



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2016 – 01:17 PM EDT

PDB ID : 4X9F  
Title : Crystal structure of Dscam1 isoform 6.9, N-terminal four Ig domains  
Authors : Chen, Q.; Yu, Y.; Li, S.A.; Cheng, L.  
Deposited on : 2014-12-11  
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

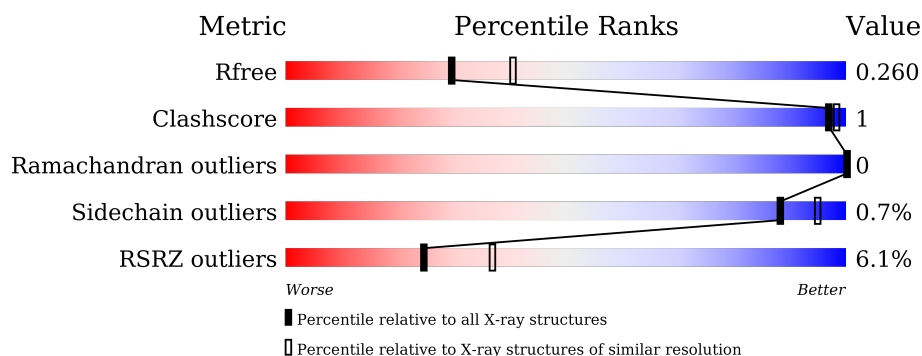
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	394	<div> <div>11%</div> <div> <div></div> <div>96%</div> <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	A	406	-	-	-	X
4	MAN	A	405	-	-	-	X
7	EPE	A	417	-	-	-	X
7	EPE	A	418	-	-	-	X

## 2 Entry composition [i](#)

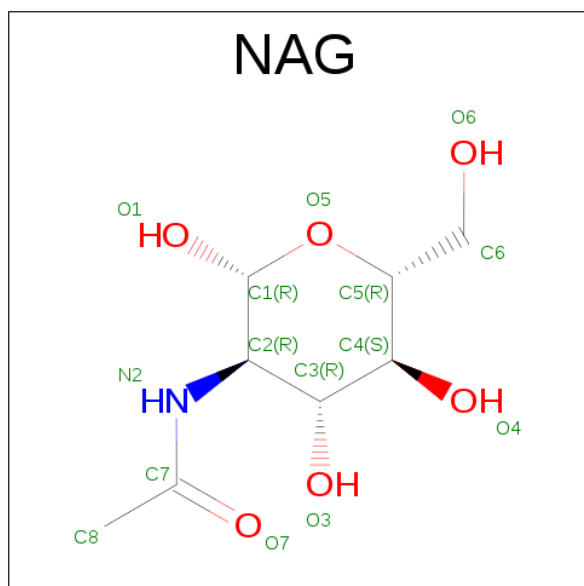
There are 8 unique types of molecules in this entry. The entry contains 6598 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Down Syndrome Cell Adhesion Molecule isoform 6.9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3064	1928	532	591	13			
1	B	390	Total	C	N	O	S	0	1	0
			3053	1922	532	586	13			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



