



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:23 PM GMT

PDB ID : 1TFM  
Title : CRYSTAL STRUCTURE OF A RIBOSOME INACTIVATING PROTEIN IN ITS NATURALLY INHIBITED FORM  
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Deposited on : 2004-05-27  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

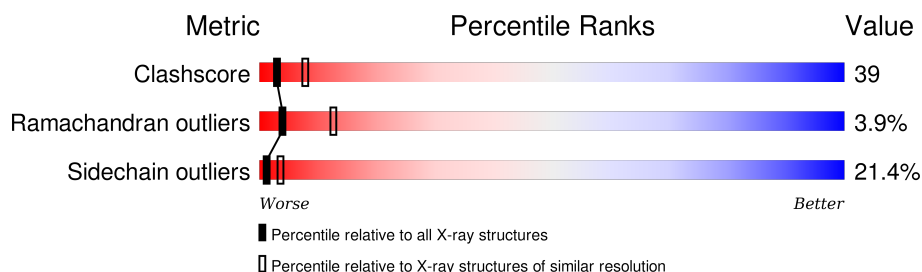
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

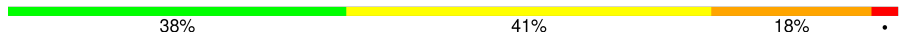

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	255	

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	NAG	B	259	-	-	X	-
4	BMA	B	260	X	-	-	-
5	NAG	A	241	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GAL	B	267	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4101 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 Himalayan mistletoe ribosome-inactivating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1875	1191	319	361	4			

- Molecule 2 is a protein called Himalayan mistletoe ribosome-inactivating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			1938	1199	343	384	12			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

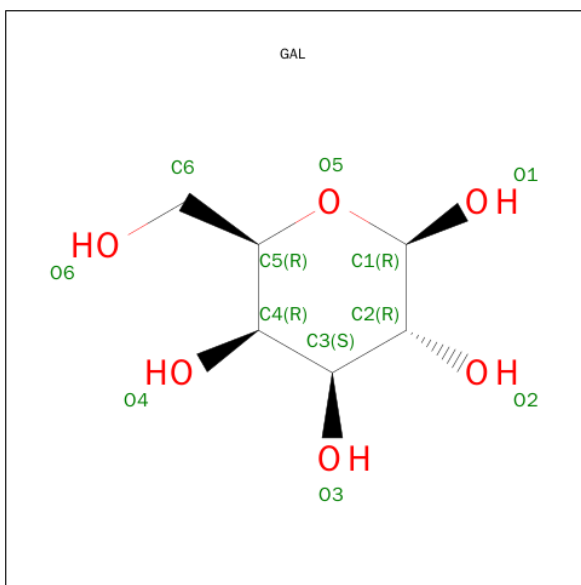
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

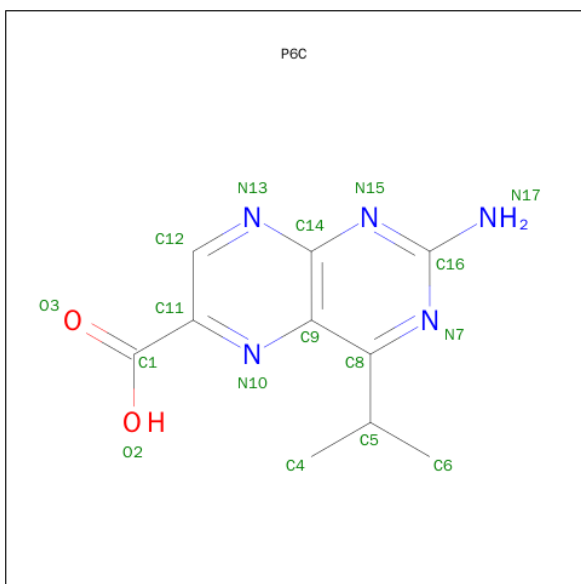
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	2	Total	C	O	0	0
			23	12	11		

- Molecule 8 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 9 is 2-AMINO-4-ISOPROPYL-PTERIDINE-6-CARBOXYLIC ACID (three-letter code: P6C) (formula:  $C_{10}H_{11}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			17	10	5	2		

- Molecule 10 is water.

