



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:23 PM GMT

PDB ID : 2V5M  
Title : STRUCTURAL BASIS FOR DSCAM ISOFORM SPECIFICITY  
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Deposited on : 2007-07-06  
Resolution : 1.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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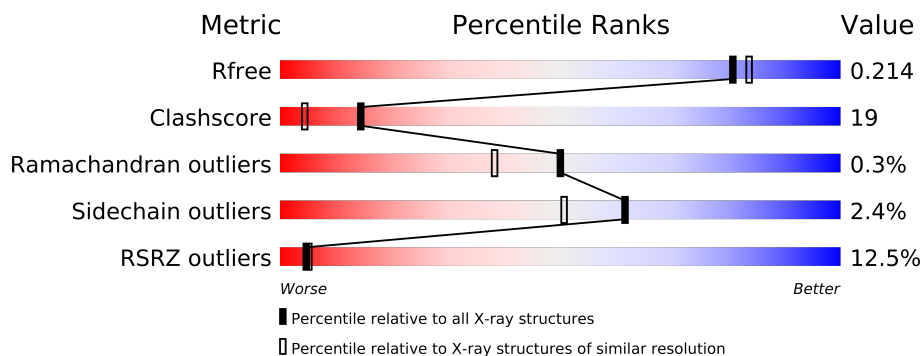
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. 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	388	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3915 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 DSCAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3144	1980	545	606	13	0	25	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	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
			Total	C	N	O		
2	A	2	28	16	2	10	0	0

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

There are 40 discrepancies between the modelled and reference sequences:

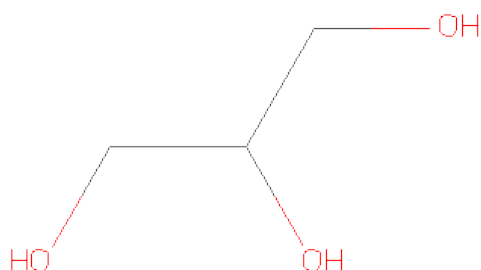
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ILE	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	211	ALA	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	213	ARG	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	214	THR	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	215	PRO	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	216	ALA	THR	VARIANT 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
A	239	PHE	TYR	VARIANT SEE REMARK 99	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	239	PHE	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

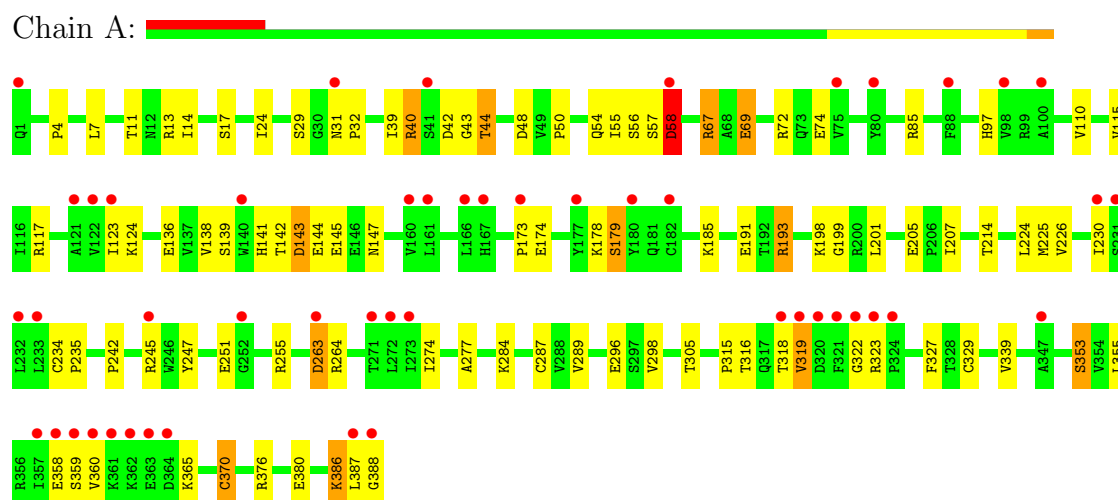
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	709	Total	O	0	0
			709	709		

