



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D7W  
Title : Mistletoe Lectin I in Complex with Zeatin  
Authors : Meyer, A.; Rypniewski, W.; Szymanski, M.; Voelter, W.; Barciszewski, J.; Betzel, C.  
Deposited on : 2008-05-22  
Resolution : 2.49 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 (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

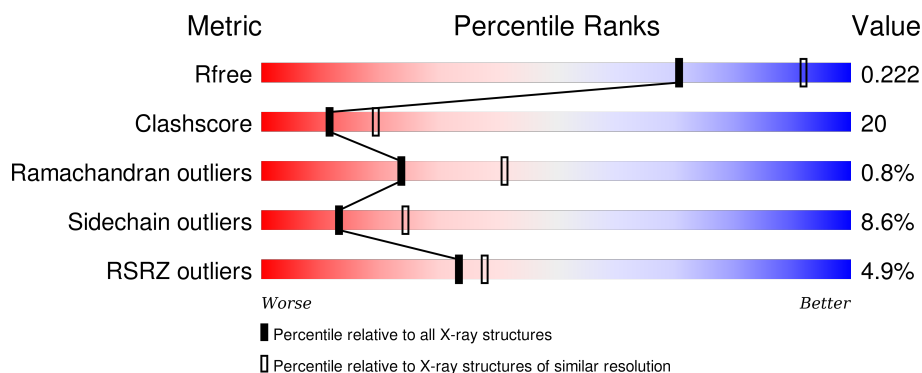
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>4%</div> <div>74%</div> <div>18%</div> <div>6%</div> <div>•</div> </div>
2	B	265	<div> <div>5%</div> <div>70%</div> <div>22%</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
3	NAG	B	600	X	-	-	-
3	NAG	B	604	X	-	-	-
3	NAG	B	605	X	-	-	-
4	SO4	A	661	-	-	-	X
5	ZEA	B	701[A]	-	-	X	X
6	ZEZ	B	702[B]	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4382 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 Beta-galactoside-specific lectin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	3	0
			1945	1228	330	383	4			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	THR	VAL	SEE REMARK 999	UNP P81446
A	9	ASP	THR	SEE REMARK 999	UNP P81446
A	10	GLN	HIS	SEE REMARK 999	UNP P81446
A	19	SER	ARG	SEE REMARK 999	UNP P81446
A	36	ASN	GLU	SEE REMARK 999	UNP P81446
A	45	VAL	ILE	SEE REMARK 999	UNP P81446
A	49	GLU	ASP	SEE REMARK 999	UNP P81446
A	50	GLY	ALA	SEE REMARK 999	UNP P81446
A	61	ALA	GLU	SEE REMARK 999	UNP P81446
A	65	THR	SER	SEE REMARK 999	UNP P81446
A	81	GLU	GLN	SEE REMARK 999	UNP P81446
A	84	ASN	ASP	SEE REMARK 999	UNP P81446
A	90	SER	ARG	SEE REMARK 999	UNP P81446
A	94	ALA	ARG	SEE REMARK 999	UNP P81446
A	99	GLN	HIS	SEE REMARK 999	UNP P81446
A	100	ASP	LEU	SEE REMARK 999	UNP P81446
A	102	SER	THR	SEE REMARK 999	UNP P81446
A	106	SER	ARG	SEE REMARK 999	UNP P81446
A	109	GLN	LEU	SEE REMARK 999	UNP P81446
A	148	GLN	SER	SEE REMARK 999	UNP P81446
A	150	LYS	ARG	SEE REMARK 999	UNP P81446
A	208	HIS	GLN	SEE REMARK 999	UNP P81446
A	219	ALA	ARG	SEE REMARK 999	UNP P81446
A	223	ALA	PRO	SEE REMARK 999	UNP P81446
A	226	VAL	ASN	SEE REMARK 999	UNP P81446
A	227	ILE	PHE	SEE REMARK 999	UNP P81446
A	233	ILE	VAL	SEE REMARK 999	UNP P81446

- Molecule 2 is a protein called Beta-galactoside-specific lectin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	1	0
			2005	1244	353	396	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	511	MET	-	SEE REMARK 999	UNP P81446
B	512	THR	-	SEE REMARK 999	UNP P81446