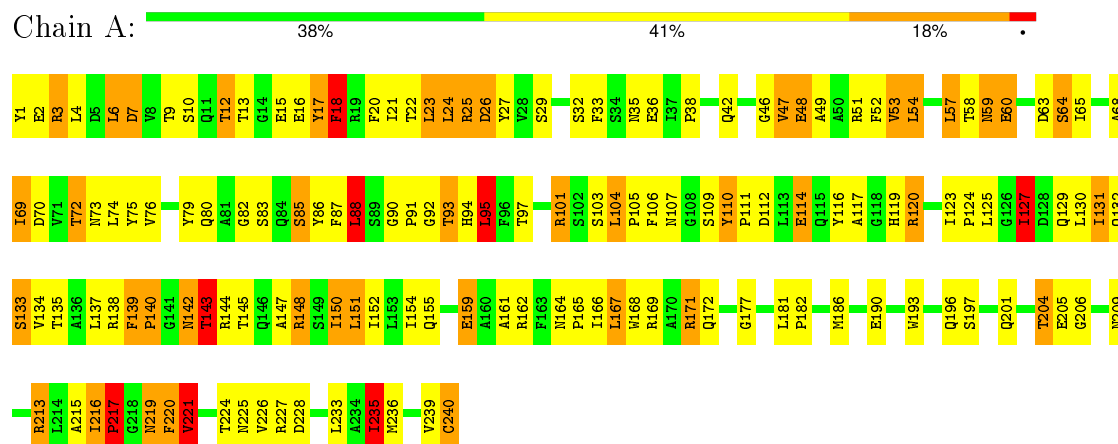
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	51	Total 51	O 51	0	0
10	B	55	Total 55	O 55	0	0

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

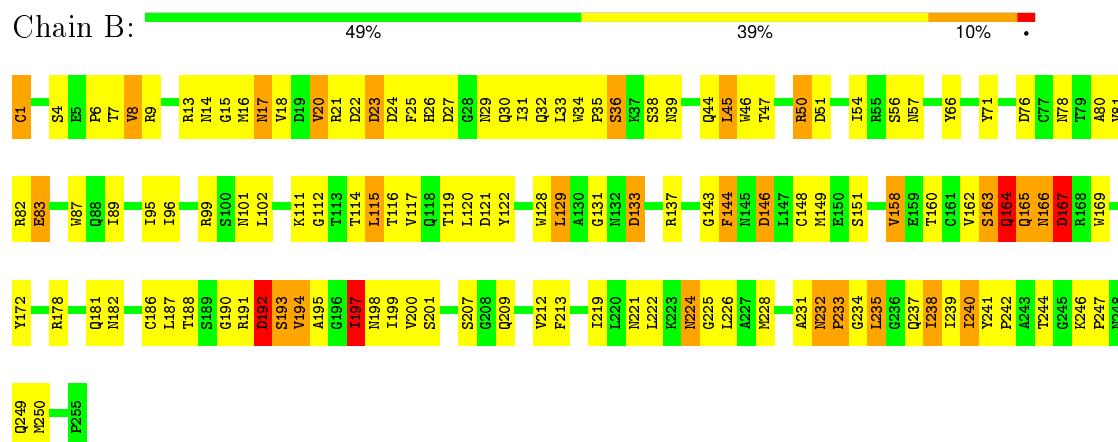
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Himalayan mistletoe ribosome-inactivating protein



- Molecule 2: Himalayan mistletoe ribosome-inactivating protein





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.42Å 109.42Å 309.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.234 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, P6C, BGC, BMA, 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	0.70	5/1913 (0.3%)	1.01	14/2602 (0.5%)
2	B	0.50	0/1978	0.94	7/2697 (0.3%)
All	All	0.60	5/3891 (0.1%)	0.97	21/5299 (0.4%)