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: DSCAM



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.17Å 99.17Å 163.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 29.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-1.95) 98.6 (29.71-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.205 0.179 , 0.214	Depositor DCC
$R_{free}$ test set	3006 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 59598 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: GOL, 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	0.67	2/3291 (0.1%)	1.35	24/4458 (0.5%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	LYS	C-O	5.77	1.34	1.23
1	A	387	LEU	C-O	5.43	1.33	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	NE-CZ-NH2	-22.43	109.08	120.30
1	A	193	ARG	NE-CZ-NH1	18.34	129.47	120.30
1	A	198	LYS	CD-CE-NZ	8.24	130.65	111.70
1	A	72	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	A	85	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	67	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	40	ARG	N-CA-CB	-6.87	98.23	110.60
1	A	72	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	138	VAL	CA-CB-CG2	-6.62	100.97	110.90
1	A	380	GLU	OE1-CD-OE2	-6.23	115.83	123.30
1	A	264	ARG	NE-CZ-NH1	6.09	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69[A]	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	69[B]	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	353	SER	N-CA-CB	-5.85	101.73	110.50
1	A	40	ARG	CA-CB-CG	5.83	126.24	113.40
1	A	370	CYS	CA-CB-SG	-5.50	104.09	114.00
1	A	17	SER	N-CA-CB	5.46	118.68	110.50
1	A	179	SER	N-CA-CB	-5.43	102.35	110.50
1	A	255	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	386	LYS	CD-CE-NZ	5.19	123.64	111.70
1	A	263[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	263[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	143[A]	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	143[B]	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58[A]	ASP	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	3144	0	3111	120	0
2	A	56	0	50	3	0
3	A	6	0	6	1	0
4	A	709	0	0	66	6
All	All	3915	0	3167	122	6

