



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 01:07 PM EST

PDB ID : 3HLY  
Title : Crystal Structure of the Flavodoxin-like domain from *Synechococcus* sp Q5MZIP6\_SYNP6 protein. Northeast Structural Genomics Consortium Target SnR135d.  
Authors : Vorobiev, S.; Su, M.; Lee, D.; Ciccocanti, C.; Sahdev, S.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-05-28  
Resolution : 2.40 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

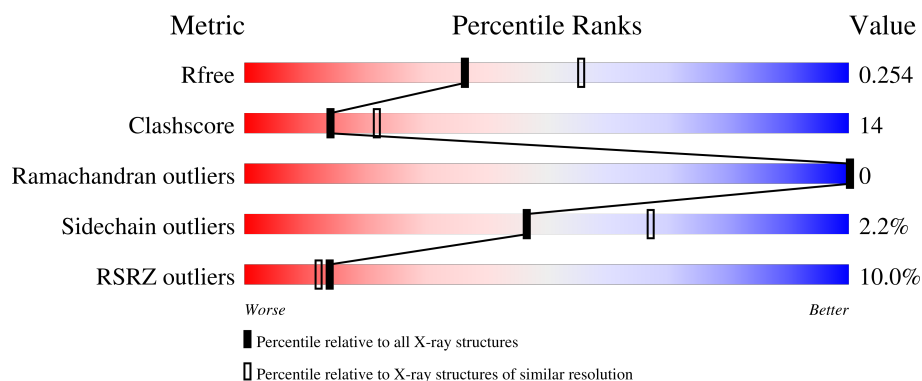
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	161	
1	B	161	
1	C	161	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3284 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 Flavodoxin-like domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	Se	0	0	0
			1062	671	182	207	1	1			
1	B	144	Total	C	N	O	S	Se	0	0	0
			1033	657	175	199	1	1			
1	C	153	Total	C	N	O	S	Se	0	0	0
			1084	688	181	212	1	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	MSE	-	expression tag	UNP Q5MZIP6
A	415	GLU	-	expression tag	UNP Q5MZIP6
A	416	HIS	-	expression tag	UNP Q5MZIP6
A	417	HIS	-	expression tag	UNP Q5MZIP6
A	418	HIS	-	expression tag	UNP Q5MZIP6
A	419	HIS	-	expression tag	UNP Q5MZIP6
A	420	HIS	-	expression tag	UNP Q5MZIP6
A	421	HIS	-	expression tag	UNP Q5MZIP6
B	261	MSE	-	expression tag	UNP Q5MZIP6
B	415	GLU	-	expression tag	UNP Q5MZIP6
B	416	HIS	-	expression tag	UNP Q5MZIP6
B	417	HIS	-	expression tag	UNP Q5MZIP6
B	418	HIS	-	expression tag	UNP Q5MZIP6
B	419	HIS	-	expression tag	UNP Q5MZIP6
B	420	HIS	-	expression tag	UNP Q5MZIP6
B	421	HIS	-	expression tag	UNP Q5MZIP6
C	261	MSE	-	expression tag	UNP Q5MZIP6
C	415	GLU	-	expression tag	UNP Q5MZIP6
C	416	HIS	-	expression tag	UNP Q5MZIP6
C	417	HIS	-	expression tag	UNP Q5MZIP6
C	418	HIS	-	expression tag	UNP Q5MZIP6
C	419	HIS	-	expression tag	UNP Q5MZIP6
C	420	HIS	-	expression tag	UNP Q5MZIP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	421	HIS	-	expression tag	UNP Q5MZIP6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	0	0
3	B	35	Total O 35 35	0	0
3	C	26	Total O 26 26	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.27Å 97.90Å 118.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.94 – 2.40 32.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (32.94-2.40) 97.8 (32.94-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.93 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, $R_{free}$	0.225 , 0.250 0.228 , 0.254	Depositor DCC
$R_{free}$ test set	873 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.40	0/1081	0.66	0/1475
1	B	0.36	0/1052	0.63	0/1438
1	C	0.33	0/1102	0.59	0/1506
All	All	0.37	0/3235	0.62	0/4419

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	1062	0	1029	27	0
1	B	1033	0	998	30	0
1	C	1084	0	1028	35	0
2	B	1	0	0	0	0
3	A	43	0	0	1	0
3	B	35	0	0	2	0
3	C	26	0	0	2	0
All	All	3284	0	3055	87	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 14.