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	5
2	B	0	6
4	B	1	0
All	All	1	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	LEU	C-O	13.56	1.49	1.23
1	A	92	GLY	C-N	9.93	1.56	1.34
1	A	18	PHE	C-N	7.22	1.50	1.34
1	A	17	TYR	C-N	5.53	1.46	1.34
1	A	127	ILE	C-N	5.35	1.46	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ILE	CB-CG1-CD1	19.49	168.48	113.90
1	A	142	ASN	CA-C-N	-8.08	99.43	117.20
1	A	17	TYR	O-C-N	-7.67	110.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	O-C-N	-6.59	112.15	122.70
1	A	142	ASN	O-C-N	6.45	133.02	122.70
1	A	88	LEU	CA-CB-CG	6.17	129.48	115.30
2	B	165	GLN	CA-C-N	6.12	130.66	117.20
2	B	51	ASP	CB-CG-OD2	6.09	123.78	118.30
2	B	167	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	6	LEU	CA-CB-CG	6.05	129.23	115.30
2	B	165	GLN	CB-CA-C	5.93	122.26	110.40
1	A	112	ASP	CB-CG-OD2	5.92	123.63	118.30
2	B	133	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	17	TYR	CA-C-N	5.77	129.90	117.20
2	B	192	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	143	THR	O-C-N	-5.65	113.66	122.70
1	A	143	THR	CA-C-N	5.41	129.10	117.20
1	A	7	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	26	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	146	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	228	ASP	CB-CG-OD2	5.10	122.89	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	260	BMA	C3

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASN	Mainchain
1	A	18	PHE	Sidechain
1	A	217	PRO	Mainchain
1	A	90	GLY	Peptide
1	A	95	LEU	Mainchain
2	B	129	LEU	Mainchain
2	B	164	GLN	Mainchain
2	B	232	ASN	Peptide
2	B	235	LEU	Peptide
2	B	66	TYR	Sidechain
2	B	80	ALA	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	1875	0	1849	167	0
2	B	1938	0	1851	128	0
3	B	28	0	25	3	0
4	B	50	0	43	8	0
5	A	14	0	13	1	0
6	B	39	0	34	3	0
7	B	23	0	21	0	0
8	B	11	0	10	7	0
9	A	17	0	10	0	0
10	A	51	0	0	5	0
10	B	55	0	0	0	0
All	All	4101	0	3856	305	0

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 39.

