



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:18 pm GMT

PDB ID : 1M2T  
Title : Mistletoe Lectin I from Viscum album in Complex with Adenine Monophosphate. Crystal Structure at 1.9 Å Resolution  
Authors : Krauspenhaar, R.; Rypniewski, W.; Kalkura, N.; Moore, K.; DeLucas, L.; Stoeva, S.; Mikhailov, A.; Voelter, W.; Betzel, C.  
Deposited on : 2002-06-25  
Resolution : 1.89 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

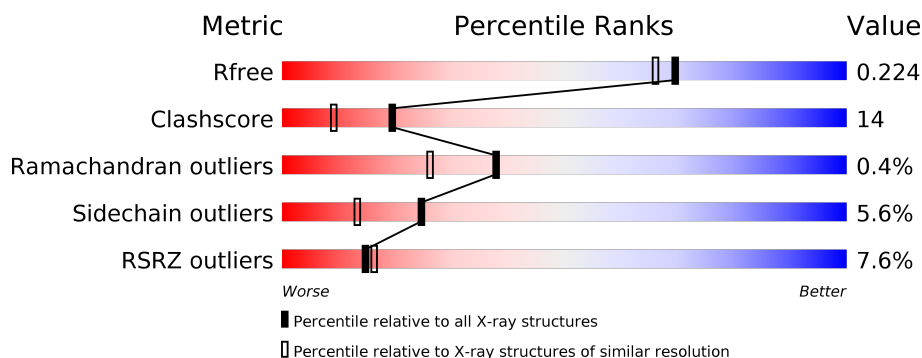
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	254	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>7%</div> <div></div> </div> </div>
2	B	263	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>17%</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
4	FUC	A	501	-	-	X	-
6	GOL	A	702	-	-	X	-
6	GOL	B	701	-	-	X	-
6	GOL	B	704	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4572 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 mistletoe lectin I A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1912	1211	323	374	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	THR	VAL	CONFLICT	UNP P81446
A	9	ASP	THR	CONFLICT	UNP P81446
A	10	GLN	HIS	CONFLICT	UNP P81446
A	15	ALA	GLU	CONFLICT	UNP P81446
A	19	SER	ARG	CONFLICT	UNP P81446
A	23	VAL	LEU	CONFLICT	UNP P81446
A	36	ASN	GLU	CONFLICT	UNP P81446
A	45	VAL	ILE	CONFLICT	UNP P81446
A	49	GLU	ASP	CONFLICT	UNP P81446
A	50	GLY	ALA	CONFLICT	UNP P81446
A	61	ALA	GLN	CONFLICT	UNP P81446
A	63	GLY	GLN	CONFLICT	UNP P81446
A	65	THR	SER	CONFLICT	UNP P81446
A	66	ILE	VAL	CONFLICT	UNP P81446
A	75	LEU	ALA	CONFLICT	UNP P81446
A	81	GLU	GLN	CONFLICT	UNP P81446
A	84	ASN	ASP	CONFLICT	UNP P81446
A	90	SER	ARG	CONFLICT	UNP P81446
A	94	ALA	ARG	CONFLICT	UNP P81446
A	99	GLN	HIS	CONFLICT	UNP P81446
A	100	ASP	LEU	CONFLICT	UNP P81446
A	102	SER	THR	CONFLICT	UNP P81446
A	106	SER	ARG	CONFLICT	UNP P81446
A	109	GLN	LEU	CONFLICT	UNP P81446
A	148	GLN	SER	CONFLICT	UNP P81446
A	150	LYS	ARG	CONFLICT	UNP P81446
A	176	ALA	TYR	CONFLICT	UNP P81446

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Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	ARG	CONFLICT	UNP P81446
A	223	ALA	PRO	CONFLICT	UNP P81446
A	226	VAL	ASN	CONFLICT	UNP P81446
A	227	ILE	PHE	CONFLICT	UNP P81446
A	233	ILE	VAL	CONFLICT	UNP P81446

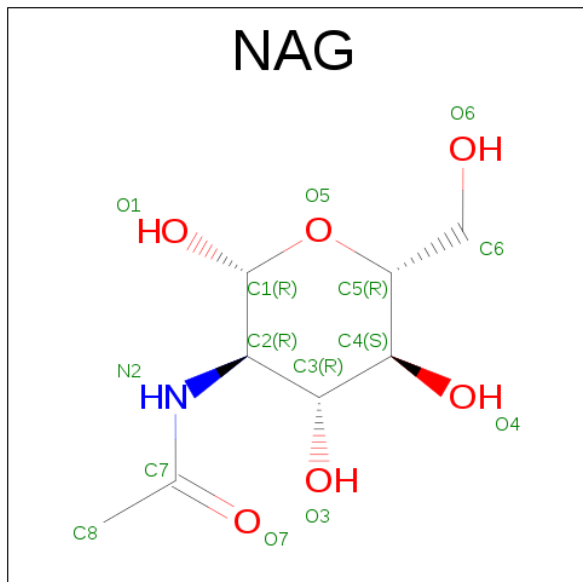
- Molecule 2 is a protein called mistletoe lectin I B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			1995	1239	352	392	12			