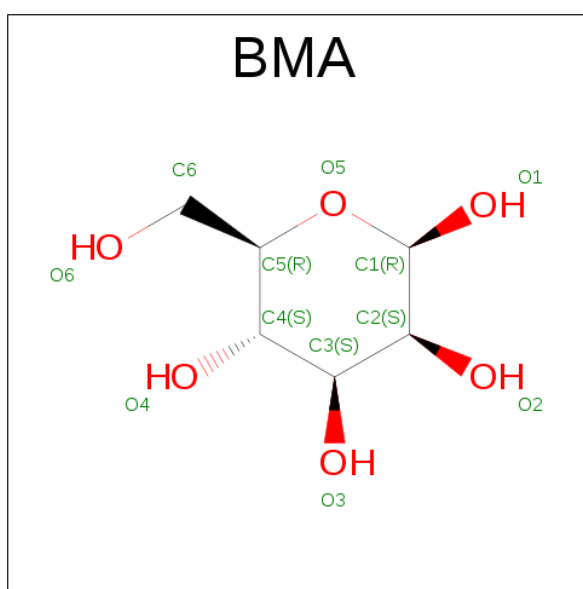
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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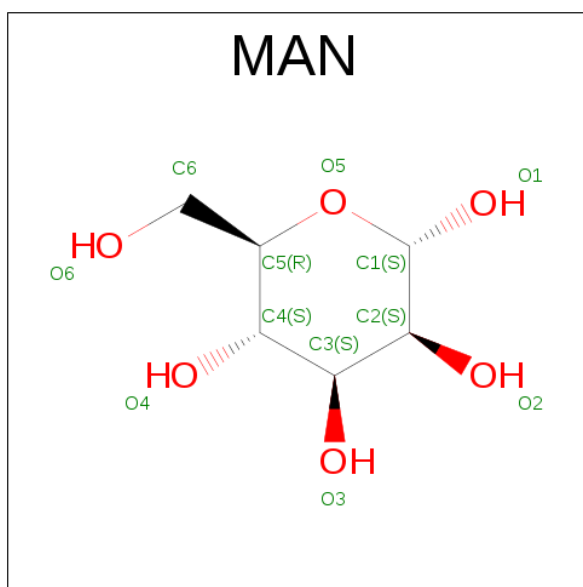
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



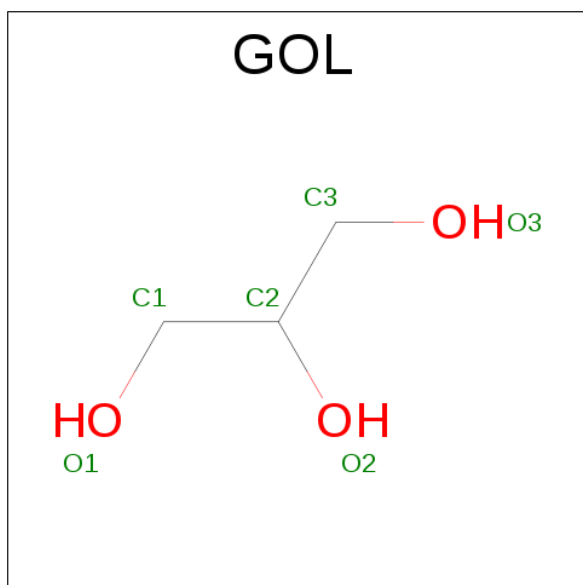
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



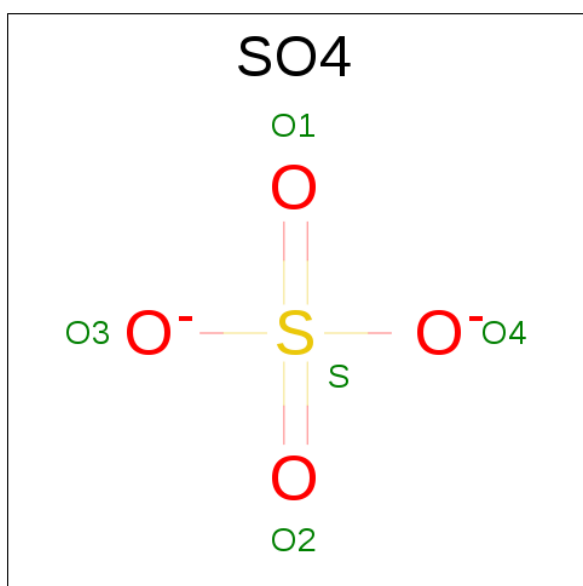
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