All (305) 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:18:PHE:HB3	1:A:167:LEU:HD21	1.26	1.16
3:B:256:NAG:H62	3:B:257:NAG:H2	1.16	1.09
1:A:101:ARG:HH11	1:A:101:ARG:HG2	1.11	1.08
4:B:259:NAG:H3	4:B:259:NAG:H83	1.36	1.06
1:A:240:CYS:OXT	1:A:240:CYS:SG	2.14	1.04
1:A:139:PHE:HB3	1:A:140:PRO:HD2	1.42	0.99
2:B:34:TRP:CE2	8:B:267:GAL:C1	2.46	0.99
1:A:119:HIS:O	1:A:123:ILE:HD13	1.65	0.94
2:B:194:VAL:HG12	2:B:194:VAL:O	1.67	0.92
1:A:18:PHE:CB	1:A:167:LEU:HD21	1.99	0.92
2:B:224:ASN:HD22	2:B:224:ASN:C	1.72	0.91
1:A:110:TYR:HB3	1:A:111:PRO:HD3	1.53	0.91
1:A:225:ASN:ND2	1:A:227:ARG:H	1.67	0.91
2:B:244:THR:HG22	2:B:249:GLN:CD	1.91	0.91
1:A:53:VAL:HG12	1:A:69:ILE:HG13	1.55	0.89
2:B:224:ASN:ND2	2:B:226:LEU:H	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HG22	1:A:94:HIS:H	1.38	0.88
2:B:14:ASN:HD22	2:B:178:ARG:HH22	1.14	0.87
1:A:225:ASN:HD22	1:A:227:ARG:H	0.87	0.87
4:B:260:BMA:H2	4:B:261:BMA:O2	1.74	0.87
1:A:127:ILE:H	1:A:127:ILE:HD12	1.37	0.86
1:A:225:ASN:HD22	1:A:227:ARG:N	1.73	0.86
2:B:164:GLN:O	2:B:164:GLN:HG3	1.73	0.85
1:A:139:PHE:HB3	1:A:140:PRO:CD	2.07	0.85
2:B:244:THR:HG23	2:B:246:LYS:H	1.40	0.85
1:A:220:PHE:H	1:A:220:PHE:HD1	1.23	0.84
2:B:224:ASN:HD22	2:B:226:LEU:H	1.26	0.84
1:A:120:ARG:H	1:A:120:ARG:CD	1.91	0.83
1:A:197:SER:OG	1:A:236:MET:HB3	1.79	0.83
1:A:3:ARG:HG3	1:A:27:TYR:CE2	2.15	0.82
1:A:127:ILE:HD11	1:A:177:GLY:HA2	1.60	0.82
2:B:144:PHE:HE2	2:B:233:PRO:HD3	1.44	0.82
1:A:48:GLU:CG	1:A:49:ALA:H	1.90	0.82
2:B:34:TRP:CZ2	2:B:111:LYS:HE3	2.15	0.81
1:A:110:TYR:HD2	10:A:251:HOH:O	1.62	0.81
1:A:220:PHE:CD1	1:A:220:PHE:N	2.49	0.80
1:A:220:PHE:HD1	1:A:220:PHE:N	1.80	0.80
3:B:256:NAG:C6	3:B:257:NAG:H2	2.08	0.80
2:B:21:ARG:HH12	2:B:30:GLN:HE21	1.27	0.80
1:A:216:ILE:CG2	1:A:217:PRO:HD2	2.13	0.79
6:B:263:NAG:H62	6:B:264:BMA:C1	2.13	0.78
1:A:127:ILE:HD12	1:A:127:ILE:N	1.97	0.78
2:B:148:CYS:O	2:B:158:VAL:HA	1.83	0.77
2:B:14:ASN:ND2	2:B:178:ARG:HH22	1.81	0.77
2:B:188:THR:HG23	2:B:209:GLN:HG2	1.65	0.77
1:A:101:ARG:HH11	1:A:101:ARG:CG	1.94	0.77
1:A:110:TYR:CB	1:A:111:PRO:HD3	2.14	0.77
1:A:1:TYR:HD2	1:A:2:GLU:H	1.33	0.76
2:B:34:TRP:CZ2	8:B:267:GAL:C1	2.68	0.76
2:B:197:ILE:HB	2:B:238:ILE:O	1.86	0.76
6:B:263:NAG:H62	6:B:264:BMA:O5	1.85	0.75
3:B:256:NAG:H62	3:B:257:NAG:C2	2.09	0.75
1:A:18:PHE:CZ	1:A:171:ARG:NH2	2.51	0.74
4:B:259:NAG:H3	4:B:259:NAG:C8	2.15	0.73
1:A:216:ILE:HG22	1:A:217:PRO:HG2	1.71	0.73