There are 26 discrepancies between the modelled and reference sequences:

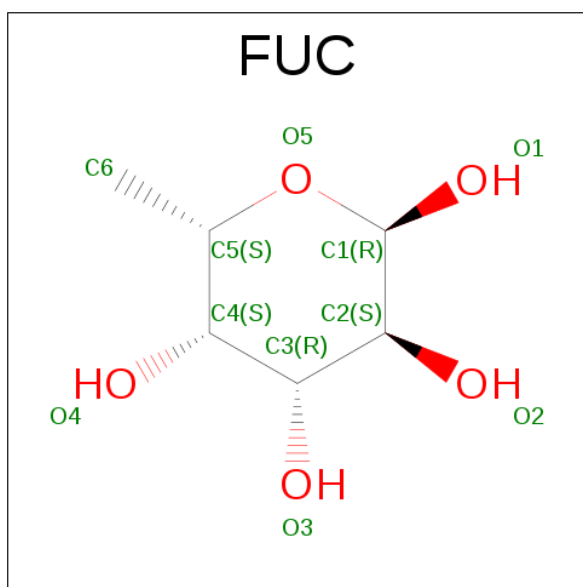
Chain	Residue	Modelled	Actual	Comment	Reference
B	249	ALA	ASP	CONFLICT	UNP P81830
B	253	THR	SER	CONFLICT	UNP P81830
B	258	ILE	THR	CONFLICT	UNP P81830
B	268	THR	ARG	CONFLICT	UNP P81830
B	301	LYS	ARG	CONFLICT	UNP P81830
B	342	GLY	ASP	CONFLICT	UNP P81830
B	390	THR	VAL	CONFLICT	UNP P81830
B	403	ALA	ASN	CONFLICT	UNP P81830
B	408	TYR	TRP	CONFLICT	UNP P81830
B	413	THR	ASP	CONFLICT	UNP P81830
B	414	ALA	SER	CONFLICT	UNP P81830
B	415	GLY	SER	CONFLICT	UNP P81830
B	417	GLU	LYS	CONFLICT	UNP P81830
B	?	-	GLY	DELETION	UNP P81830
B	420	ARG	LYS	CONFLICT	UNP P81830
B	434	LEU	ASN	CONFLICT	UNP P81830
B	436	SER	ASP	CONFLICT	UNP P81830
B	441	ASN	SER	CONFLICT	UNP P81830
B	446	ILE	VAL	CONFLICT	UNP P81830
B	457	ALA	-	INSERTION	UNP P81830
B	459	SER	ALA	CONFLICT	UNP P81830
B	?	-	SER	DELETION	UNP P81830
B	489	SER	LYS	CONFLICT	UNP P81830
B	491	GLN	ARG	CONFLICT	UNP P81830
B	501	ASN	LYS	CONFLICT	UNP P81830
B	510	PRO	PHE	CONFLICT	UNP P81830

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



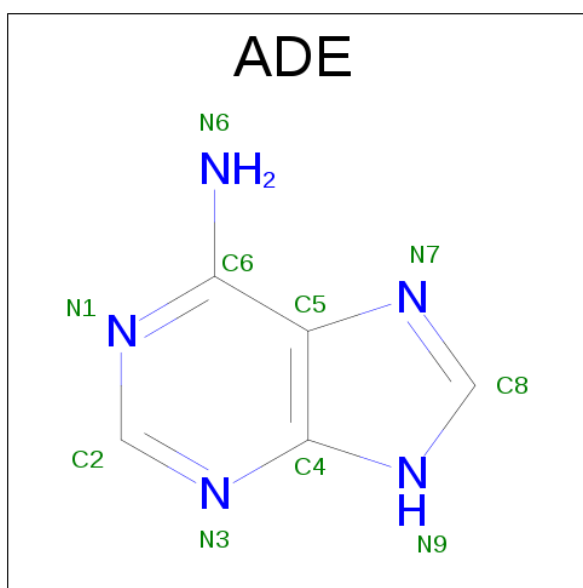
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SUGAR (FUCOSE) (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ADENINE (three-letter code: ADE) (formula:  $C_5H_5N_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			10	5	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is water.