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



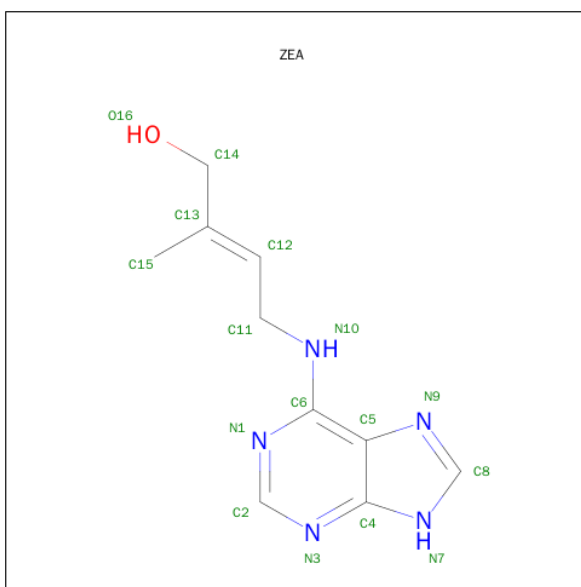
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



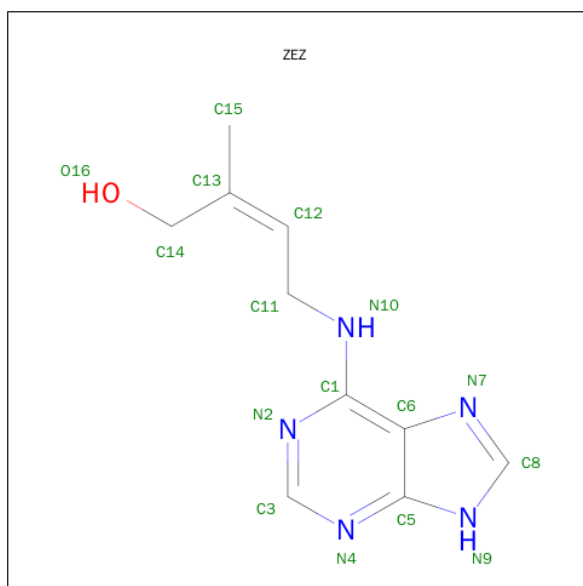
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (2E)-2-METHYL-4-(9H-PURIN-6-YLAMINO)BUT-2-EN-1-OL (three-letter code: ZEA) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O).



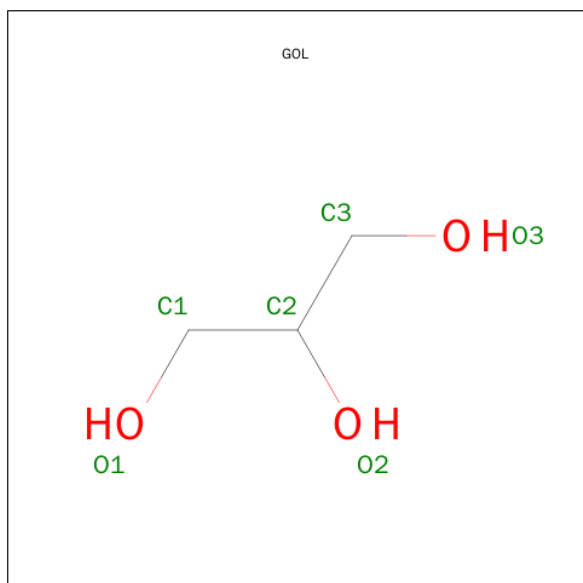
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	1
			16	10	5	1		

- Molecule 6 is (2Z)-2-METHYL-4-(9H-PURIN-6-YLAMINO)BUT-2-EN-1-OL (three-letter code: ZEZ) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	1
			16	10	5	1		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

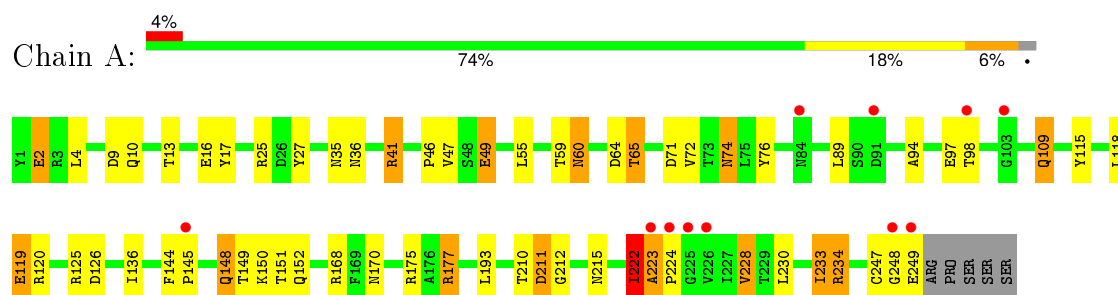
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	97	Total	O	0	0
			97	97		
8	B	185	Total	O	0	0
			185	185		