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 19.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:VAL:HB	4:A:2284:HOH:O	1.26	1.26
1:A:14:ILE:HG23	4:A:2037:HOH:O	1.50	1.10
1:A:235:PRO:CD	4:A:2482:HOH:O	2.00	1.07
1:A:57[B]:SER:O	1:A:58[B]:ASP:HB2	1.52	1.07
1:A:235:PRO:CG	4:A:2482:HOH:O	2.04	1.05
1:A:245[B]:ARG:HD2	4:A:2498:HOH:O	1.56	1.03
1:A:11:THR:OG1	4:A:2022:HOH:O	1.77	1.02
1:A:141:HIS:HD2	1:A:147:ASN:HD22	1.10	0.95
1:A:235:PRO:CB	4:A:2482:HOH:O	2.13	0.94
1:A:235:PRO:HD2	4:A:2482:HOH:O	1.61	0.92
2:A:401:NAG:H81	4:A:2683:HOH:O	1.73	0.89
1:A:55:ILE:C	1:A:56[B]:SER:N	2.25	0.89
1:A:191:GLU:HG3	4:A:2152:HOH:O	1.73	0.88
1:A:141:HIS:HD2	1:A:147:ASN:ND2	1.73	0.86
1:A:57[B]:SER:O	1:A:58[B]:ASP:CB	2.23	0.85
1:A:245[B]:ARG:HG2	1:A:247:TYR:CE2	2.12	0.84
1:A:67:ARG:HA	2:A:401:NAG:H83	1.60	0.83
1:A:42:ASP:OD2	1:A:44:THR:HG22	1.79	0.83
1:A:274:ILE:CG2	4:A:2554:HOH:O	2.30	0.80
1:A:57[A]:SER:O	1:A:58[A]:ASP:CB	2.30	0.80
1:A:225[B]:MET:HE2	1:A:305:THR:OG1	1.80	0.79
1:A:245[B]:ARG:HG2	1:A:247:TYR:CZ	2.17	0.79
1:A:144[B]:GLU:OE1	4:A:2347:HOH:O	1.99	0.79
1:A:225[B]:MET:CE	1:A:305:THR:OG1	2.32	0.77
1:A:141:HIS:CD2	1:A:147:ASN:HD22	1.98	0.76
1:A:144[B]:GLU:HB2	1:A:178[B]:LYS:HE3	1.67	0.76
1:A:358[B]:GLU:OE2	4:A:2654:HOH:O	2.05	0.75
1:A:235:PRO:HB2	4:A:2482:HOH:O	1.80	0.74
1:A:145[B]:GLU:HG3	4:A:2350:HOH:O	1.86	0.74
1:A:245[B]:ARG:CD	4:A:2498:HOH:O	2.25	0.74
1:A:319:VAL:HG22	1:A:360:VAL:HG11	1.69	0.73
1:A:315:PRO:HD2	4:A:2592:HOH:O	1.87	0.73
1:A:329:CYS:HG	1:A:370:CYS:HG	1.33	0.73
1:A:319:VAL:CG2	1:A:360:VAL:HG11	2.20	0.72
1:A:14:ILE:HD11	4:A:2022:HOH:O	1.90	0.71
1:A:388:GLY:C	4:A:2598:HOH:O	2.28	0.71
1:A:245[B]:ARG:CG	1:A:247:TYR:CE2	2.75	0.70
1:A:13[A]:ARG:NH1	4:A:2028:HOH:O	2.21	0.70
1:A:376:ARG:HD2	4:A:2030:HOH:O	1.92	0.69
1:A:57[A]:SER:O	1:A:58[A]:ASP:HB2	1.93	0.69
1:A:296:GLU:OE2	4:A:2567:HOH:O	2.10	0.68
1:A:263[B]:ASP:OD1	4:A:2527:HOH:O	2.12	0.68
1:A:143[A]:ASP:OD2	1:A:179:SER:HB3	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:ASP:C	1:A:42:ASP:OD2	2.34	0.66
1:A:54:GLN:HG2	4:A:2115:HOH:O	1.94	0.65
1:A:274:ILE:HG21	4:A:2554:HOH:O	1.93	0.65
1:A:14:ILE:CG2	4:A:2037:HOH:O	2.24	0.63
1:A:13[A]:ARG:HD3	4:A:2028:HOH:O	1.99	0.62
1:A:97:HIS:HD2	4:A:2010:HOH:O	1.82	0.61
1:A:143[B]:ASP:CG	4:A:2341:HOH:O	2.38	0.61
1:A:143[B]:ASP:OD1	1:A:179:SER:N	2.29	0.60
1:A:230[B]:ILE:HD12	4:A:2554:HOH:O	2.00	0.60
1:A:274:ILE:HG22	4:A:2554:HOH:O	1.99	0.59
1:A:318:THR:HA	1:A:386:LYS:O	2.02	0.59
1:A:50:PRO:HG3	4:A:2120:HOH:O	2.03	0.58
1:A:11:THR:HG22	4:A:2008:HOH:O	2.04	0.58
1:A:13[B]:ARG:NH2	4:A:2030:HOH:O	2.36	0.58
1:A:11:THR:N	4:A:2022:HOH:O	2.36	0.57
1:A:144[B]:GLU:HB2	1:A:178[B]:LYS:CE	2.36	0.56
1:A:245[B]:ARG:HG2	1:A:247:TYR:OH	2.05	0.56
1:A:225[A]:MET:HE2	4:A:2471:HOH:O	2.07	0.55
1:A:14:ILE:HA	4:A:2037:HOH:O	2.06	0.55
1:A:245[B]:ARG:CG	1:A:247:TYR:CZ	2.89	0.55
1:A:323:ARG:NH1	4:A:2601:HOH:O	2.37	0.54
1:A:178[B]:LYS:HG3	4:A:2341:HOH:O	2.08	0.54
1:A:298:VAL:HG11	4:A:2480:HOH:O	2.07	0.54
1:A:42:ASP:OD2	1:A:43:GLY:N	2.40	0.54
1:A:234:CYS:HG	1:A:287:CYS:CB	2.20	0.54
1:A:365:LYS:HE2	4:A:2659:HOH:O	2.08	0.53
1:A:67:ARG:HD3	4:A:2162:HOH:O	2.06	0.53
1:A:117[B]:ARG:HG2	1:A:173:PRO:HD3	1.91	0.52
1:A:245[B]:ARG:HD3	1:A:247:TYR:CZ	2.44	0.52
1:A:224:LEU:HB3	4:A:2472:HOH:O	2.08	0.52
1:A:74:GLU:HG2	4:A:2186:HOH:O	2.11	0.50
1:A:316:THR:CG2	4:A:2004:HOH:O	2.58	0.50
1:A:143[B]:ASP:OD1	4:A:2341:HOH:O	2.19	0.50
1:A:44:THR:HG21	4:A:2093:HOH:O	2.11	0.49
1:A:319:VAL:CG2	1:A:360:VAL:CG1	2.90	0.49
1:A:57[A]:SER:O	1:A:58[A]:ASP:HB3	2.09	0.49
1:A:230[A]:ILE:HD11	4:A:2472:HOH:O	2.12	0.49
1:A:13[B]:ARG:CZ	4:A:2030:HOH:O	2.60	0.48
1:A:242:PRO:HB2	1:A:289[A]:VAL:HG23	1.94	0.48
1:A:284:LYS:CE	4:A:2556:HOH:O	2.61	0.48
1:A:56[B]:SER:HB3	4:A:2135:HOH:O	2.13	0.48
1:A:7:LEU:HD21	4:A:2069:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ALA:HB2	4:A:2554:HOH:O	2.14	0.47
2:A:502:NAG:O4	4:A:2708:HOH:O	2.08	0.47
1:A:322:GLY:HA2	1:A:359:SER:OG	2.15	0.47
1:A:365:LYS:HG3	4:A:2659:HOH:O	2.14	0.46
1:A:234:CYS:O	3:A:601:GOL:H32	2.16	0.46
1:A:13[A]:ARG:NH1	4:A:2029:HOH:O	2.49	0.46
1:A:4:PRO:HA	1:A:29:SER:O	2.15	0.46
1:A:54:GLN:HG2	4:A:2119:HOH:O	2.17	0.45
1:A:339:VAL:HG13	1:A:370:CYS:SG	2.56	0.45
1:A:298:VAL:CG1	4:A:2480:HOH:O	2.66	0.44
1:A:31:ASN:HD22	1:A:32:PRO:HA	1.82	0.44
1:A:144[B]:GLU:CB	1:A:178[B]:LYS:HE3	2.43	0.44
1:A:277:ALA:CB	4:A:2554:HOH:O	2.65	0.44
1:A:123:ILE:HD11	1:A:201:LEU:HD21	1.99	0.44
1:A:39:ILE:HD12	1:A:43:GLY:HA2	2.01	0.42
1:A:225[B]:MET:HG3	1:A:226:VAL:N	2.34	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HG21	1.74	0.42
1:A:207:ILE:HD12	4:A:2163:HOH:O	2.19	0.42
1:A:245[B]:ARG:HG3	1:A:247:TYR:CE2	2.54	0.42
1:A:327:PHE:HE1	4:A:2593:HOH:O	2.01	0.42
1:A:142:THR:HB	1:A:178[B]:LYS:HE2	2.00	0.42
1:A:139:SER:OG	1:A:141:HIS:HE1	2.02	0.41
1:A:69[B]:GLU:CD	4:A:2162:HOH:O	2.58	0.41
1:A:40:ARG:CD	4:A:2100:HOH:O	2.68	0.41
1:A:142:THR:CB	1:A:178[B]:LYS:HE2	2.51	0.41
1:A:214:THR:HB	4:A:2453:HOH:O	2.19	0.41
1:A:205[A]:GLU:OE2	4:A:2438:HOH:O	2.22	0.41
1:A:40:ARG:HD3	4:A:2100:HOH:O	2.20	0.41
1:A:242:PRO:HB2	1:A:289[A]:VAL:CG2	2.50	0.40
1:A:173:PRO:HD2	1:A:174:GLU:OE1	2.22	0.40
1:A:136[B]:GLU:HG2	1:A:185:LYS:O	2.21	0.40
1:A:55:ILE:O	1:A:56[B]:SER:N	2.52	0.40
1:A:110:VAL:HG12	1:A:199:GLY:HA3	2.02	0.40