1:A:166:ILE:HG23	1:A:186:MET:HE2	1.70	0.73
8:B:267:GAL:HO4	8:B:267:GAL:HO6	0.74	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HG2	1:A:101:ARG:NH1	1.91	0.73
1:A:120:ARG:H	1:A:120:ARG:HD3	1.54	0.73
1:A:94:HIS:O	1:A:95:LEU:HB2	1.88	0.72
2:B:244:THR:OG1	2:B:246:LYS:HG3	1.90	0.72
2:B:81:VAL:HG12	2:B:83:GLU:HG2	1.70	0.72
1:A:25:ARG:HD2	1:A:161:ALA:O	1.89	0.72
1:A:48:GLU:CG	1:A:49:ALA:N	2.50	0.72
2:B:71:TYR:HA	2:B:116:THR:HG22	1.72	0.71
4:B:259:NAG:H83	4:B:259:NAG:C3	2.20	0.70
1:A:58:THR:OG1	1:A:64:SER:HB2	1.90	0.70
2:B:221:ASN:HD22	2:B:224:ASN:H	1.40	0.69
1:A:10:SER:H	1:A:12:THR:CG2	2.05	0.69
1:A:239:VAL:O	1:A:240:CYS:HB3	1.92	0.69
1:A:114:GLU:OE2	1:A:114:GLU:N	2.26	0.68
2:B:54:ILE:CD1	2:B:87:TRP:HB2	2.23	0.68
1:A:18:PHE:CE2	1:A:171:ARG:NE	2.59	0.68
2:B:213:PHE:CE1	2:B:219:ILE:HD11	2.28	0.68
2:B:193:SER:O	2:B:194:VAL:HG23	1.92	0.68
2:B:144:PHE:CE2	2:B:233:PRO:HD3	2.28	0.67
1:A:48:GLU:HG2	1:A:49:ALA:N	2.07	0.67
2:B:194:VAL:CG1	2:B:194:VAL:O	2.40	0.66
1:A:216:ILE:HG22	1:A:217:PRO:CD	2.25	0.66
2:B:95:ILE:HD13	2:B:128:TRP:CD1	2.30	0.66
1:A:216:ILE:HG22	1:A:217:PRO:CG	2.25	0.65
2:B:17:ASN:HD21	2:B:36:SER:HA	1.60	0.65
2:B:192:ASP:OD1	2:B:192:ASP:N	2.26	0.65
2:B:34:TRP:CH2	2:B:111:LYS:HE3	2.32	0.65
2:B:34:TRP:NE1	8:B:267:GAL:C1	2.59	0.65
1:A:159:GLU:HA	1:A:159:GLU:OE1	1.97	0.65
2:B:166:ASN:C	2:B:166:ASN:HD22	1.98	0.65
1:A:3:ARG:HG3	1:A:27:TYR:CZ	2.32	0.64
1:A:120:ARG:H	1:A:120:ARG:NE	1.96	0.64
1:A:9:THR:O	1:A:9:THR:HG23	1.97	0.64
2:B:21:ARG:NH1	2:B:30:GLN:HE21	1.95	0.63
2:B:99:ARG:HD2	2:B:99:ARG:O	1.98	0.63
2:B:34:TRP:CZ3	2:B:111:LYS:HG2	2.34	0.63
2:B:14:ASN:HD22	2:B:178:ARG:NH2	1.94	0.63
1:A:150:ILE:HG22	1:A:151:LEU:N	2.14	0.63
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.34	0.63
2:B:244:THR:HG22	2:B:249:GLN:NE2	2.13	0.62
1:A:127:ILE:H	1:A:127:ILE:CD1	2.05	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:HH11	1:A:3:ARG:HA	1.64	0.62
1:A:155:GLN:HG2	1:A:190:GLU:OE2	1.98	0.62
2:B:169:TRP:CZ3	2:B:187:LEU:HD13	2.34	0.62
1:A:101:ARG:CG	1:A:101:ARG:NH1	2.58	0.61
2:B:224:ASN:HD22	2:B:225:GLY:N	1.97	0.61
4:B:258:NAG:H61	4:B:259:NAG:C1	2.31	0.61
2:B:25:PHE:HE1	2:B:56:SER:HG	1.46	0.61
2:B:213:PHE:HE1	2:B:219:ILE:HD11	1.66	0.60
1:A:110:TYR:O	1:A:114:GLU:HG2	2.02	0.60
1:A:166:ILE:HG23	1:A:186:MET:CE	2.31	0.60
1:A:10:SER:H	1:A:12:THR:HG22	1.67	0.60
2:B:172:TYR:CE1	2:B:178:ARG:HD2	2.38	0.59