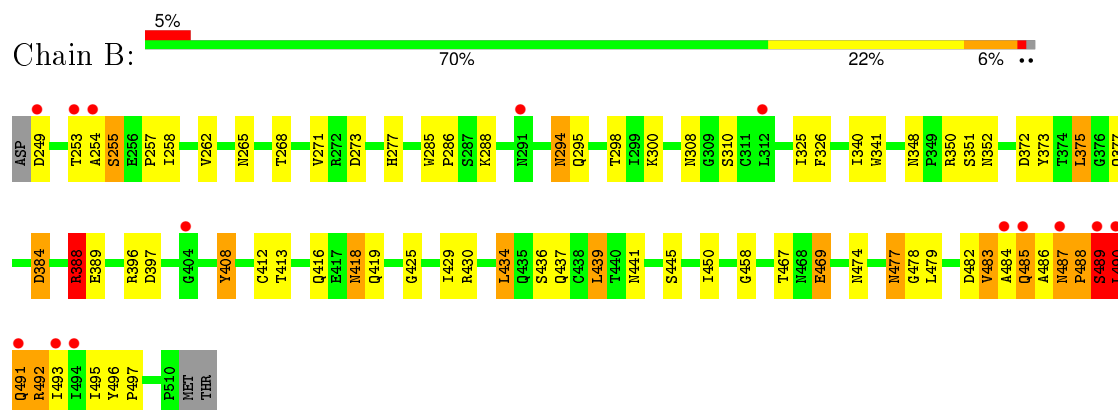
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Beta-galactoside-specific lectin 1



#### • Molecule 2: Beta-galactoside-specific lectin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.64Å 106.64Å 311.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.49 19.85 – 2.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.49) 99.9 (19.85-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.224 0.180 , 0.222	Depositor DCC
$R_{free}$ test set	1858 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 37477 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4382	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 3.11% 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, 0.375 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: ZEZ, GOL, ZEA, NAG, SO4

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	1.02	0/1983	0.98	6/2702 (0.2%)
2	B	1.06	3/2044 (0.1%)	1.02	9/2789 (0.3%)
All	All	1.04	3/4027 (0.1%)	1.00	15/5491 (0.3%)

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
2	B	0	4
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	489	SER	CB-OG	8.33	1.53	1.42
2	B	489	SER	N-CA	6.67	1.59	1.46
2	B	469	GLU	CG-CD	5.71	1.60	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CB-CG-OD1	9.12	126.50	118.30
1	A	211	ASP	CB-CG-OD2	-7.62	111.44	118.30
2	B	384	ASP	CB-CG-OD2	6.74	124.37	118.30
2	B	388	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	234	ARG	NE-CZ-NH1	-6.37	117.11	120.30
2	B	492	ARG	N-CA-C	-6.35	93.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	273[A]	ASP	CB-CG-OD2	5.82	123.54	118.30
2	B	273[B]	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	177	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	350	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	396	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	222	ILE	CG1-CB-CG2	-5.60	99.08	111.40
2	B	350	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	118	LEU	CB-CG-CD2	-5.41	101.80	111.00
2	B	384	ASP	CB-CG-OD1	-5.06	113.75	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	CYS	Peptide
2	B	483	VAL	Peptide
2	B	488	PRO	Peptide
2	B	490	LEU	Peptide
2	B	491	GLN	Peptide

## 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	1945	0	1902	54	0
2	B	2005	0	1938	103	0
3	A	14	0	13	1	0
3	B	70	0	65	10	0
4	A	10	0	0	2	0
5	B	16	0	13	6	0
6	B	16	0	13	8	0
7	A	12	0	16	1	0
7	B	12	0	16	3	0
8	A	97	0	0	10	1
8	B	185	0	0	5	1
All	All	4382	0	3976	162	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 20.