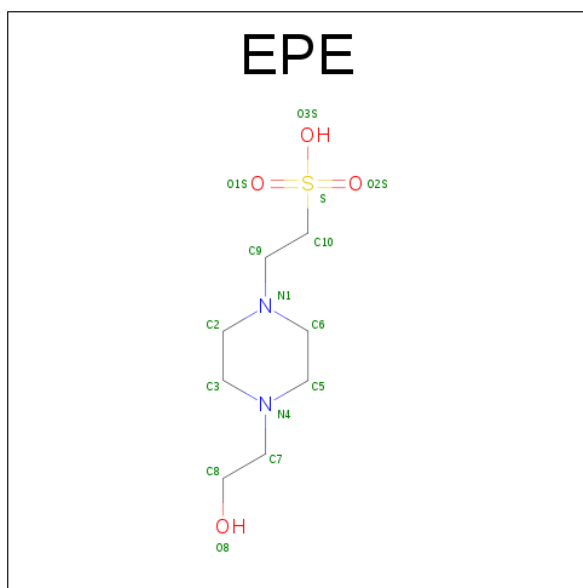
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	A	1	Total S 1 1	0	0
6	A	1	Total O 1 1	0	0
6	A	1	Total O 1 1	0	0
6	A	1	Total O 1 1	0	0
6	A	1	Total O 1 1	0	0
6	B	1	Total S 1 1	0	0
6	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	B	1	Total S 1 1	0	0
6	B	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 15 8 2 4 1	0	0
7	A	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 8 is water.

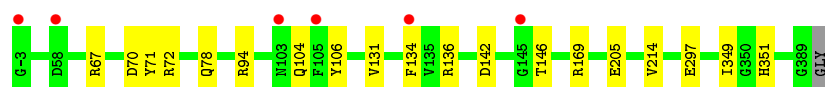


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	123	Total 123	O 123	0	0
8	B	89	Total 89	O 89	0	0

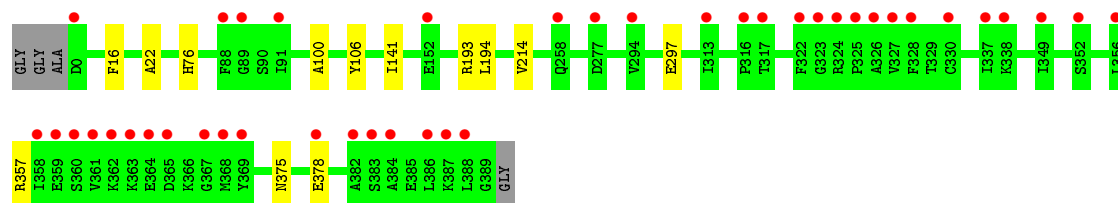
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Down Syndrome Cell Adhesion Molecule isoform 6.9



- Molecule 1: Down Syndrome Cell Adhesion Molecule isoform 6.9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.69Å 90.50Å 169.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.30 – 2.35 49.79 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.30-2.35) 99.3 (49.79-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.211 , 0.260 0.213 , 0.260	Depositor DCC
$R_{free}$ test set	2103 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: GOL, BMA, NAG, SO4, EPE, MAN

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	0.24	0/3127	0.44	0/4238
1	B	0.23	0/3116	0.43	0/4223
All	All	0.24	0/6243	0.44	0/8461

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	3064	0	3029	10	1
1	B	3053	0	3025	6	0
2	A	56	0	48	1	0
2	B	56	0	48	0	0
3	A	22	0	18	0	0
3	B	22	0	18	0	0
4	A	22	0	20	0	0
4	B	22	0	20	0	0
5	A	18	0	24	0	0
5	B	6	0	8	0	0
6	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
7	A	30	0	34	0	1
8	A	123	0	0	3	0
8	B	89	0	0	0	0
All	All	6598	0	6292	16	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 1.

All (16) 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:70:ASP:OD2	8:A:501:HOH:O	2.12	0.68
1:A:71:TYR:O	1:A:72:ARG:NE	2.31	0.63
1:B:106:TYR:O	1:B:193[A]:ARG:NH1	2.34	0.60
1:A:142:ASP:OD1	1:A:146:THR:N	2.35	0.59
1:A:169:ARG:NH1	6:A:416:SO4:O1	2.39	0.56
1:A:214:VAL:HG23	1:A:297:GLU:HG2	1.89	0.55
1:A:67:ARG:HA	2:A:401:NAG:H83	1.96	0.47
1:B:214:VAL:HG23	1:B:297:GLU:HG2	1.97	0.45
1:A:78:GLN:NE2	8:A:508:HOH:O	2.47	0.44
1:A:349:ILE:HD11	1:A:351:HIS:HB3	1.99	0.44
1:A:106:TYR:HB3	1:A:131:VAL:HG11	2.01	0.42
1:B:16:PHE:CG	1:B:22:ALA:HB2	2.54	0.42
1:B:375:ASN:OD1	1:B:378:GLU:N	2.43	0.41
1:A:94:ARG:NH2	8:A:509:HOH:O	2.49	0.41
1:B:76:HIS:HB3	1:B:100:ALA:HB3	2.03	0.40
1:B:141:ILE:HD12	1:B:194:LEU:HD13	2.04	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:NH1	7:A:418:EPE:O1S[4_455]	2.09	0.11