1:A:110:TYR:CB	1:A:111:PRO:CD	2.81	0.59
1:A:51:ARG:HG3	1:A:51:ARG:O	2.03	0.58
1:A:162:ARG:HD3	1:A:193:TRP:CD2	2.38	0.58
1:A:116:TYR:HD2	1:A:143:THR:HG23	1.69	0.58
1:A:59:ASN:C	1:A:59:ASN:HD22	2.06	0.58
1:A:169:ARG:NH2	10:A:261:HOH:O	2.36	0.58
2:B:224:ASN:ND2	2:B:224:ASN:C	2.46	0.58
1:A:164:ASN:N	1:A:165:PRO:CD	2.66	0.58
2:B:244:THR:OG1	2:B:246:LYS:CG	2.52	0.57
1:A:69:ILE:CG2	1:A:76:VAL:HG22	2.34	0.57
1:A:196:GLN:HE21	1:A:233:LEU:HD22	1.70	0.57
1:A:117:ALA:HB2	1:A:147:ALA:HB1	1.87	0.57
1:A:70:ASP:OD1	1:A:72:THR:HB	2.05	0.56
1:A:13:THR:O	1:A:16:GLU:HB2	2.05	0.56
1:A:134:VAL:CG2	1:A:135:THR:N	2.68	0.56
1:A:79:TYR:CZ	1:A:137:LEU:HD22	2.40	0.56
1:A:53:VAL:HG12	1:A:69:ILE:CG1	2.31	0.56
1:A:220:PHE:O	1:A:221:VAL:HG23	2.06	0.56
1:A:215:ALA:O	1:A:216:ILE:HG13	2.06	0.56
1:A:48:GLU:HG3	1:A:49:ALA:H	1.66	0.56
1:A:240:CYS:OXT	2:B:1:CYS:SG	2.65	0.55
2:B:193:SER:O	2:B:194:VAL:CG2	2.55	0.55
1:A:216:ILE:HG23	1:A:217:PRO:HD2	1.87	0.55
2:B:16:MET:CE	2:B:35:PRO:HG3	2.36	0.55
1:A:116:TYR:HD2	1:A:143:THR:CG2	2.19	0.55
6:B:263:NAG:C6	6:B:264:BMA:C1	2.80	0.55
1:A:201:GLN:HB3	1:A:240:CYS:OXT	2.07	0.55
1:A:162:ARG:HD3	1:A:193:TRP:CE2	2.41	0.55
2:B:162:VAL:HG12	2:B:163:SER:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:CG1	1:A:69:ILE:HG13	2.31	0.54
1:A:10:SER:HA	1:A:131:ILE:HD11	1.88	0.54
1:A:70:ASP:HB3	1:A:73:ASN:OD1	2.08	0.54
2:B:24:ASP:HB3	2:B:29:ASN:ND2	2.22	0.54
1:A:10:SER:CA	1:A:131:ILE:HD11	2.37	0.54
1:A:119:HIS:O	1:A:123:ILE:CD1	2.49	0.54
2:B:32:GLN:OE1	8:B:267:GAL:H4	2.08	0.53
2:B:166:ASN:HD22	2:B:167:ASP:N	2.05	0.53
1:A:38:PRO:HB2	1:A:235:ILE:HG12	1.90	0.53
1:A:110:TYR:CG	1:A:111:PRO:HD3	2.42	0.53
1:A:117:ALA:HB2	1:A:147:ALA:CB	2.38	0.53
2:B:195:ALA:HA	2:B:239:ILE:HB	1.91	0.53
1:A:159:GLU:CA	1:A:159:GLU:OE1	2.56	0.53
1:A:159:GLU:OE2	1:A:190:GLU:HG2	2.09	0.53
2:B:102:LEU:HB2	2:B:117:VAL:HB	1.90	0.53
1:A:134:VAL:HG23	1:A:135:THR:N	2.24	0.53
1:A:105:PRO:HB2	1:A:116:TYR:OH	2.09	0.52
2:B:213:PHE:CE1	2:B:219:ILE:CD1	2.92	0.52
1:A:196:GLN:HB3	1:A:233:LEU:HD22	1.90	0.52
1:A:18:PHE:O	1:A:22:THR:HB	2.09	0.52
2:B:22:ASP:O	2:B:23:ASP:HB2	2.10	0.52
2:B:54:ILE:HD11	2:B:87:TRP:HB2	1.91	0.52
1:A:59:ASN:OD1	1:A:134:VAL:CG2	2.58	0.52
2:B:34:TRP:CH2	8:B:267:GAL:H5	2.45	0.51
1:A:105:PRO:HG2	1:A:116:TYR:CE2	2.45	0.51
2:B:31:ILE:HG22	2:B:115:LEU:CD2	2.41	0.51
2:B:20:VAL:O	2:B:20:VAL:HG22	2.10	0.51
2:B:16:MET:HE2	2:B:35:PRO:HG3	1.93	0.51