All (162) 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)
2:B:308:ASN:HD21	3:B:600:NAG:C1	1.22	1.53
2:B:485:GLN:HG2	2:B:486:ALA:CB	1.42	1.50
2:B:485:GLN:CG	2:B:486:ALA:HB2	1.44	1.47
2:B:484:ALA:HB1	2:B:492:ARG:O	1.30	1.22
1:A:223:ALA:CB	1:A:224:PRO:HD3	1.79	1.13
2:B:488:PRO:HB2	2:B:489:SER:CB	1.81	1.11
2:B:488:PRO:HB2	2:B:489:SER:HB2	1.13	1.10
1:A:223:ALA:HB1	1:A:224:PRO:HD3	1.11	1.10
2:B:488:PRO:CB	2:B:489:SER:HB2	1.95	0.97
2:B:288:LYS:H	2:B:295:GLN:HE22	1.07	0.96
2:B:265:ASN:HD22	2:B:430:ARG:HH22	1.13	0.96
2:B:416:GLN:HE21	2:B:418:ASN:HD21	1.15	0.94
3:B:603:NAG:HO4	3:B:604:NAG:C1	1.71	0.94
2:B:408:TYR:HD2	2:B:491:GLN:HB3	1.29	0.93
2:B:484:ALA:H	2:B:485:GLN:C	1.72	0.93
1:A:234:ARG:HH21	5:B:701[A]:ZEA:H153	1.34	0.92
2:B:477:ASN:HD22	2:B:479:LEU:H	1.16	0.91
2:B:258:ILE:HD12	2:B:298:THR:OG1	1.71	0.90
1:A:223:ALA:CB	1:A:224:PRO:CD	2.50	0.89
1:A:223:ALA:HB1	1:A:224:PRO:CD	2.02	0.89
1:A:13:THR:O	8:A:748:HOH:O	1.91	0.88
2:B:477:ASN:ND2	2:B:479:LEU:H	1.72	0.88
2:B:490:LEU:N	2:B:491:GLN:HA	1.89	0.88
2:B:474:ASN:HD22	2:B:477:ASN:H	1.22	0.88
2:B:408:TYR:CD2	2:B:491:GLN:HB3	2.09	0.87
2:B:434:LEU:HD12	2:B:436:SER:H	1.41	0.85
1:A:222:ILE:HD13	1:A:228:VAL:HB	1.55	0.85
3:B:602:NAG:HO4	3:B:605:NAG:C1	1.91	0.83
2:B:484:ALA:CB	2:B:492:ARG:O	2.22	0.80
2:B:490:LEU:H	2:B:491:GLN:HG2	1.48	0.78
7:B:650:GOL:H32	8:B:853:HOH:O	1.83	0.76
2:B:489:SER:C	2:B:491:GLN:HA	2.04	0.76
2:B:258:ILE:N	2:B:258:ILE:HD13	2.03	0.74
2:B:441:ASN:HD22	2:B:495:ILE:HD13	1.52	0.73
1:A:9:ASP:HA	1:A:136:ILE:HD11	1.70	0.73
6:B:702[B]:ZEE:O16	6:B:702[B]:ZEE:H11	1.90	0.71
2:B:288:LYS:NZ	2:B:294:ASN:HD21	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:ARG:HG3	6:B:702[B]:ZEE:N7	2.05	0.71
2:B:388:ARG:HG3	5:B:701[A]:ZEA:N9	2.05	0.71
2:B:425:GLY:HA2	6:B:702[B]:ZEE:H15A	1.73	0.71
2:B:425:GLY:HA2	5:B:701[A]:ZEA:H142	1.73	0.71
2:B:490:LEU:N	2:B:491:GLN:HG2	2.08	0.68
2:B:485:GLN:CB	2:B:486:ALA:HB2	2.22	0.68
2:B:445:SER:HB3	8:B:833:HOH:O	1.93	0.68
2:B:484:ALA:H	2:B:485:GLN:CA	2.08	0.67
2:B:288:LYS:H	2:B:295:GLN:NE2	1.86	0.65
1:A:119:GLU:OE1	1:A:125:ARG:HD3	1.96	0.65
2:B:477:ASN:C	2:B:477:ASN:HD22	2.00	0.64
2:B:288:LYS:N	2:B:295:GLN:HE22	1.89	0.64
2:B:434:LEU:HG	2:B:437:GLN:HG2	1.78	0.64
2:B:484:ALA:N	2:B:485:GLN:CA	2.60	0.64
2:B:288:LYS:HZ1	2:B:294:ASN:HD21	1.46	0.64
2:B:467:THR:HB	2:B:469:GLU:OE1	1.98	0.64
1:A:234:ARG:HH21	6:B:702[B]:ZEE:H14A	1.63	0.64
2:B:265:ASN:ND2	2:B:430:ARG:HH22	1.89	0.63
2:B:474:ASN:ND2	2:B:477:ASN:H	1.96	0.63
2:B:258:ILE:CD1	2:B:298:THR:HG23	2.28	0.63
1:A:25:ARG:HH12	1:A:170:ASN:HD21	1.45	0.63
2:B:375:LEU:HD22	2:B:458:GLY:HA2	1.80	0.62
1:A:71:ASP:HB3	1:A:74:ASN:HD21	1.64	0.62
2:B:450:ILE:HD12	2:B:493:ILE:HG22	1.81	0.62
2:B:257:PRO:C	2:B:258:ILE:HD13	2.20	0.62
2:B:384:ASP:HB3	2:B:388:ARG:HH12	1.65	0.62
1:A:2:GLU:HG3	1:A:27:TYR:CE2	2.35	0.61
2:B:485:GLN:HG2	2:B:486:ALA:HB2	0.67	0.61
2:B:308:ASN:ND2	3:B:600:NAG:O5	2.20	0.61
2:B:489:SER:N	2:B:490:LEU:HB2	2.16	0.60
2:B:483:VAL:HA	2:B:484:ALA:HB2	1.82	0.60
2:B:408:TYR:HD2	2:B:491:GLN:CB	2.08	0.60
2:B:429:ILE:CG2	2:B:439:LEU:HD22	2.32	0.60
2:B:485:GLN:HG2	2:B:486:ALA:HB3	1.70	0.60
2:B:373:TYR:HE1	3:B:602:NAG:H81	1.67	0.59
4:A:661:SO4:O4	2:B:249:ASP:N	2.36	0.59
1:A:248:GLY:HA2	1:A:249:GLU:C	2.23	0.58
2:B:372:ASP:H	2:B:377:GLN:HE22	1.51	0.58
1:A:60:ASN:HD21	1:A:64:ASP:H	1.50	0.58
1:A:215:ASN:HD21	2:B:257:PRO:HD3	1.69	0.58
1:A:212:GLY:HA2	1:A:233:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:HA	1:A:152:GLN:HE21	1.68	0.57
3:B:602:NAG:H83	3:B:602:NAG:H3	1.84	0.57
1:A:215:ASN:ND2	2:B:255:SER:HB3	2.18	0.57
