:3037:HOH:O	1.97	0.65
1:B:270:LYS:HE2	3:B:3048:HOH:O	1.98	0.63
1:B:36:GLU:H	1:B:36:GLU:CD	2.02	0.62
1:B:143:TYR:HD1	1:B:161:PHE:CD1	2.17	0.62
1:B:144:GLN:OE1	1:B:247:ARG:HG2	1.99	0.61
1:B:62:GLN:HE22	1:B:109:LYS:NZ	1.97	0.60
1:B:243:LEU:HD22	1:B:250:VAL:HB	1.83	0.60
1:B:200:HIS:CE1	1:B:244:PRO:HD3	2.36	0.60
1:A:185:HIS:HD2	1:A:188:ASP:OD2	1.85	0.59
1:B:52:THR:HG22	1:B:131:MET:HB2	1.85	0.59
1:B:56:SER:HB2	1:B:138:LEU:HG	1.83	0.59
1:A:37:GLU:CD	1:A:37:GLU:H	2.06	0.59
1:A:54:PRO:HG3	1:A:172:TYR:CD2	2.38	0.58
1:B:171:GLY:O	1:B:172:TYR:HB2	2.07	0.55
1:B:159:GLN:O	1:B:163:ARG:HG3	2.06	0.55
1:A:228:GLU:O	1:A:232:GLN:HG3	2.06	0.55
1:A:142:TYR:CE2	1:A:161:PHE:CZ	2.90	0.54
1:A:25:VAL:HG23	1:A:115:ARG:NH2	2.24	0.53
1:B:89:LEU:HG	1:B:96:LEU:HD11	1.90	0.53
1:A:236:GLN:HG2	3:A:378:HOH:O	2.08	0.52
1:B:239:ASN:C	1:B:241:GLU:H	2.12	0.52
1:A:171:GLY:O	1:A:172:TYR:HB2	2.10	0.52
1:B:38:ILE:HG23	1:B:89:LEU:CD2	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:VAL:HG21	1:A:253:TRP:HA	1.91	0.51
1:B:35:MET:HE2	1:B:38:ILE:HD12	1.92	0.51
1:A:186:ARG:HG3	1:A:187:MET:HE2	1.94	0.50
1:A:111:HIS:HB2	1:A:172:TYR:CZ	2.47	0.50
1:A:31:CYS:O	1:A:35:MET:HE3	2.12	0.50
1:A:63:GLU:HB3	1:A:233:LEU:HD21	1.94	0.50
1:B:239:ASN:ND2	1:B:241:GLU:HB2	2.28	0.49
1:A:69:SER:O	1:A:70:GLN:HB3	2.12	0.49
1:B:143:TYR:CD1	1:B:161:PHE:CD1	2.99	0.49
1:A:64:VAL:O	1:A:68:VAL:HG23	2.13	0.49
1:A:142:TYR:HD2	1:A:161:PHE:CZ	2.19	0.48
1:B:142:TYR:HE1	3:B:3071:HOH:O	1.97	0.48
1:B:167:ASN:O	1:B:168:ASP:HB2	2.13	0.47
1:A:185:HIS:CD2	1:A:188:ASP:OD2	2.67	0.46
1:B:68:VAL:HG11	1:B:210:LEU:HB3	1.98	0.46
1:A:159:GLN:HG2	3:A:350:HOH:O	2.16	0.46
1:A:159:GLN:O	1:A:163:ARG:HG3	2.16	0.46
1:B:62:GLN:NE2	1:B:109:LYS:NZ	2.63	0.46
1:B:21:GLU:HG3	3:B:3024:HOH:O	2.17	0.45
1:A:138:LEU:HD23	1:A:138:LEU:C	2.37	0.45
1:B:120:ASP:O	1:B:125:ASP:HB2	2.17	0.45
1:A:34:LYS:HG3	1:A:35:MET:HE2	1.99	0.44
1:B:86:LEU:HB2	1:B:109:LYS:CD	2.47	0.44
1:B:26:ARG:HE	1:B:26:ARG:HB2	1.53	0.44
1:A:219:ASP:OD1	1:A:222:GLN:HG3	2.18	0.44
1:B:135:PRO:HB2	1:B:265:PHE:HZ	1.82	0.43
1:B:67:LEU:HD23	1:B:230:CYS:SG	2.58	0.43
1:A:54:PRO:HG3	1:A:172:TYR:HD2	1.83	0.42
1:B:38:ILE:HG23	1:B:89:LEU:HD23	2.01	0.42
1:B:219:ASP:HA	3:B:3025:HOH:O	2.19	0.42
1:A:69:SER:O	1:A:70:GLN:CB	2.68	0.42
1:B:40:ASN:O	1:B:41:PHE:C	2.58	0.42
1:B:41:PHE:HZ	1:B:99:ILE:HG22	1.84	0.42
1:A:129:ILE:HD11	1:A:214:LEU:HD21	2.03	0.41
1:B:260:SER:O	1:B:264:LYS:HG3	2.19	0.41
1:A:53:TYR:CG	1:A:54:PRO:HD2	2.56	0.41
1:B:239:ASN:O	1:B:241:GLU:N	2.49	0.41
1:B:243:LEU:HD21	1:B:284:LEU:HB2	2.02	0.40
1:B:199:MET:O	1:B:199:MET:HG2	2.20	0.40