## 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	392/394 (100%)	385 (98%)	7 (2%)	0	100	100
1	B	389/394 (99%)	381 (98%)	8 (2%)	0	100	100
All	All	781/788 (99%)	766 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	338/337 (100%)	334 (99%)	4 (1%)	78	89
1	B	338/337 (100%)	337 (100%)	1 (0%)	94	98
All	All	676/674 (100%)	671 (99%)	5 (1%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	134	PHE
1	A	136	ARG
1	A	205	GLU
1	B	357	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 15 are modelled with single atom - leaving 22 for Mogul analysis.

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	401	1,2	14,14,15	0.68	1 (7%)	15,19,21	0.58	0
2	NAG	A	402	3,2	14,14,15	0.37	0	15,19,21	0.66	0
3	BMA	A	403	2,4	11,11,12	0.90	1 (9%)	15,15,17	1.25	2 (13%)
4	MAN	A	404	3	11,11,12	0.48	0	15,15,17	1.41	2 (13%)
4	MAN	A	405	3	11,11,12	0.97	1 (9%)	15,15,17	1.17	2 (13%)
2	NAG	A	406	1,2	14,14,15	0.36	0	15,19,21	0.32	0
2	NAG	A	407	3,2	14,14,15	0.33	0	15,19,21	0.25	0
3	BMA	A	408	2	11,11,12	0.64	0	15,15,17	1.19	3 (20%)
5	GOL	A	409	-	5,5,5	0.34	0	5,5,5	0.52	0
5	GOL	A	410	-	5,5,5	0.35	0	5,5,5	0.22	0
7	EPE	A	417	-	15,15,15	0.85	1 (6%)	19,20,20	2.29	9 (47%)
7	EPE	A	418	-	15,15,15	0.88	1 (6%)	19,20,20	3.49	11 (57%)
5	GOL	A	419	-	5,5,5	0.38	0	5,5,5	0.23	0
2	NAG	B	401	1,2	14,14,15	0.47	0	15,19,21	0.41	0
2	NAG	B	402	3,2	14,14,15	0.26	0	15,19,21	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	B	403	2	11,11,12	0.71	0	15,15,17	0.88	1 (6%)
2	NAG	B	404	1,2	14,14,15	0.40	0	15,19,21	0.30	0
2	NAG	B	405	3,2	14,14,15	0.25	0	15,19,21	0.41	0
3	BMA	B	406	2,4	11,11,12	0.58	0	15,15,17	1.14	2 (13%)
4	MAN	B	407	3	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
4	MAN	B	408	3	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
5	GOL	B	409	-	5,5,5	0.34	0	5,5,5	0.13	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	NAG	A	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	402	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	403	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	404	3	-	0/2/19/22	0/1/1/1
4	MAN	A	405	3	-	0/2/19/22	0/1/1/1
2	NAG	A	406	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	407	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	408	2	-	0/2/19/22	0/1/1/1
5	GOL	A	409	-	-	0/4/4/4	0/0/0/0
5	GOL	A	410	-	-	0/4/4/4	0/0/0/0
7	EPE	A	417	-	-	0/9/19/19	0/1/1/1
7	EPE	A	418	-	-	0/9/19/19	0/1/1/1
5	GOL	A	419	-	-	0/4/4/4	0/0/0/0
2	NAG	B	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	402	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	403	2	-	0/2/19/22	0/1/1/1
2	NAG	B	404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	405	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	406	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	407	3	-	0/2/19/22	0/1/1/1
4	MAN	B	408	3	-	0/2/19/22	0/1/1/1
5	GOL	B	409	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	MAN	O5-C1	-2.37	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAG	O5-C1	-2.28	1.40	1.43
3	A	403	BMA	O5-C1	-2.21	1.40	1.43
7	A	417	EPE	C10-S	2.74	1.81	1.77
7	A	418	EPE	C10-S	2.80	1.81	1.77