2:B:388:ARG:HG2	5:B:701[A]:ZEA:H10	1.69	0.57
2:B:388:ARG:HG2	6:B:702[B]:ZEZ:HN10	1.69	0.57
2:B:348:ASN:ND2	2:B:351:SER:H	2.02	0.57
2:B:352:ASN:ND2	8:B:859:HOH:O	2.39	0.56
2:B:408:TYR:CD2	2:B:491:GLN:CB	2.86	0.56
2:B:486:ALA:H	2:B:487:ASN:CA	2.19	0.56
1:A:148:GLN:HG2	8:A:730:HOH:O	2.07	0.55
1:A:150:LYS:CD	8:A:754:HOH:O	2.55	0.55
1:A:148:GLN:HB3	1:A:151:THR:H	1.72	0.55
2:B:388:ARG:HG2	6:B:702[B]:ZEZ:N10	2.21	0.54
2:B:388:ARG:HG2	5:B:701[A]:ZEA:N10	2.21	0.54
2:B:434:LEU:HD11	2:B:436:SER:HB2	1.90	0.54
2:B:341:TRP:CZ2	3:B:605:NAG:C8	2.91	0.54
1:A:115:TYR:O	1:A:119:GLU:HB2	2.07	0.54
2:B:413:THR:H	2:B:419:GLN:HE22	1.56	0.54
1:A:150:LYS:HD3	8:A:754:HOH:O	2.09	0.52
1:A:74:ASN:ND2	1:A:76:TYR:H	2.07	0.52
1:A:16:GLU:N	8:A:748:HOH:O	2.42	0.52
2:B:341:TRP:CZ2	3:B:605:NAG:H82	2.44	0.52
1:A:211:ASP:OD2	2:B:340:ILE:HD12	2.09	0.52
1:A:27:TYR:O	1:A:27:TYR:CD1	2.63	0.51
2:B:258:ILE:CD1	2:B:298:THR:OG1	2.53	0.51
2:B:262:VAL:HG22	2:B:268:THR:HG22	1.91	0.51
1:A:222:ILE:CD1	1:A:228:VAL:HB	2.33	0.51
1:A:27:TYR:C	1:A:27:TYR:CD1	2.84	0.51
1:A:41:ARG:HG2	8:A:663:HOH:O	2.10	0.51
2:B:416:GLN:HG2	2:B:418:ASN:ND2	2.26	0.51
1:A:223:ALA:HB3	1:A:224:PRO:CD	2.39	0.50
2:B:308:ASN:HD22	3:B:600:NAG:C1	2.10	0.50
1:A:65:THR:HG22	8:A:662:HOH:O	2.10	0.49
2:B:258:ILE:HD12	2:B:298:THR:CB	2.43	0.49
2:B:326:PHE:CZ	7:B:650:GOL:H11	2.47	0.49
1:A:168:ARG:HH12	7:A:652:GOL:H32	1.76	0.49
1:A:60:ASN:ND2	1:A:64:ASP:H	2.09	0.49
1:A:35:ASN:O	1:A:36:ASN:HB2	2.13	0.49
1:A:119:GLU:OE1	4:A:660:SO4:O2	2.31	0.48
1:A:47:VAL:HG11	1:A:94:ALA:O	2.13	0.48
2:B:488:PRO:HB2	2:B:489:SER:CA	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:CYS:HA	2:B:419:GLN:HE22	1.79	0.48
2:B:486:ALA:N	2:B:487:ASN:O	2.47	0.48
2:B:372:ASP:H	2:B:377:GLN:NE2	2.11	0.47
1:A:234:ARG:NH2	5:B:701[A]:ZEA:H153	2.15	0.47
2:B:258:ILE:HD11	2:B:298:THR:HG23	1.97	0.47
1:A:46:PRO:O	1:A:49:GLU:HB2	2.15	0.47
1:A:60:ASN:HD22	1:A:60:ASN:C	2.17	0.46
2:B:486:ALA:H	2:B:487:ASN:HB3	1.80	0.46
2:B:482:ASP:O	2:B:484:ALA:HA	2.15	0.46
1:A:59:THR:HA	1:A:64:ASP:O	2.16	0.45
2:B:484:ALA:N	2:B:485:GLN:HA	2.28	0.45
2:B:434:LEU:C	2:B:434:LEU:HD12	2.37	0.45
2:B:487:ASN:OD1	2:B:488:PRO:O	2.34	0.45
2:B:477:ASN:C	2:B:477:ASN:ND2	2.68	0.45
2:B:496:TYR:CD2	2:B:497:PRO:HD2	2.52	0.44
1:A:234:ARG:HE	6:B:702[B]:ZEE:H14A	1.83	0.44
1:A:109:GLN:HG2	1:A:109:GLN:H	1.50	0.44
7:B:650:GOL:C3	8:B:853:HOH:O	2.55	0.44
2:B:416:GLN:HE21	2:B:418:ASN:ND2	1.97	0.43
3:A:500:NAG:H83	3:A:500:NAG:O3	2.18	0.43
1:A:210:THR:O	1:A:211:ASP:HB2	2.19	0.43
2:B:429:ILE:HG21	2:B:439:LEU:HD22	2.00	0.43
1:A:126:ASP:HB3	1:A:193:LEU:HD11	2.01	0.43
2:B:271:VAL:HB	2:B:294:ASN:HB2	2.00	0.42
2:B:418:ASN:C	2:B:418:ASN:HD22	2.22	0.42
3:B:603:NAG:O4	3:B:604:NAG:O5	2.04	0.42
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.79	0.41
2:B:477:ASN:HD22	2:B:478:GLY:N	2.18	0.41
2:B:300:LYS:HB3	2:B:300:LYS:HE3	1.92	0.41
2:B:277:HIS:HB3	8:B:860:HOH:O	2.19	0.41
1:A:71:ASP:HB3	1:A:74:ASN:ND2	2.35	0.41
2:B:285:TRP:CD1	2:B:286:PRO:HD2	2.56	0.41
2:B:490:LEU:N	2:B:491:GLN:CA	2.73	0.41
2:B:477:ASN:HD22	2:B:479:LEU:N	1.99	0.41
1:A:9:ASP:HB2	8:A:733:HOH:O	2.21	0.41
2:B:310:SER:HB3	2:B:325:ILE:HG13	2.01	0.41
1:A:25:ARG:HH22	1:A:170:ASN:ND2	2.19	0.40
1:A:65:THR:CG2	8:A:662:HOH:O	2.68	0.40
2:B:425:GLY:CA	6:B:702[B]:ZEE:H15A	2.47	0.40
1:A:17:TYR:N	8:A:748:HOH:O	1.59	0.40
1:A:74:ASN:HD22	1:A:74:ASN:C	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.92	0.40
2:B:348:ASN:HD22	2:B:351:SER:CB	2.35	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)
8:A:754:HOH:O	8:B:781:HOH:O[6_554]	2.02	0.18