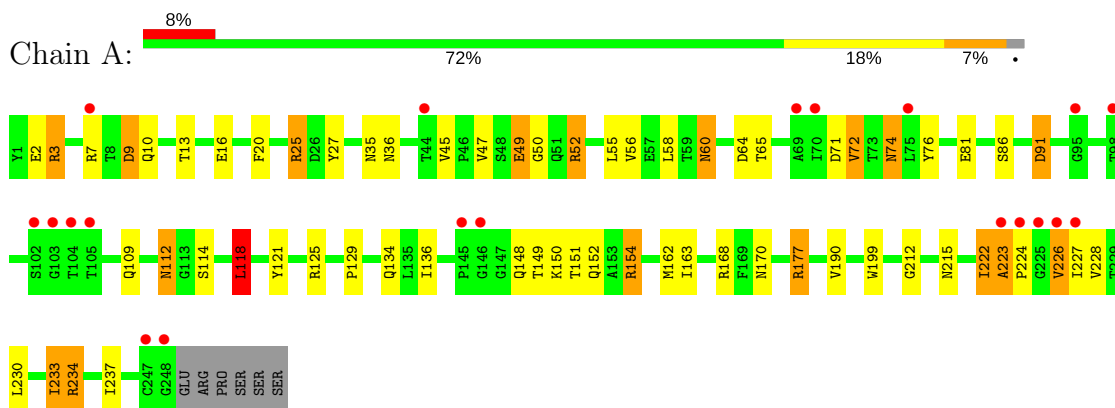
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O	0	0
			203	203		
7	B	300	Total	O	0	0
			300	300		



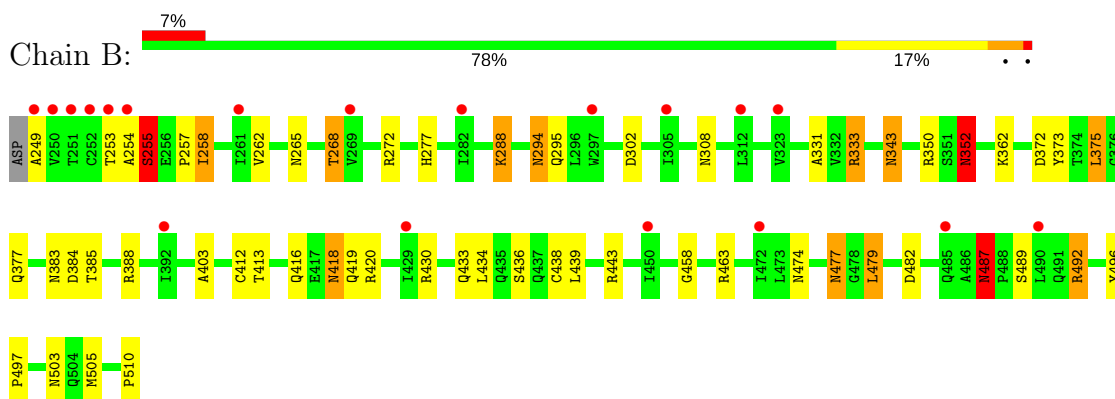
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: mistletoe lectin I A chain



- Molecule 2: mistletoe lectin I B chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.12Å 107.12Å 309.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.89 24.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-1.89) 99.7 (24.97-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.210 , 0.240 0.197 , 0.224	Depositor DCC
$R_{free}$ test set	4159 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, ADE, NAG, FUC

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	0.55	0/1950	1.22	19/2659 (0.7%)
2	B	0.66	1/2034 (0.0%)	1.26	11/2774 (0.4%)
All	All	0.61	1/3984 (0.0%)	1.24	30/5433 (0.6%)

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	2
2	B	0	8
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	510	PRO	N-CD	5.64	1.55	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	3	ARG	NE-CZ-NH1	11.21	125.90	120.30
2	B	420	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	A	52	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	A	125	ARG	NE-CZ-NH1	-10.29	115.15	120.30
2	B	333	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	B	333	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	25	ARG	NE-CZ-NH2	-7.94	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	A	9	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	3	ARG	CD-NE-CZ	7.36	133.90	123.60
1	A	118	LEU	CA-CB-CG	6.50	130.25	115.30
2	B	362	LYS	CA-CB-CG	6.46	127.61	113.40
1	A	52	ARG	NE-CZ-NH1	-6.24	117.18	120.30
2	B	383	ASN	CB-CG-OD1	6.12	133.85	121.60
1	A	91	ASP	CB-CG-OD2	5.83	123.55	118.30
2	B	350	ARG	NE-CZ-NH2	5.79	123.19	120.30
2	B	463	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	B	443	ARG	CD-NE-CZ	5.63	131.49	123.60
1	A	109	GLN	CA-CB-CG	-5.63	101.01	113.40
1	A	222	ILE	CB-CA-C	5.59	122.78	111.60
2	B	492	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	154	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	154	ARG	CD-NE-CZ	5.31	131.04	123.60
1	A	25	ARG	NH1-CZ-NH2	5.26	125.19	119.40
2	B	268	THR	CA-CB-OG1	5.22	119.97	109.00
1	A	162	MET	CA-CB-CG	-5.18	104.49	113.30
1	A	72	VAL	N-CA-CB	-5.16	100.14	111.50
2	B	443	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	177	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ARG	Mainchain
1	A	86	SER	Mainchain
2	B	255	SER	Mainchain
2	B	288	LYS	Mainchain
2	B	343	ASN	Mainchain
2	B	352	ASN	Mainchain
2	B	384	ASP	Mainchain
2	B	438	CYS	Mainchain
2	B	479	LEU	Mainchain
2	B	487	ASN	Mainchain