2:B:20:VAL:HB	2:B:31:ILE:HD13	1.93	0.51
1:A:65:ILE:HD12	1:A:65:ILE:C	2.31	0.51
2:B:31:ILE:HG22	2:B:115:LEU:HD22	1.91	0.51
2:B:17:ASN:HD21	2:B:36:SER:CA	2.22	0.51
2:B:46:TRP:HB3	2:B:54:ILE:CG2	2.39	0.51
2:B:16:MET:HB2	2:B:33:LEU:HG	1.93	0.51
1:A:182:PRO:HB3	1:A:186:MET:SD	2.51	0.51
2:B:8:VAL:HG13	2:B:131:GLY:H	1.75	0.50
1:A:70:ASP:CG	1:A:72:THR:HG22	2.31	0.50
1:A:18:PHE:HB3	1:A:167:LEU:CD2	2.17	0.50
1:A:69:ILE:HG22	1:A:76:VAL:HG22	1.94	0.50
1:A:69:ILE:HA	1:A:75:TYR:O	2.12	0.50
2:B:8:VAL:HG13	2:B:9:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:CD1	2:B:128:TRP:HB2	2.42	0.49
1:A:119:HIS:CD2	1:A:119:HIS:N	2.80	0.49
1:A:120:ARG:CD	1:A:120:ARG:N	2.69	0.49
1:A:9:THR:CG2	1:A:9:THR:O	2.59	0.49
2:B:231:ALA:O	2:B:232:ASN:HB2	2.11	0.49
2:B:181:GLN:HA	2:B:181:GLN:OE1	2.12	0.49
2:B:144:PHE:HE2	2:B:233:PRO:CD	2.20	0.49
1:A:166:ILE:HG12	1:A:186:MET:HG3	1.95	0.49
2:B:213:PHE:CE1	2:B:219:ILE:HG12	2.48	0.49
2:B:34:TRP:CG	2:B:35:PRO:HD2	2.48	0.49
2:B:246:LYS:HB3	2:B:247:PRO:CD	2.42	0.49
1:A:119:HIS:H	1:A:119:HIS:CD2	2.29	0.49
2:B:224:ASN:ND2	2:B:226:LEU:N	2.50	0.49
1:A:116:TYR:CD2	1:A:143:THR:CG2	2.96	0.48
1:A:221:VAL:HG12	1:A:221:VAL:O	2.13	0.48
1:A:204:THR:HG21	2:B:6:PRO:HD2	1.94	0.48
2:B:221:ASN:ND2	2:B:224:ASN:H	2.08	0.48
1:A:52:PHE:CG	1:A:95:LEU:HD21	2.48	0.48
1:A:204:THR:OG1	1:A:205:GLU:N	2.45	0.48
1:A:26:ASP:O	1:A:29:SER:HB2	2.13	0.48
2:B:133:ASP:HB3	2:B:137:ARG:HH12	1.79	0.48
2:B:18:VAL:HG12	2:B:46:TRP:CZ2	2.48	0.48
1:A:85:SER:HB2	1:A:87:PHE:HE1	1.79	0.48
1:A:93:THR:HG22	1:A:94:HIS:N	2.19	0.47
1:A:120:ARG:NE	1:A:120:ARG:N	2.61	0.47
2:B:241:TYR:CD2	2:B:242:PRO:HD2	2.49	0.47
1:A:70:ASP:OD1	1:A:72:THR:CB	2.63	0.47
1:A:224:THR:HG21	2:B:133:ASP:HB2	1.97	0.47
2:B:89:ILE:HD13	2:B:95:ILE:HG13	1.96	0.47
2:B:186:CYS:O	2:B:199:ILE:HA	2.15	0.47
1:A:88:LEU:HB3	1:A:106:PHE:O	2.14	0.47
1:A:82:GLY:HA3	1:A:138:ARG:NH2	2.30	0.47
2:B:34:TRP:CD1	2:B:35:PRO:HD2	2.50	0.46
2:B:224:ASN:HD22	2:B:226:LEU:N	2.05	0.46
1:A:129:GLN:O	1:A:133:SER:HB2	2.15	0.46
4:B:258:NAG:C6	4:B:259:NAG:C1	2.94	0.46
1:A:116:TYR:CD2	1:A:143:THR:HG23	2.49	0.46
4:B:259:NAG:C3	4:B:259:NAG:C8	2.82	0.46
1:A:10:SER:HA	1:A:131:ILE:CD1	2.46	0.46
2:B:35:PRO:HD3	2:B:111:LYS:HG3	1.97	0.46
2:B:20:VAL:O	2:B:20:VAL:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG21	2:B:6:PRO:CD	2.46	0.46
2:B:213:PHE:CD1	2:B:219:ILE:HG12	2.51	0.46