## 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	249/254 (98%)	236 (95%)	12 (5%)	1 (0%)	39	61
2	B	261/265 (98%)	245 (94%)	13 (5%)	3 (1%)	17	31
All	All	510/519 (98%)	481 (94%)	25 (5%)	4 (1%)	24	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ALA
2	B	254	ALA
2	B	489	SER
2	B	487	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	213/216 (99%)	190 (89%)	23 (11%)	8	15
2	B	220/222 (99%)	206 (94%)	14 (6%)	22	39
All	All	433/438 (99%)	396 (92%)	37 (8%)	13	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	LEU
1	A	10	GLN
1	A	41	ARG
1	A	49	GLU
1	A	55	LEU
1	A	60	ASN
1	A	65	THR
1	A	72	VAL
1	A	74	ASN
1	A	89	LEU
1	A	97	GLU
1	A	98	THR
1	A	109	GLN
1	A	119	GLU
1	A	120	ARG
1	A	148	GLN
1	A	175[A]	ARG
1	A	177	ARG
1	A	222	ILE
1	A	228	VAL
1	A	230	LEU
1	A	233	ILE
2	B	253	THR
2	B	255	SER
2	B	294	ASN
2	B	375	LEU
2	B	388	ARG
2	B	389	GLU
2	B	397	ASP
2	B	408	TYR
2	B	418	ASN
2	B	434	LEU