## 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	1912	0	1877	49	0
2	B	1995	0	1937	57	0
3	A	28	0	26	9	0
3	B	56	0	52	13	0
4	A	10	0	10	7	0
4	B	10	0	10	0	0
5	A	10	0	4	1	0
6	A	24	0	23	6	0
6	B	24	0	25	6	0
7	A	203	0	0	4	0
7	B	300	0	0	10	1
All	All	4572	0	3964	116	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 14.

All (116) 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:112:ASN:HD21	3:A:500:NAG:C1	1.59	1.13
2:B:503:ASN:HD21	6:B:701:GOL:H31	1.16	1.08
2:B:416:GLN:HE21	2:B:418:ASN:HD21	1.04	1.00
2:B:288:LYS:H	2:B:295:GLN:HE22	1.11	0.97
2:B:343:ASN:HD21	3:B:602:NAG:C1	1.78	0.96
4:A:501:FUC:H61	3:A:502:NAG:H3	1.49	0.94
2:B:308:ASN:HD21	3:B:600:NAG:C1	1.81	0.92
1:A:112:ASN:ND2	3:A:500:NAG:C1	2.39	0.86
2:B:265:ASN:HD22	2:B:430:ARG:HH22	1.25	0.83
2:B:503:ASN:ND2	6:B:701:GOL:H31	1.95	0.81
3:B:603:NAG:O4	3:B:604:NAG:C1	2.29	0.80
4:A:501:FUC:C6	3:A:502:NAG:H3	2.14	0.77
1:A:226:VAL:HG23	1:A:227:ILE:H	1.52	0.75
2:B:308:ASN:HD21	3:B:600:NAG:C2	2.00	0.75
2:B:474:ASN:HD22	2:B:477:ASN:H	1.33	0.74
1:A:226:VAL:CG2	1:A:227:ILE:H	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:ASP:H	2:B:377:GLN:HE22	1.37	0.73
2:B:413:THR:H	2:B:419:GLN:HE22	1.36	0.73
1:A:226:VAL:CG2	1:A:227:ILE:N	2.52	0.72
2:B:416:GLN:HE21	2:B:418:ASN:ND2	1.85	0.72
6:A:702:GOL:H11	2:B:388:ARG:HG2	1.73	0.71
2:B:288:LYS:H	2:B:295:GLN:NE2	1.89	0.70
2:B:258:ILE:HG23	7:B:822:HOH:O	1.93	0.69
1:A:149:THR:HA	1:A:152:GLN:HE21	1.56	0.68
2:B:487:ASN:HD21	2:B:489:SER:HB2	1.59	0.68
2:B:288:LYS:NZ	2:B:294:ASN:HD21	1.94	0.65
2:B:403:ALA:HB2	7:B:994:HOH:O	1.96	0.64
1:A:215:ASN:ND2	2:B:255:SER:HB3	2.13	0.64
1:A:2:GLU:HG3	1:A:27:TYR:CE2	2.33	0.64
2:B:288:LYS:N	2:B:295:GLN:HE22	1.90	0.64
4:A:501:FUC:H63	3:A:502:NAG:H5	1.80	0.64
3:A:500:NAG:H3	4:A:501:FUC:H2	1.81	0.62
2:B:413:THR:H	2:B:419:GLN:NE2	1.97	0.62
2:B:343:ASN:ND2	3:B:602:NAG:C1	2.59	0.62
2:B:302:ASP:HB2	2:B:333:ARG:HH22	1.64	0.62
2:B:308:ASN:ND2	3:B:600:NAG:C1	2.59	0.61
2:B:436:SER:HB2	7:B:912:HOH:O	2.01	0.60
1:A:71:ASP:HB3	1:A:74:ASN:HD21	1.66	0.60
3:B:603:NAG:HO4	3:B:604:NAG:C1	2.12	0.60
1:A:121:TYR:O	1:A:150:LYS:HG3	2.02	0.59
1:A:234:ARG:HE	6:A:702:GOL:H31	1.66	0.59
3:A:500:NAG:O3	4:A:501:FUC:C1	2.51	0.59
2:B:477:ASN:HD22	2:B:479:LEU:H	1.50	0.59
1:A:226:VAL:HG22	1:A:227:ILE:N	2.18	0.58
2:B:412:CYS:HA	2:B:419:GLN:HE22	1.67	0.58
2:B:331:ALA:HA	6:B:705:GOL:H31	1.85	0.58
1:A:25:ARG:HH12	1:A:170:ASN:HD21	1.53	0.57
2:B:474:ASN:ND2	2:B:477:ASN:H	2.02	0.56
2:B:372:ASP:H	2:B:377:GLN:NE2	2.01	0.56
1:A:91:ASP:CG	1:A:112:ASN:HB3	2.27	0.54
2:B:277:HIS:HE1	7:B:913:HOH:O	1.90	0.54
7:A:9560:HOH:O	2:B:505:MET:HE2	2.08	0.54
1:A:47:VAL:HA	1:A:52:ARG:HG2	1.89	0.54
2:B:492:ARG:HD3	7:B:971:HOH:O	2.07	0.53
1:A:65:THR:HG22	7:A:9608:HOH:O	2.08	0.53