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	Distance(Å)	Clash(Å)
3:B:3005:HOH:O	3:B:3065:HOH:O[4.556]	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	245/284 (86%)	238 (97%)	6 (2%)	1 (0%)	43	46
1	B	239/284 (84%)	213 (89%)	21 (9%)	5 (2%)	11	4
All	All	484/568 (85%)	451 (93%)	27 (6%)	6 (1%)	19	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	B	157	THR
1	B	245	VAL
1	B	126	SER
1	B	240	ALA
1	B	172	TYR

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	229/258 (89%)	223 (97%)	6 (3%)	59	70
1	B	224/258 (87%)	202 (90%)	22 (10%)	12	7
All	All	453/516 (88%)	425 (94%)	28 (6%)	26	24

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	86	LEU
1	A	210	LEU
1	A	236	GLN
1	A	267	LEU
1	A	284	LEU
1	B	21	GLU
1	B	23	HIS
1	B	26	ARG
1	B	34	LYS
1	B	45	PRO
1	B	59	SER
1	B	70	GLN
1	B	119	SER
1	B	139	VAL
1	B	169	LYS
1	B	184	GLU
1	B	189	SER
1	B	210	LEU
1	B	212	ARG
1	B	217	SER
1	B	220	LYS
1	B	233	LEU
1	B	236	GLN
1	B	239	ASN
1	B	243	LEU
1	B	264	LYS
1	B	271	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	185	HIS
1	B	62	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z > 2$
2	GOL	B	3000	-	5,5,5	0.73	0	5,5,5	0.73	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	GOL	B	3000	-	-	0/4/4/4	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	251/284 (88%)	-0.27	2 (0%) 83 86	17, 27, 45, 62	0
1	B	245/284 (86%)	0.37	27 (11%) 6 7	20, 43, 78, 95	0
All	All	496/568 (87%)	0.05	29 (5%) 22 25	17, 34, 73, 95	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	6.0
1	B	218	CYS	5.9
1	B	275	LYS	5.0
1	B	221	ALA	4.6
1	B	241	GLU	4.2
1	B	71	GLY	4.2
1	B	67	LEU	3.8
1	B	156	GLY	3.7
1	B	239	ASN	3.3
1	B	245	VAL	3.3
1	B	226	LEU	3.1
1	B	229	HIS	3.1
1	B	236	GLN	3.1
1	B	19	TYR	3.0
1	B	230	CYS	3.0
1	B	237	CYS	2.9
1	B	238	CYS	2.9
1	B	216	VAL	2.7
1	B	244	PRO	2.5
1	B	223	LEU	2.4
1	B	228	GLU	2.4
1	A	70	GLN	2.4
1	B	219	ASP	2.3
1	B	217	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	243	LEU	2.3
1	B	224	GLU	2.2
1	B	214	LEU	2.1
1	A	146	HIS	2.1
1	B	93	GLN	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 ⓘ

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	3000	6/6	0.33	6.17	54,58,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.