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Mol	Chain	Res	Type
2	B	439	LEU
2	B	477	ASN
2	B	485	GLN
2	B	490	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	74	ASN
1	A	85	GLN
1	A	109	GLN
1	A	152	GLN
1	A	161	GLN
1	A	170	ASN
1	A	215	ASN
2	B	265	ASN
2	B	294	ASN
2	B	295	GLN
2	B	308	ASN
2	B	348	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

### 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 ⓘ

14 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	1	14,14,15	1.44	2 (14%)	15,19,21	2.60	6 (40%)
7	GOL	A	648	-	5,5,5	0.49	0	5,5,5	0.57	0
7	GOL	A	652	-	5,5,5	0.39	0	5,5,5	0.84	0
4	SO4	A	660	-	4,4,4	0.34	0	6,6,6	0.65	0
4	SO4	A	661	-	4,4,4	0.24	0	6,6,6	0.16	0
3	NAG	B	600	2	14,14,15	0.99	1 (7%)	15,19,21	2.51	6 (40%)
3	NAG	B	602	3,2	14,14,15	1.02	1 (7%)	15,19,21	2.55	7 (46%)
3	NAG	B	603	3,2	14,14,15	1.22	1 (7%)	15,19,21	1.35	3 (20%)
3	NAG	B	604	3	14,14,15	0.45	0	15,19,21	2.73	5 (33%)
3	NAG	B	605	3	14,14,15	0.54	0	15,19,21	0.59	0
7	GOL	B	650	-	5,5,5	0.91	0	5,5,5	1.25	0
7	GOL	B	651	-	5,5,5	0.59	0	5,5,5	0.54	0
5	ZEA	B	701[A]	-	12,17,17	0.97	0	12,22,22	3.81	7 (58%)
6	ZEZ	B	702[B]	-	12,17,17	0.95	0	12,22,22	3.87	7 (58%)