All (87) 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:321:PRO:HA	1:A:355:ASP:HA	1.25	1.13
1:C:309:VAL:HG21	1:C:335:ILE:HG12	1.60	0.83
1:A:321:PRO:HA	1:A:355:ASP:CA	2.12	0.74
1:A:349:ASP:HB3	1:A:379:VAL:HG22	1.71	0.72
1:A:341:ASN:ND2	1:B:341:ASN:HD22	1.89	0.71
1:A:341:ASN:ND2	1:B:341:ASN:HB3	2.06	0.70
1:C:373:ALA:HB1	1:C:398:LEU:HD13	1.75	0.69
1:A:276:ARG:HD3	3:A:704:HOH:O	1.95	0.66
1:B:295:VAL:HG13	1:B:300:VAL:HB	1.80	0.62
1:A:302:PRO:O	1:A:306:ILE:HG13	2.02	0.59
1:A:271:TYR:CE1	1:A:321:PRO:HD3	2.37	0.59
1:B:328:VAL:O	1:B:332:LEU:HD13	2.03	0.59
1:B:275:ASP:HB2	3:B:641:HOH:O	2.03	0.59
1:C:309:VAL:HG11	1:C:335:ILE:HG23	1.86	0.58
1:C:414:LEU:HD23	1:C:414:LEU:H	1.68	0.58
1:C:362:LEU:HD11	1:C:372:THR:HG22	1.85	0.57
1:C:279:GLN:O	1:C:283:ARG:HG3	2.05	0.56
1:B:269:SER:O	1:B:270:ASP:HB2	2.05	0.56
1:B:320:PRO:HG3	1:B:332:LEU:HD21	1.88	0.56
1:B:387:ILE:HD13	3:B:634:HOH:O	2.05	0.56
1:B:285:LEU:HD13	1:B:395:GLY:O	2.05	0.56
1:B:340:HIS:O	1:B:343:GLN:HG2	2.05	0.56
1:C:304:GLU:HA	1:C:304:GLU:OE1	2.06	0.56
1:C:274:SER:HB2	1:C:350:SER:HB2	1.88	0.55
1:A:313:ARG:HG2	1:A:402:LEU:HD22	1.87	0.55
1:A:373:ALA:HB1	1:A:398:LEU:HD13	1.89	0.55
1:C:306:ILE:HG13	1:C:338:ALA:HB2	1.89	0.54
1:A:271:TYR:CZ	1:A:352:GLY:HA3	2.42	0.54
1:B:305:LEU:O	1:B:309:VAL:HG23	2.09	0.52
1:A:341:ASN:HD21	1:B:341:ASN:HB3	1.73	0.52
1:B:275:ASP:O	1:B:279:GLN:HG3	2.10	0.51
1:C:336:PHE:CZ	1:C:364:GLN:HB3	2.44	0.51
1:B:303:GLN:O	1:B:306:ILE:HG22	2.10	0.51
1:C:313:ARG:O	1:C:343:GLN:HB2	2.11	0.50
1:A:295:VAL:HG13	1:A:300:VAL:HB	1.92	0.50
1:B:379:VAL:CG2	1:B:381:ASP:O	2.59	0.50
1:B:370:LEU:HD12	1:B:370:LEU:N	2.27	0.50
1:B:370:LEU:HD12	1:B:370:LEU:H	1.76	0.50
1:B:379:VAL:HG21	1:B:383:PRO:HG3	1.92	0.50
1:C:340:HIS:H	1:C:340:HIS:CD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:SER:HB2	1:A:291:ALA:O	2.13	0.49
1:C:295:VAL:HG11	1:C:305:LEU:HD13	1.94	0.49
1:C:334:THR:HG22	3:C:700:HOH:O	2.12	0.49
1:B:269:SER:O	1:B:270:ASP:CB	2.61	0.49
1:B:351:TYR:CZ	1:B:381:ASP:HA	2.49	0.48
1:A:379:VAL:HG23	1:A:379:VAL:O	2.14	0.48
1:C:271:TYR:CZ	1:C:352:GLY:HA3	2.48	0.48
1:C:349:ASP:HB2	1:C:379:VAL:HG12	1.96	0.48
1:A:264:LEU:HD12	1:A:293:GLU:O	2.14	0.47
1:A:305:LEU:O	1:A:309:VAL:HG23	2.15	0.47
1:A:320:PRO:HG3	1:A:332:LEU:HD11	1.96	0.46
1:A:356:GLU:HB3	1:A:361:LEU:HD21	1.97	0.46
1:C:316:VAL:HA	1:C:346:GLY:O	2.16	0.46
1:C:309:VAL:CG1	1:C:335:ILE:HG23	2.46	0.46
1:B:339:ALA:HA	1:B:343:GLN:OE1	2.15	0.46
1:A:341:ASN:ND2	1:B:341:ASN:ND2	2.62	0.45
1:C:305:LEU:O	1:C:309:VAL:HG23	2.16	0.45
1:C:329:ALA:C	1:C:331:ALA:H	2.19	0.45
1:C:290:VAL:HG21	1:C:399:GLY:HA2	1.99	0.45
1:B:326:GLU:O	1:B:330:THR:HG23	2.17	0.44
1:A:281:ILE:HG13	1:A:391:CYS:HB3	1.98	0.44
1:C:345:ILE:HD11	1:C:347:LEU:HD21	1.98	0.44
1:C:340:HIS:CD2	1:C:340:HIS:N	2.86	0.44
1:B:349:ASP:HB2	1:B:379:VAL:CG1	2.48	0.44
1:C:407:ALA:O	1:C:411:MSE:HB2	2.18	0.44
1:A:340:HIS:O	1:A:343:GLN:HG2	2.17	0.43
1:A:341:ASN:HD21	1:B:341:ASN:H	1.65	0.43
1:C:336:PHE:HZ	1:C:364:GLN:HB3	1.83	0.43
1:B:349:ASP:HB2	1:B:379:VAL:HG12	2.00	0.43
1:A:313:ARG:HH21	1:A:405:ALA:HB3	1.84	0.43
1:B:346:GLY:HA3	1:B:374:PHE:CZ	2.53	0.43
1:C:305:LEU:HD11	1:C:335:ILE:HD11	2.01	0.43
1:C:301:ASP:HA	1:C:302:PRO:HD2	1.90	0.42
1:C:373:ALA:CB	1:C:398:LEU:HD13	2.44	0.42
1:C:379:VAL:O	1:C:379:VAL:HG13	2.18	0.42
1:C:348:PHE:CB	1:C:377:ILE:HB	2.48	0.42
1:A:265:ILE:HD12	1:A:294:MSE:HE3	2.01	0.42
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.84	0.42
1:B:268:LEU:HD23	1:B:298:ARG:HE	1.85	0.42
1:C:338:ALA:HB3	3:C:700:HOH:O	2.20	0.41
1:C:345:ILE:HG23	1:C:345:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:THR:HA	1:C:320:PRO:HD3	1.94	0.41
1:C:410:THR:O	1:C:414:LEU:HD23	2.21	0.41
1:C:341:ASN:CB	1:C:369:GLY:HA3	2.51	0.40
1:A:300:VAL:HG22	1:A:301:ASP:N	2.36	0.40
1:B:288:THR:OG1	1:B:290:VAL:HG23	2.22	0.40
1:B:328:VAL:O	1:B:331:ALA:HB3	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	143/161 (89%)	136 (95%)	7 (5%)	0	100	100
1	B	142/161 (88%)	135 (95%)	7 (5%)	0	100	100
1	C	151/161 (94%)	138 (91%)	13 (9%)	0	100	100
All	All	436/483 (90%)	409 (94%)	27 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	107/127 (84%)	106 (99%)	1 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	102/127 (80%)	99 (97%)	3 (3%)	37	58
1	C	105/127 (83%)	102 (97%)	3 (3%)	37	58
All	All	314/381 (82%)	307 (98%)	7 (2%)	47	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	VAL
1	B	285	LEU
1	B	324	PRO
1	B	355	ASP
1	C	287	LYS
1	C	340	HIS
1	C	403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	341	ASN
1	B	341	ASN
1	B	389	GLN