2:B:343:ASN:HD21	3:B:602:NAG:C2	2.20	0.53
2:B:249:ALA:N	7:B:923:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:NAG:HO3	4:A:501:FUC:C1	2.23	0.52
2:B:433:GLN:O	2:B:434:LEU:HD23	2.09	0.51
1:A:154:ARG:HD3	7:A:9731:HOH:O	2.09	0.51
1:A:9:ASP:HA	1:A:136:ILE:HD11	1.93	0.51
1:A:20:PHE:HZ	1:A:56:VAL:HG13	1.76	0.50
2:B:302:ASP:HB2	2:B:333:ARG:NH2	2.27	0.50
2:B:403:ALA:HB1	7:B:1001:HOH:O	2.11	0.50
2:B:262:VAL:HG22	2:B:268:THR:HG22	1.94	0.50
2:B:413:THR:N	2:B:419:GLN:HE22	2.08	0.50
1:A:60:ASN:HD22	1:A:60:ASN:C	2.16	0.49
1:A:74:ASN:ND2	1:A:76:TYR:H	2.11	0.48
1:A:212:GLY:HA2	1:A:233:ILE:HG23	1.96	0.48
1:A:148:GLN:HG3	1:A:150:LYS:HB3	1.97	0.46
2:B:418:ASN:C	2:B:418:ASN:HD22	2.18	0.46
3:A:500:NAG:C3	4:A:501:FUC:H2	2.46	0.46
1:A:148:GLN:HG3	1:A:151:THR:H	1.80	0.46
1:A:215:ASN:HD21	2:B:257:PRO:HD3	1.80	0.45
2:B:262:VAL:CG2	2:B:385:THR:HG22	2.46	0.45
2:B:288:LYS:HZ1	2:B:294:ASN:HD21	1.63	0.45
1:A:148:GLN:HB2	6:A:601:GOL:O2	2.16	0.45
3:B:603:NAG:O4	3:B:604:NAG:C2	2.64	0.45
2:B:308:ASN:HD21	3:B:600:NAG:H2	1.80	0.45
1:A:129:PRO:O	1:A:134:GLN:HG2	2.17	0.45
1:A:168:ARG:HD3	1:A:199:TRP:CD2	2.52	0.45
1:A:60:ASN:HD21	1:A:64:ASP:H	1.64	0.44
2:B:482:ASP:OD1	6:B:701:GOL:H2	2.18	0.44
1:A:114:SER:O	1:A:118:LEU:HB2	2.18	0.44
1:A:65:THR:HB	6:A:600:GOL:H31	2.00	0.44
1:A:25:ARG:HH22	1:A:170:ASN:ND2	2.14	0.44
2:B:265:ASN:ND2	2:B:430:ARG:HH22	2.04	0.44
1:A:71:ASP:HB3	1:A:74:ASN:ND2	2.31	0.44
1:A:49:GLU:OE1	1:A:50:GLY:N	2.51	0.44
1:A:52:ARG:O	1:A:72:VAL:HB	2.17	0.44
2:B:375:LEU:HD22	2:B:458:GLY:HA2	2.00	0.43
1:A:74:ASN:ND2	1:A:76:TYR:HB2	2.33	0.43
1:A:13:THR:OG1	1:A:16:GLU:HG3	2.19	0.43
2:B:496:TYR:CG	2:B:497:PRO:HD2	2.54	0.43
3:B:600:NAG:H2	7:B:957:HOH:O	2.18	0.43
1:A:190:VAL:HG23	7:A:9576:HOH:O	2.19	0.42
2:B:482:ASP:OD2	6:B:701:GOL:H2	2.18	0.42
1:A:233:ILE:HD11	1:A:237:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:HD22	1:A:76:TYR:H	1.67	0.42
1:A:177:ARG:NH1	6:B:704:GOL:H12	2.35	0.42
1:A:234:ARG:HB3	6:A:702:GOL:C3	2.50	0.42
2:B:477:ASN:HD22	2:B:477:ASN:C	2.23	0.42
2:B:352:ASN:HA	2:B:352:ASN:HD22	1.73	0.41
1:A:45:VAL:HG13	1:A:49:GLU:HG3	2.02	0.41
1:A:76:TYR:HA	5:A:9550:ADE:C2	2.55	0.41
1:A:25:ARG:NH1	1:A:170:ASN:HD21	2.18	0.41
1:A:223:ALA:HB3	1:A:224:PRO:HD3	2.01	0.41
2:B:385:THR:HA	7:B:995:HOH:O	2.19	0.41
2:B:288:LYS:HZ3	2:B:294:ASN:HD21	1.67	0.41
3:B:602:NAG:C7	7:B:961:HOH:O	2.68	0.41
1:A:35:ASN:O	1:A:36:ASN:HB2	2.21	0.40
2:B:272:ARG:HH11	2:B:272:ARG:HD2	1.77	0.40
2:B:373:TYR:HE1	3:B:602:NAG:H81	1.86	0.40
1:A:58:LEU:HD11	1:A:163:ILE:HD11	2.03	0.40
1:A:234:ARG:HE	6:A:702:GOL:C3	2.32	0.40
2:B:474:ASN:HB3	2:B:477:ASN:ND2	2.37	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)
7:B:768:HOH:O	7:B:768:HOH:O[12_554]	1.76	0.44