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	BMA	O2-C2-C3	-2.59	104.96	110.19
4	A	404	MAN	O2-C2-C3	-2.33	105.49	110.19
3	B	406	BMA	O2-C2-C3	-2.24	105.67	110.19
4	A	405	MAN	O2-C2-C3	-2.24	105.68	110.19
3	A	408	BMA	O2-C2-C3	-2.19	105.78	110.19
4	B	408	MAN	O2-C2-C3	-2.14	105.86	110.19
4	B	407	MAN	O2-C2-C3	-2.14	105.87	110.19
3	B	403	BMA	O2-C2-C3	-2.07	106.01	110.19
3	A	408	BMA	O5-C1-C2	2.01	114.11	110.89
7	A	418	EPE	O3S-S-C10	2.09	109.33	104.99
4	A	405	MAN	C1-O5-C5	2.16	115.31	112.14
3	B	406	BMA	O5-C1-C2	2.24	114.47	110.89
7	A	417	EPE	C7-N4-C3	2.36	116.38	111.25
7	A	417	EPE	C7-N4-C5	2.53	116.75	111.25
7	A	418	EPE	C7-N4-C3	2.54	116.78	111.25
7	A	417	EPE	C2-C3-N4	2.56	115.65	110.65
3	A	408	BMA	C1-O5-C5	2.63	116.00	112.14
7	A	417	EPE	O2S-S-C10	2.70	108.77	106.87
4	B	407	MAN	C1-O5-C5	2.70	116.11	112.14
3	A	403	BMA	C1-O5-C5	2.75	116.18	112.14
4	B	408	MAN	C1-O5-C5	2.88	116.38	112.14
7	A	417	EPE	O3S-S-C10	3.10	111.44	104.99
7	A	417	EPE	C5-C6-N1	3.22	116.93	110.65
7	A	417	EPE	C6-N1-C2	3.25	116.15	108.87
7	A	418	EPE	C7-N4-C5	3.48	118.83	111.25
7	A	417	EPE	C5-N4-C3	3.52	116.75	108.87
4	A	404	MAN	C1-O5-C5	3.64	117.49	112.14
7	A	418	EPE	C2-C3-N4	3.86	118.19	110.65
7	A	418	EPE	C6-C5-N4	4.10	118.65	110.65
7	A	418	EPE	C3-C2-N1	4.27	118.99	110.65
7	A	418	EPE	C5-C6-N1	4.29	119.03	110.65
7	A	417	EPE	O1S-S-C10	4.44	110.01	106.87
7	A	418	EPE	C6-N1-C2	4.65	119.28	108.87
7	A	418	EPE	O1S-S-C10	5.49	110.75	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	418	EPE	O2S-S-C10	6.17	111.22	106.87
7	A	418	EPE	C5-N4-C3	6.22	122.80	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAG	1	0
7	A	418	EPE	0	1