All (6) 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)
4:A:2185:HOH:O	4:A:2211:HOH:O[8_665]	1.50	0.70
4:A:2400:HOH:O	4:A:2400:HOH:O[2_765]	1.74	0.46
4:A:2029:HOH:O	4:A:2450:HOH:O[5_755]	1.82	0.38
4:A:2429:HOH:O	4:A:2429:HOH:O[6_565]	2.00	0.20

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:2279:HOH:O	4:A:2316:HOH:O[5_755]	2.02	0.18
4:A:2198:HOH:O	4:A:2267:HOH:O[6_555]	2.04	0.16

## 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	411/388 (106%)	398 (97%)	11 (3%)	2 (0%)	38 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58[A]	ASP
1	A	58[B]	ASP

### 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	356/332 (107%)	348 (98%)	8 (2%)	64 55

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ASP
1	A	124	LYS
1	A	193	ARG
1	A	251	GLU
1	A	319	VAL

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Mol	Chain	Res	Type
1	A	353	SER
1	A	355	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	31	ASN
1	A	97	HIS
1	A	111	ASN
1	A	141	HIS
1	A	147	ASN

### 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 ⓘ

4 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	401	1,2	12,14,15	0.82	0	15,19,21	3.14	9 (60%)
2	NAG	A	402	2	12,14,15	0.58	0	15,19,21	2.59	7 (46%)
2	NAG	A	501	1,2	12,14,15	0.57	0	15,19,21	2.07	4 (26%)
2	NAG	A	502	2	12,14,15	0.69	0	15,19,21	1.17	1 (6%)