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	1	-	0/6/23/26	0/1/1/1
7	GOL	A	648	-	-	0/4/4/4	0/0/0/0
7	GOL	A	652	-	-	0/4/4/4	0/0/0/0
4	SO4	A	660	-	-	0/0/0/0	0/0/0/0
4	SO4	A	661	-	-	0/0/0/0	0/0/0/0
3	NAG	B	600	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	602	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	603	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	604	3	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	605	3	1/1/5/7	0/6/23/26	0/1/1/1
7	GOL	B	650	-	-	0/4/4/4	0/0/0/0
7	GOL	B	651	-	-	0/4/4/4	0/0/0/0
5	ZEA	B	701[A]	-	-	0/8/8/8	0/2/2/2
6	ZEZ	B	702[B]	-	-	0/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	NAG	O5-C1	-2.38	1.39	1.43
3	A	500	NAG	C3-C2	2.15	1.57	1.52
3	B	600	NAG	C4-C5	2.29	1.57	1.53
3	B	602	NAG	O7-C7	2.40	1.28	1.23
3	A	500	NAG	C1-C2	4.61	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701[A]	ZEA	N3-C2-N1	-9.89	121.32	128.89
6	B	702[B]	ZEZ	N4-C3-N2	-9.89	121.32	128.89
3	B	600	NAG	C2-N2-C7	-7.03	114.01	123.04
3	B	602	NAG	O3-C3-C4	-4.95	99.20	110.34
3	A	500	NAG	C3-C4-C5	-4.73	101.95	110.20
5	B	701[A]	ZEA	C4-C5-N9	-4.21	105.61	109.48
6	B	702[B]	ZEZ	C5-C6-N7	-4.21	105.61	109.48
3	B	604	NAG	C2-N2-C7	-4.10	117.77	123.04
6	B	702[B]	ZEZ	C15-C13-C12	-3.82	116.01	123.50
5	B	701[A]	ZEA	C12-C11-N10	-3.62	100.76	112.93
6	B	702[B]	ZEZ	C12-C11-N10	-3.62	100.76	112.93
3	B	600	NAG	C4-C3-C2	-3.51	105.78	111.23
3	B	603	NAG	C3-C4-C5	-2.47	105.89	110.20
3	B	604	NAG	C6-C5-C4	-2.45	106.97	113.02
3	B	603	NAG	C1-O5-C5	-2.31	109.32	112.25
3	B	603	NAG	C4-C3-C2	-2.29	107.67	111.23
5	B	701[A]	ZEA	C11-C12-C13	-2.08	123.17	126.96
6	B	702[B]	ZEZ	C11-C12-C13	-2.08	123.17	126.96
3	B	604	NAG	O3-C3-C4	-2.04	105.74	110.34
3	B	602	NAG	O6-C6-C5	-2.04	104.59	111.33
3	B	600	NAG	O4-C4-C5	2.04	114.66	109.24
3	B	602	NAG	O4-C4-C5	2.11	114.82	109.24
3	B	600	NAG	O4-C4-C3	2.14	115.16	110.34
3	B	600	NAG	C8-C7-N2	2.21	120.33	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701[A]	ZEA	C15-C13-C14	2.28	121.27	114.85
6	B	702[B]	ZEZ	C15-C13-C14	2.28	121.27	114.85
3	A	500	NAG	O4-C4-C5	2.41	115.63	109.24
5	B	701[A]	ZEA	O16-C14-C13	2.42	116.85	111.76
3	B	602	NAG	C8-C7-N2	2.47	120.84	116.11
3	A	500	NAG	C8-C7-N2	2.68	121.23	116.11
3	B	604	NAG	C3-C4-C5	2.74	114.97	110.20
3	B	602	NAG	O5-C5-C6	2.76	113.33	107.35
3	A	500	NAG	O5-C5-C6	3.03	113.91	107.35
3	B	600	NAG	O3-C3-C4	3.12	117.35	110.34
3	B	602	NAG	C1-O5-C5	3.47	116.65	112.25
3	A	500	NAG	O3-C3-C2	3.89	116.83	109.11
3	B	602	NAG	C2-N2-C7	5.07	129.55	123.04
5	B	701[A]	ZEA	C2-N1-C6	5.18	120.21	116.48
6	B	702[B]	ZEZ	C3-N2-C1	5.18	120.21	116.48
3	A	500	NAG	C1-O5-C5	5.66	119.43	112.25
3	B	604	NAG	C1-O5-C5	8.41	122.93	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	605	NAG	C1
3	B	600	NAG	C1
3	B	604	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAG	1	0
7	A	652	GOL	1	0
4	A	660	SO4	1	0
4	A	661	SO4	1	0
3	B	600	NAG	3	0
3	B	602	NAG	3	0
3	B	603	NAG	2	0
3	B	604	NAG	2	0
3	B	605	NAG	3	0
7	B	650	GOL	3	0
5	B	701[A]	ZEA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702[B]	ZEZ	8	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	249/254 (98%)	-0.09	11 (4%) 38 43	32, 45, 71, 84	0
2	B	262/265 (98%)	-0.08	14 (5%) 30 34	26, 38, 63, 90	1 (0%)
All	All	511/519 (98%)	-0.09	25 (4%) 33 38	26, 42, 70, 90	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	PRO	5.3
1	A	225	GLY	5.0
1	A	248	GLY	4.5
2	B	489	SER	4.3
1	A	249	GLU	4.1
2	B	487	ASN	4.0
2	B	491	GLN	3.6
2	B	253	THR	3.6
1	A	226	VAL	3.5
2	B	493	ILE	3.4
2	B	249	ASP	3.1
1	A	84	ASN	3.0
2	B	485	GLN	3.0
1	A	98	THR	2.8
2	B	254	ALA	2.7
2	B	404	GLY	2.7
1	A	223	ALA	2.5
2	B	490	LEU	2.5
2	B	291	ASN	2.4
1	A	103	GLY	2.4
2	B	312	LEU	2.4
1	A	145	PRO	2.4
2	B	484	ALA	2.3
1	A	91	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	494	ILE	2.1

## 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	ZEZ	B	702[B]	16/16	0.69	0.39	11.46	38,51,53,54	16
5	ZEA	B	701[A]	16/16	0.74	0.35	9.00	27,51,53,54	16
4	SO4	A	661	5/5	0.94	0.51	3.78	121,122,122,123	0
7	GOL	B	650	6/6	0.88	0.19	1.79	35,46,53,55	0
7	GOL	A	648	6/6	0.95	0.15	0.85	48,52,54,57	0
4	SO4	A	660	5/5	0.95	0.18	0.76	71,73,77,79	0
7	GOL	A	652	6/6	0.93	0.14	0.11	61,68,68,73	0
7	GOL	B	651	6/6	0.96	0.14	-0.19	38,41,47,51	0
3	NAG	B	603	14/15	0.97	0.12	-0.47	33,37,42,44	0
3	NAG	B	600	14/15	0.68	0.35	-	68,87,89,90	0
3	NAG	B	605	14/15	0.77	0.42	-	83,95,99,100	0
3	NAG	A	500	14/15	0.86	0.32	-	89,94,102,104	0
3	NAG	B	604	14/15	0.71	0.44	-	71,89,93,93	0
3	NAG	B	602	14/15	0.95	0.16	-	43,52,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.