## 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	393/394 (99%)	0.13	6 (1%) 76 85	31, 47, 71, 140	0
1	B	390/394 (98%)	0.69	42 (10%) 8 13	37, 58, 97, 196	0
All	All	783/788 (99%)	0.41	48 (6%) 25 37	31, 51, 90, 196	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	ILE	7.7
1	B	324	ARG	6.2
1	B	322	PHE	5.8
1	B	361	VAL	5.6
1	B	325	PRO	5.5
1	B	384	ALA	5.2
1	B	337	ILE	4.9
1	B	369	TYR	4.8
1	B	388	LEU	4.6
1	A	105	PHE	3.9
1	B	359	GLU	3.7
1	B	328	PHE	3.7
1	B	383	SER	3.4
1	A	-3	GLY	3.4
1	B	349	ILE	3.3
1	B	386	LEU	3.3
1	B	356	LEU	3.2
1	B	313	ILE	3.1
1	B	327	VAL	3.0
1	B	330	CYS	2.9
1	B	367	GLY	2.9
1	B	0	ASP	2.8
1	B	364	GLU	2.8
1	B	362	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	323	GLY	2.7
1	B	378	GLU	2.7
1	A	58	ASP	2.7
1	B	382	ALA	2.7
1	B	360	SER	2.6
1	B	326	ALA	2.6
1	B	317	THR	2.5
1	A	145	GLY	2.5
1	B	338	LYS	2.5
1	B	294	VAL	2.5
1	A	134	PHE	2.4
1	B	152	GLU	2.4
1	B	352	SER	2.4
1	B	258	GLN	2.3
1	B	316	PRO	2.3
1	B	89	GLY	2.2
1	B	387	LYS	2.1
1	B	91	ILE	2.1
1	A	103	ASN	2.1
1	B	277	ASP	2.1
1	B	88	PHE	2.1
1	B	363	LYS	2.0
1	B	365	ASP	2.0
1	B	368	MET	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 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EPE	A	418	15/15	0.32	1.00	17.72	120,142,188,191	0
7	EPE	A	417	15/15	0.61	0.86	14.35	75,142,159,170	0
2	NAG	A	406	14/15	0.85	0.16	2.57	67,81,89,94	0
4	MAN	A	405	11/12	0.81	0.25	2.11	63,67,94,109	0
4	MAN	A	404	11/12	0.81	0.24	1.71	69,76,85,87	0
5	GOL	A	410	6/6	0.85	0.20	1.48	68,70,72,74	0
5	GOL	B	409	6/6	0.92	0.18	0.66	48,49,54,67	0
2	NAG	A	401	14/15	0.88	0.16	0.09	32,49,62,68	0
5	GOL	A	409	6/6	0.88	0.12	-0.71	43,47,56,56	0
2	NAG	B	401	14/15	0.96	0.12	-1.14	41,53,63,63	0
2	NAG	B	404	14/15	0.88	0.13	-1.37	53,71,75,78	0
3	BMA	B	406	11/12	0.80	0.17	-	87,94,104,110	0
6	SO4	B	414	1/5	0.69	0.15	-	82,82,82,82	0
2	NAG	B	405	14/15	0.91	0.14	-	64,74,93,94	0
5	GOL	A	419	6/6	0.65	0.37	-	73,88,90,118	0
6	SO4	B	412	1/5	0.75	0.35	-	50,50,50,50	0
2	NAG	A	407	14/15	0.75	0.28	-	102,112,121,121	0
6	SO4	A	416	1/5	-0.39	2.78	-	89,89,89,89	0
2	NAG	A	402	14/15	0.85	0.16	-	52,68,76,79	0
6	SO4	A	412	1/5	0.89	0.23	-	70,70,70,70	0
6	SO4	A	413	1/5	0.65	1.74	-	77,77,77,77	0
6	SO4	B	413	1/5	0.76	0.51	-	82,82,82,82	0
2	NAG	B	402	14/15	0.83	0.16	-	49,78,100,101	0
4	MAN	B	407	11/12	0.76	0.39	-	98,105,114,114	0
6	SO4	B	417	1/5	0.58	0.21	-	66,66,66,66	0
6	SO4	B	410	1/5	0.12	0.64	-	108,108,108,108	0
6	SO4	A	414	1/5	0.02	0.97	-	76,76,76,76	0
3	BMA	A	403	11/12	0.89	0.26	-	63,71,87,99	0
6	SO4	B	416	1/5	0.70	0.32	-	64,64,64,64	0
6	SO4	B	411	1/5	0.60	1.19	-	95,95,95,95	0
6	SO4	B	415	1/5	-0.32	0.80	-	82,82,82,82	0
3	BMA	A	408	11/12	0.53	0.34	-	91,111,119,121	0
6	SO4	B	418	1/5	0.80	0.55	-	67,67,67,67	0
3	BMA	B	403	11/12	0.75	0.24	-	96,109,114,115	0
6	SO4	A	411	1/5	0.59	0.38	-	66,66,66,66	0
4	MAN	B	408	11/12	0.79	0.21	-	83,96,105,117	0
6	SO4	A	415	1/5	0.26	1.34	-	85,85,85,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.