



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:53 AM GMT

PDB ID : 2V5S
Title : STRUCTURAL BASIS FOR DSCAM ISOFORM SPECIFICITY
Authors : Meijers, R.; Puettmann-Holgado, R.; Skiniotis, G.; Liu, J.-H.; Walz, T.;
Schmucker, D.; Wang, J.-H.
Deposited on : 2007-07-09
Resolution : 2.30 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

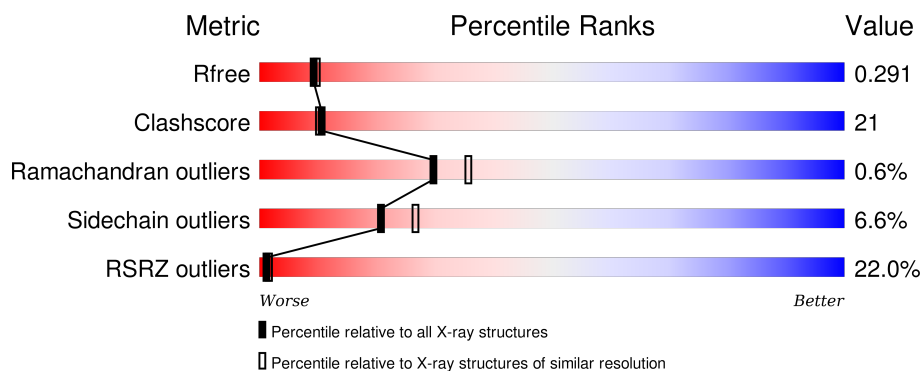
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	394	<div> <div>19%</div> <div>68%</div> <div>27%</div> <div>••</div> </div>
1	B	394	<div> <div>24%</div> <div>70%</div> <div>23%</div> <div>6%</div> <div>•</div> </div>

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
2	NAG	B	1391	X	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 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 DSCAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	19	0
			3110	1962	538	597	13			
1	B	394	Total	C	N	O	S	0	21	0
			3159	1994	545	607	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	EXPRESSION TAG	UNP Q9NBA1
A	-4	TYR	-	EXPRESSION TAG	UNP Q9NBA1
A	-3	PHE	-	EXPRESSION TAG	UNP Q9NBA1
A	-2	GLN	-	EXPRESSION TAG	UNP Q9NBA1
A	-1	GLY	-	EXPRESSION TAG	UNP Q9NBA1
A	0	ASP	-	EXPRESSION TAG	UNP Q9NBA1
A	207	ILE	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	211	ALA	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	213	ARG	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	214	THR	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	215	PRO	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	216	ALA	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	218	VAL	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	219	GLN	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	222	LEU	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	223	GLU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	224	LEU	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	225	MET	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	226	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	227	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
A	228	HIS	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	229	THR	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	230	ILE	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	232	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1

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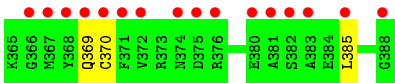
Chain	Residue	Modelled	Actual	Comment	Reference
A	239	PHE	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	-5	ALA	-	EXPRESSION TAG	UNP Q9NBA1
B	-4	TYR	-	EXPRESSION TAG	UNP Q9NBA1
B	-3	PHE	-	EXPRESSION TAG	UNP Q9NBA1
B	-2	GLN	-	EXPRESSION TAG	UNP Q9NBA1
B	-1	GLY	-	EXPRESSION TAG	UNP Q9NBA1
B	0	ASP	-	EXPRESSION TAG	UNP Q9NBA1
B	207	ILE	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	211	ALA	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
B	213	ARG	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	214	THR	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	215	PRO	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	216	ALA	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	218	VAL	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	219	GLN	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	222	LEU	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	223	GLU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	224	LEU	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	225	MET	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	226	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	227	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
B	228	HIS	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	229	THR	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	230	ILE	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	232	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	239	PHE	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0
3	B	127	Total 127	O 127	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.77Å 166.84Å 125.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.90 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.99-2.30) 94.7 (19.90-2.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.287 0.235 , 0.291	Depositor DCC
R_{free} test set	2254 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.3	EDS
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 44901 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8332e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG

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	0.46	0/3243	1.17	12/4394 (0.3%)
1	B	0.48	1/3299 (0.0%)	1.18	8/4470 (0.2%)
All	All	0.47	1/6542 (0.0%)	1.18	20/8864 (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	A	0	4
1	B	0	7
2	B	1	0
All	All	1	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-2	GLN	CD-OE1	6.29	1.37	1.24

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	MET	N-CA-C	-9.04	86.58	111.00
1	A	183	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	B	143[A]	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	143[B]	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	213	ARG	NE-CZ-NH2	-7.28	116.66	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1391	NAG	C1

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	THR	Peptide
1	A	321	PHE	Peptide
1	A	41	SER	Peptide
1	A	59	GLY	Peptide
1	B	32	PRO	Peptide

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	3110	0	3088	119	2
1	B	3159	0	3123	146	2
2	A	56	0	50	2	0
2	B	56	0	50	33	0
3	A	119	0	0	27	1
3	B	127	0	0	19	0
All	All	6627	0	6311	269	3

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 21.