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	2	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	O6-C6-C5	-6.84	87.82	111.36
2	A	402	NAG	O5-C5-C6	6.13	113.41	106.98
2	A	401	NAG	C3-C4-C5	5.56	120.12	110.20
2	A	501	NAG	C6-C5-C4	-5.08	100.72	113.00
2	A	401	NAG	C6-C5-C4	-4.34	102.51	113.00
2	A	501	NAG	O5-C5-C6	-4.34	102.43	106.98
2	A	401	NAG	O5-C5-C6	3.91	111.08	106.98
2	A	402	NAG	C3-C2-N2	-3.83	105.93	111.76
2	A	402	NAG	C6-C5-C4	-3.41	104.75	113.00
2	A	402	NAG	C2-N2-C7	-3.29	117.57	123.09
2	A	401	NAG	O7-C7-C8	-2.86	116.45	122.04
2	A	401	NAG	O5-C5-C4	2.66	114.03	110.65
2	A	401	NAG	C2-N2-C7	2.49	127.26	123.09
2	A	501	NAG	O4-C4-C3	-2.39	104.99	110.35
2	A	502	NAG	O5-C5-C4	-2.31	107.72	110.65
2	A	401	NAG	C4-C3-C2	-2.25	105.81	111.32
2	A	401	NAG	O7-C7-N2	2.21	126.51	121.90
2	A	501	NAG	C3-C4-C5	2.20	114.13	110.20
2	A	402	NAG	O4-C4-C5	2.16	114.97	109.28
2	A	402	NAG	C4-C3-C2	-2.15	106.05	111.32
2	A	402	NAG	O5-C5-C4	2.08	113.29	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	$\# Z  > 2$
3	GOL	A	601	-	5,5,5	0.42	0	5,5,5	5.05	3 (60%)

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
3	GOL	A	601	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	GOL	C3-C2-C1	-10.06	66.86	111.26
3	A	601	GOL	O2-C2-C1	4.30	127.83	108.22
3	A	601	GOL	O2-C2-C3	2.27	118.58	108.22

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, 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	388/388 (100%)	0.86	49 (12%) 4 5	49, 58, 68, 81	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	GLY	6.7
1	A	321	PHE	5.9
1	A	318	THR	4.7
1	A	387	LEU	4.4
1	A	360	VAL	4.2
1	A	362	LYS	4.2
1	A	319	VAL	4.1
1	A	359	SER	4.0
1	A	122	VAL	3.9
1	A	323	ARG	3.9
1	A	361	LYS	3.9
1	A	322	GLY	3.8
1	A	347	ALA	3.8
1	A	320	ASP	3.7
1	A	233	LEU	3.5
1	A	58[A]	ASP	3.4
1	A	363	GLU	3.4
1	A	161	LEU	3.0
1	A	271	THR	3.0
1	A	272	LEU	3.0
1	A	123	ILE	3.0
1	A	324	PRO	3.0
1	A	364	ASP	3.0
1	A	358[A]	GLU	3.0
1	A	88	PHE	3.0
1	A	166	LEU	2.9
1	A	232	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	177	TYR	2.7
1	A	231	SER	2.7
1	A	140	TRP	2.6
1	A	263[A]	ASP	2.5
1	A	357	ILE	2.5
1	A	75	VAL	2.4
1	A	160	VAL	2.4
1	A	230[A]	ILE	2.3
1	A	167	HIS	2.3
1	A	100	ALA	2.3
1	A	31	ASN	2.3
1	A	180	TYR	2.2
1	A	121	ALA	2.2
1	A	182	CYS	2.2
1	A	98	VAL	2.2
1	A	1	GLN	2.1
1	A	80	TYR	2.1
1	A	273	ILE	2.1
1	A	252	GLY	2.1
1	A	41	SER	2.1
1	A	173	PRO	2.1
1	A	245[A]	ARG	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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	402	14/15	0.21	4.06	59,66,74,80	0
2	NAG	A	502	14/15	0.22	2.14	64,68,83,85	0
2	NAG	A	501	14/15	0.21	1.27	62,69,77,84	0
2	NAG	A	401	14/15	0.12	-0.37	43,53,62,71	0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	601	6/6	0.11	-1.58	40,46,53,53	0

## 6.5 Other polymers

There are no such residues in this entry.