### 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 oligosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	144/161 (89%)	0.34	10 (6%) 24 22	22, 43, 75, 91	0
1	B	143/161 (88%)	0.41	7 (4%) 36 33	21, 47, 76, 88	0
1	C	151/161 (93%)	0.84	27 (17%) 4 4	28, 60, 107, 138	0
All	All	438/483 (90%)	0.53	44 (10%) 14 12	21, 49, 88, 138	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	SER	5.2
1	C	329	ALA	4.7
1	B	381	ASP	4.1
1	A	406	ASP	4.0
1	C	337	ALA	3.9
1	C	323	GLN	3.8
1	C	414	LEU	3.5
1	C	336	PHE	3.4
1	C	327	ALA	3.3
1	B	384	THR	3.2
1	B	303	GLN	3.2
1	C	324	PRO	3.1
1	C	413	SER	3.1
1	C	341	ASN	3.0
1	A	384	THR	3.0
1	C	325	SER	3.0
1	C	301	ASP	3.0
1	C	307	GLU	2.9
1	C	328	VAL	2.9
1	C	312	ALA	2.9
1	C	271	TYR	2.9
1	B	405	ALA	2.9
1	C	333	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	351	TYR	2.7
1	A	381	ASP	2.7
1	C	326	GLU	2.6
1	A	354	ASP	2.6
1	C	303	GLN	2.5
1	C	412	LYS	2.5
1	C	339	ALA	2.5
1	C	306	ILE	2.5
1	C	270	ASP	2.4
1	A	380	LYS	2.4
1	C	334	THR	2.3
1	C	330	THR	2.2
1	C	353	GLY	2.1
1	B	382	GLN	2.1
1	A	349	ASP	2.1
1	B	350	SER	2.1
1	A	397	ASP	2.1
1	A	301	ASP	2.0
1	B	368	LEU	2.0
1	C	332	LEU	2.0
1	A	304	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CA	B	501	1/1	0.98	0.12	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.