The worst 5 of 269 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:291[B]:ASN:ND2	1:B:294:GLY:O	1.75	1.20
1:B:294:GLY:O	2:B:1391:NAG:C1	1.91	1.19
1:B:291[A]:ASN:ND2	1:B:294:GLY:O	1.76	1.17
1:A:106:TYR:O	3:A:2019:HOH:O	1.62	1.16
2:B:1391:NAG:H82	3:B:2110:HOH:O	1.48	1.13

All (3) 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)
1:A:198:LYS:NZ	1:B:181:GLN:OE1[3_655]	1.98	0.22
3:A:2064:HOH:O	3:A:2064:HOH:O[3_655]	1.99	0.21
1:A:181:GLN:NE2	1:B:198:LYS:NZ[3_655]	2.15	0.05

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	404/394 (102%)	382 (95%)	21 (5%)	1 (0%)	52	64
1	B	411/394 (104%)	386 (94%)	20 (5%)	5 (1%)	16	16
All	All	815/788 (103%)	768 (94%)	41 (5%)	6 (1%)	30	31

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	VAL
1	B	315	PRO
1	B	156	GLY
1	B	241	ALA
1	B	291[A]	ASN

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	350/336 (104%)	329 (94%)	21 (6%)	24	31
1	B	355/336 (106%)	324 (91%)	31 (9%)	13	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	705/672 (105%)	653 (93%)	52 (7%)	21	21

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LYS
1	B	57	SER
1	B	316	THR
1	B	27	LYS
1	B	41	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	181	GLN
1	B	54	GLN
1	A	141	HIS
1	B	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

8 carbohydrates 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	NAG	A	1389	1,2	14,14,15	0.51	0	15,19,21	1.82	4 (26%)
2	NAG	A	1390	2	14,14,15	0.58	0	15,19,21	1.38	2 (13%)
2	NAG	A	1391	1,2	14,14,15	0.47	0	15,19,21	2.07	4 (26%)
2	NAG	A	1392	2	14,14,15	0.51	0	15,19,21	1.40	1 (6%)
2	NAG	B	1389	1,2	14,14,15	0.50	0	15,19,21	1.11	0
2	NAG	B	1390	2	14,14,15	0.48	0	15,19,21	1.35	3 (20%)
2	NAG	B	1391	1,2	14,14,15	1.03	1 (7%)	15,19,21	5.77	10 (66%)
2	NAG	B	1392	2	14,14,15	0.63	0	15,19,21	1.75	3 (20%)

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	NAG	A	1389	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1390	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1391	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1392	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1389	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1390	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1391	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1392	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1391	NAG	C1-C2	3.15	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1391	NAG	C6-C5-C4	-6.06	98.07	113.02
2	B	1391	NAG	O7-C7-C8	-3.87	114.95	122.06
2	A	1391	NAG	O3-C3-C4	-3.47	102.52	110.34
2	A	1389	NAG	C3-C4-C5	-3.47	104.16	110.20
2	B	1392	NAG	O7-C7-C8	-3.21	116.17	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1391	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1389	NAG	2	0
2	B	1389	NAG	1	0
2	B	1391	NAG	29	0
2	B	1392	NAG	4	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	388/394 (98%)	1.19	76 (19%) 1 2	56, 65, 72, 81	7 (1%)
1	B	394/394 (100%)	1.37	96 (24%) 1 1	52, 65, 73, 82	5 (1%)
All	All	782/788 (99%)	1.28	172 (21%) 1 1	52, 65, 72, 82	12 (1%)

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	8.5
1	A	55	ILE	8.4
1	B	58	ASP	7.8
1	A	385	LEU	6.5
1	A	88	PHE	6.2

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 ⓘ

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(Å ²)	Q<0.9
2	NAG	B	1391	14/15	-0.03	1.00	7.58	96,107,112,114	0
2	NAG	A	1391	14/15	0.68	0.36	1.45	77,82,85,89	0
2	NAG	B	1389	14/15	0.83	0.19	-0.04	52,62,67,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1389	14/15	0.79	0.17	-0.07	56,63,70,78	0
2	NAG	A	1390	14/15	0.55	0.46	-	88,94,96,97	0
2	NAG	B	1390	14/15	0.69	0.34	-	71,81,85,86	0
2	NAG	A	1392	14/15	0.53	0.46	-	93,96,97,98	0
2	NAG	B	1392	14/15	0.19	0.56	-	119,122,129,129	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.