## 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	246/254 (97%)	239 (97%)	6 (2%)	1 (0%)	38	26
2	B	260/263 (99%)	256 (98%)	3 (1%)	1 (0%)	38	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	506/517 (98%)	495 (98%)	9 (2%)	2 (0%)	38	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	254	ALA
1	A	223	ALA

### 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	208/215 (97%)	194 (93%)	14 (7%)	19	9
2	B	218/219 (100%)	208 (95%)	10 (5%)	31	20
All	All	426/434 (98%)	402 (94%)	24 (6%)	25	13

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	GLN
1	A	49	GLU
1	A	55	LEU
1	A	60	ASN
1	A	74	ASN
1	A	81	GLU
1	A	112	ASN
1	A	118	LEU
1	A	222	ILE
1	A	226	VAL
1	A	228	VAL
1	A	230	LEU
1	A	233	ILE
2	B	253	THR
2	B	255	SER

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Mol	Chain	Res	Type
2	B	258	ILE
2	B	294	ASN
2	B	352	ASN
2	B	375	LEU
2	B	418	ASN
2	B	439	LEU
2	B	477	ASN
2	B	487	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	51	GLN
1	A	60	ASN
1	A	74	ASN
1	A	109	GLN
1	A	112	ASN
1	A	137	GLN
1	A	161	GLN
1	A	170	ASN
1	A	215	ASN
2	B	265	ASN
2	B	277	HIS
2	B	291	ASN
2	B	294	ASN
2	B	295	GLN
2	B	308	ASN
2	B	343	ASN
2	B	348	ASN
2	B	352	ASN
2	B	377	GLN
2	B	418	ASN
2	B	419	GLN
2	B	462	GLN
2	B	474	ASN
2	B	477	ASN
2	B	485	GLN
2	B	487	ASN
2	B	491	GLN
2	B	503	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

17 ligands 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$
3	NAG	A	500	-	14,14,15	1.24	1 (7%)	15,19,21	2.23	4 (26%)
4	FUC	A	501	-	9,10,11	0.94	0	13,14,16	1.65	4 (30%)
3	NAG	A	502	-	14,14,15	1.34	2 (14%)	15,19,21	3.07	6 (40%)
6	GOL	A	600	-	5,5,5	1.53	1 (20%)	5,5,5	1.74	2 (40%)
6	GOL	A	601	-	5,5,5	1.65	1 (20%)	5,5,5	2.01	3 (60%)
6	GOL	A	700	-	5,5,5	1.36	0	5,5,5	1.59	1 (20%)
6	GOL	A	702	-	5,5,5	1.25	1 (20%)	5,5,5	1.46	1 (20%)
5	ADE	A	9550	-	9,11,11	0.67	0	7,15,15	3.19	3 (42%)
3	NAG	B	600	-	14,14,15	1.24	1 (7%)	15,19,21	1.97	3 (20%)
4	FUC	B	601	-	9,10,11	0.82	0	13,14,16	2.26	3 (23%)
3	NAG	B	602	-	14,14,15	1.29	1 (7%)	15,19,21	1.94	3 (20%)
3	NAG	B	603	2	14,14,15	1.54	2 (14%)	15,19,21	2.92	5 (33%)
3	NAG	B	604	-	14,14,15	1.29	1 (7%)	15,19,21	2.19	4 (26%)
6	GOL	B	701	-	5,5,5	1.56	0	5,5,5	1.43	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	703	-	5,5,5	0.73	0	5,5,5	0.98	0
6	GOL	B	704	-	5,5,5	1.42	0	5,5,5	1.27	0
6	GOL	B	705	-	5,5,5	1.60	1 (20%)	5,5,5	1.95	1 (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
3	NAG	A	500	-	-	0/6/23/26	0/1/1/1
4	FUC	A	501	-	-	0/0/17/20	0/1/1/1
3	NAG	A	502	-	-	0/6/23/26	0/1/1/1
6	GOL	A	600	-	-	0/4/4/4	0/0/0/0
6	GOL	A	601	-	-	0/4/4/4	0/0/0/0
6	GOL	A	700	-	-	0/4/4/4	0/0/0/0
6	GOL	A	702	-	-	0/4/4/4	0/0/0/0
5	ADE	A	9550	-	-	0/0/0/0	0/2/2/2
3	NAG	B	600	-	-	0/6/23/26	0/1/1/1
4	FUC	B	601	-	-	0/0/17/20	0/1/1/1
3	NAG	B	602	-	-	0/6/23/26	0/1/1/1
3	NAG	B	603	2	-	0/6/23/26	0/1/1/1
3	NAG	B	604	-	-	0/6/23/26	0/1/1/1
6	GOL	B	701	-	-	0/4/4/4	0/0/0/0
6	GOL	B	703	-	-	0/4/4/4	0/0/0/0
6	GOL	B	704	-	-	0/4/4/4	0/0/0/0
6	GOL	B	705	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	NAG	C1-C2	-3.95	1.47	1.52
3	B	602	NAG	O7-C7	-3.87	1.14	1.23
3	B	604	NAG	O7-C7	-3.85	1.14	1.23
3	B	600	NAG	O7-C7	-3.51	1.15	1.23
3	A	500	NAG	O7-C7	-3.39	1.15	1.23
3	A	502	NAG	O7-C7	-3.24	1.15	1.23
3	B	603	NAG	O7-C7	-3.12	1.15	1.23
3	A	502	NAG	C1-C2	-2.26	1.49	1.52
6	A	600	GOL	O1-C1	-2.18	1.33	1.42
6	A	601	GOL	O1-C1	-2.18	1.33	1.42
6	B	705	GOL	O1-C1	-2.16	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	GOL	O3-C3	-2.14	1.33	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C1-O5-C5	-5.73	104.27	112.17
3	B	604	NAG	C1-O5-C5	-4.81	105.53	112.17
3	A	502	NAG	O7-C7-N2	-4.68	112.90	121.92
3	B	600	NAG	O5-C1-C2	-4.68	104.96	111.47
3	B	604	NAG	O5-C1-C2	-4.28	105.52	111.47
4	B	601	FUC	C1-C2-C3	-4.25	104.27	109.65
3	B	603	NAG	C4-C3-C2	-3.93	105.25	111.02
3	A	500	NAG	C1-O5-C5	-3.68	107.09	112.17
5	A	9550	ADE	C2-N3-C4	-3.51	105.09	113.33
3	A	502	NAG	C4-C3-C2	-3.46	105.95	111.02
6	A	702	GOL	C3-C2-C1	-2.92	99.92	111.52
3	B	600	NAG	C1-O5-C5	-2.56	108.64	112.17
3	A	500	NAG	O4-C4-C3	-2.47	104.99	110.36
3	A	500	NAG	O7-C7-N2	-2.20	117.67	121.92
3	B	604	NAG	C8-C7-N2	-2.10	112.32	116.11
3	B	603	NAG	O4-C4-C3	-2.08	105.83	110.36
3	B	602	NAG	C1-C2-N2	2.09	114.05	110.49
4	A	501	FUC	C3-C4-C5	2.19	113.12	109.68
6	A	601	GOL	O1-C1-C2	2.20	121.13	110.07
6	A	601	GOL	O2-C2-C3	2.21	119.26	108.84
5	A	9550	ADE	C4-C5-N7	2.24	111.58	109.41
6	A	600	GOL	O1-C1-C2	2.33	121.80	110.07
6	A	600	GOL	O2-C2-C1	2.45	120.39	108.84
6	A	601	GOL	O2-C2-C1	2.49	120.60	108.84
6	A	700	GOL	O2-C2-C3	2.51	120.67	108.84
4	A	501	FUC	O2-C2-C3	2.58	115.25	110.17
4	A	501	FUC	C2-C3-C4	2.61	115.42	110.88
3	B	603	NAG	O3-C3-C4	2.69	116.22	110.36
3	B	602	NAG	C8-C7-N2	2.75	121.08	116.11
6	B	701	GOL	O2-C2-C3	2.76	121.85	108.84
3	B	603	NAG	C3-C4-C5	2.94	115.40	110.22
4	A	501	FUC	C1-C2-C3	3.10	113.58	109.65
6	B	705	GOL	O2-C2-C3	3.48	125.25	108.84
3	B	604	NAG	C3-C4-C5	3.51	116.41	110.22
3	B	600	NAG	C3-C4-C5	3.69	116.73	110.22
4	B	601	FUC	C1-O5-C5	3.91	121.04	112.39
4	B	601	FUC	O5-C5-C4	3.97	116.17	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C8-C7-N2	4.10	123.52	116.11
3	A	502	NAG	O5-C1-C2	4.53	117.77	111.47
3	A	502	NAG	C1-C2-N2	5.17	119.32	110.49
3	A	500	NAG	C3-C4-C5	5.72	120.29	110.22
3	A	502	NAG	C1-O5-C5	5.72	120.05	112.17
5	A	9550	ADE	N3-C2-N1	6.98	134.93	128.86
3	B	603	NAG	O5-C1-C2	8.94	123.91	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAG	6	0
4	A	501	FUC	7	0
3	A	502	NAG	3	0
6	A	600	GOL	1	0
6	A	601	GOL	1	0
6	A	702	GOL	4	0
5	A	9550	ADE	1	0
3	B	600	NAG	5	0
3	B	602	NAG	5	0
3	B	603	NAG	3	0
3	B	604	NAG	3	0
6	B	701	GOL	4	0
6	B	704	GOL	1	0
6	B	705	GOL	1	0

## 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	248/254 (97%)	0.22	20 (8%) 13 14	34, 45, 65, 75	0
2	B	262/263 (99%)	0.20	19 (7%) 16 18	30, 39, 56, 75	0
All	All	510/517 (98%)	0.21	39 (7%) 15 16	30, 41, 63, 75	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	250	VAL	7.8
1	A	248	GLY	7.7
1	A	225	GLY	6.6
2	B	249	ALA	6.6
2	B	253	THR	6.1
1	A	145	PRO	5.0
1	A	223	ALA	4.8
1	A	103	GLY	4.6
2	B	252	CYS	4.6
2	B	251	THR	4.3
1	A	226	VAL	3.6
2	B	261	ILE	3.3
1	A	224	PRO	3.3
2	B	323	VAL	3.1
1	A	247	CYS	3.0
1	A	102	SER	2.9
2	B	312	LEU	2.9
2	B	254	ALA	2.9
1	A	44	THR	2.9
2	B	269	VAL	2.9
1	A	105	THR	2.7
2	B	429	ILE	2.7
2	B	282	ILE	2.5
1	A	7	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	472	ILE	2.5
1	A	104	THR	2.4
2	B	490	LEU	2.3
2	B	297	TRP	2.3
1	A	95	GLY	2.3
1	A	98	THR	2.2
1	A	69	ALA	2.2
2	B	485	GLN	2.2
1	A	146	GLY	2.2
1	A	227	ILE	2.2
2	B	450	ILE	2.1
1	A	70	ILE	2.1
2	B	392	ILE	2.1
1	A	75	LEU	2.0
2	B	305	ILE	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(Å <sup>2</sup> )	Q<0.9
6	GOL	B	704	6/6	0.82	0.24	4.96	55,58,63,63	0
6	GOL	B	701	6/6	0.90	0.26	1.99	55,57,63,68	0
6	GOL	A	702	6/6	0.88	0.17	1.86	49,50,53,54	0
3	NAG	B	602	14/15	0.81	0.25	1.02	61,64,67,71	0
6	GOL	A	700	6/6	0.92	0.12	0.39	42,48,52,55	0
6	GOL	B	703	6/6	0.94	0.12	0.32	33,37,43,47	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	705	6/6	0.95	0.10	0.20	41,57,60,62	0
3	NAG	B	603	14/15	0.93	0.09	-0.68	35,44,50,53	0
5	ADE	A	9550	10/10	0.95	0.08	-0.85	38,55,61,64	0
4	FUC	A	501	10/11	0.70	0.65	-	78,79,80,81	10
3	NAG	A	500	14/15	0.64	0.45	-	91,92,93,93	0
3	NAG	A	502	14/15	0.66	0.46	-	74,75,76,77	14
6	GOL	A	600	6/6	0.74	0.17	-	83,88,90,93	0
3	NAG	B	600	14/15	0.69	0.35	-	63,76,81,84	0
4	FUC	B	601	10/11	0.72	0.19	-	76,77,78,79	10
6	GOL	A	601	6/6	0.69	0.28	-	88,89,91,92	0
3	NAG	B	604	14/15	0.67	0.40	-	62,74,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.