1:A:196:GLN:NE2	1:A:233:LEU:HD22	2.30	0.46
1:A:17:TYR:CE1	1:A:21:ILE:HD11	2.51	0.46
1:A:86:TYR:HB3	1:A:104:LEU:CD1	2.46	0.46
2:B:133:ASP:HB3	2:B:137:ARG:NH1	2.31	0.45
2:B:21:ARG:HH12	2:B:30:GLN:NE2	2.05	0.45
2:B:81:VAL:O	2:B:82:ARG:C	2.55	0.45
2:B:13:ARG:C	2:B:15:GLY:H	2.20	0.45
2:B:7:THR:HG22	2:B:45:LEU:HB3	1.99	0.45
2:B:29:ASN:OD1	2:B:30:GLN:N	2.50	0.45
2:B:166:ASN:C	2:B:166:ASN:ND2	2.69	0.45
1:A:23:LEU:O	1:A:24:LEU:C	2.55	0.45
1:A:143:THR:HG22	1:A:144:ARG:N	2.32	0.45
1:A:68:ALA:HB1	1:A:95:LEU:HD22	1.98	0.45
2:B:8:VAL:HG13	2:B:131:GLY:N	2.32	0.45
4:B:258:NAG:H61	4:B:259:NAG:H82	1.99	0.44
1:A:10:SER:CB	1:A:60:GLU:HG2	2.47	0.44
2:B:232:ASN:C	2:B:234:GLY:H	2.21	0.44
1:A:219:ASN:HA	10:A:269:HOH:O	2.15	0.44
1:A:59:ASN:HD21	1:A:63:ASP:H	1.65	0.44
1:A:117:ALA:HB1	1:A:148:ARG:HA	2.00	0.44
1:A:225:ASN:ND2	1:A:227:ARG:HB2	2.33	0.44
1:A:196:GLN:HB3	1:A:233:LEU:CD2	2.47	0.44
2:B:162:VAL:HG12	2:B:163:SER:H	1.82	0.44
1:A:35:ASN:O	1:A:36:GLU:HB2	2.18	0.44
1:A:94:HIS:O	1:A:95:LEU:CB	2.60	0.44
2:B:240:ILE:HA	2:B:240:ILE:HD13	1.64	0.44
1:A:33:PHE:CD1	1:A:33:PHE:N	2.86	0.44
1:A:23:LEU:HA	1:A:23:LEU:HD13	1.63	0.43
2:B:164:GLN:HE21	2:B:164:GLN:HB2	1.69	0.43
1:A:213:ARG:HG2	10:A:288:HOH:O	2.17	0.43
2:B:7:THR:HA	2:B:47:THR:HA	1.99	0.43
1:A:46:GLY:O	1:A:47:VAL:HG23	2.19	0.43
1:A:35:ASN:O	1:A:36:GLU:CB	2.67	0.43
1:A:110:TYR:HB3	1:A:111:PRO:CD	2.33	0.43
1:A:86:TYR:CD1	1:A:86:TYR:N	2.87	0.43
2:B:24:ASP:C	2:B:24:ASP:OD1	2.56	0.43
1:A:159:GLU:HG3	1:A:190:GLU:HG2	2.00	0.43
2:B:188:THR:HG23	2:B:209:GLN:CG	2.40	0.43
1:A:114:GLU:O	1:A:116:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:ND2	1:A:226:VAL:N	2.67	0.43
2:B:8:VAL:CG1	2:B:131:GLY:N	2.82	0.43
1:A:110:TYR:O	1:A:111:PRO:C	2.58	0.42
2:B:143:GLY:O	2:B:144:PHE:C	2.57	0.42
1:A:85:SER:HB2	1:A:87:PHE:CE1	2.53	0.42
1:A:110:TYR:CD2	10:A:251:HOH:O	2.49	0.42
2:B:133:ASP:HB3	2:B:137:ARG:HH22	1.84	0.42
2:B:121:ASP:O	2:B:122:TYR:HB2	2.20	0.42
1:A:150:ILE:CG2	1:A:151:LEU:N	2.82	0.42
2:B:222:LEU:HG	2:B:222:LEU:O	2.18	0.42
2:B:149:MET:HB3	2:B:149:MET:HE3	1.78	0.42
2:B:213:PHE:CE1	2:B:219:ILE:CG1	3.02	0.42
2:B:17:ASN:HD22	2:B:44:GLN:NE2	2.18	0.42
2:B:232:ASN:HB3	2:B:234:GLY:H	1.85	0.42
2:B:224:ASN:O	2:B:226:LEU:HD12	2.19	0.42
1:A:143:THR:O	1:A:144:ARG:C	2.58	0.42
1:A:7:ASP:HB3	1:A:57:LEU:HD12	2.02	0.42
2:B:8:VAL:CG1	2:B:9:ARG:O	2.68	0.41
2:B:26:HIS:O	2:B:27:ASP:C	2.58	0.41
2:B:200:VAL:HG13	2:B:201:SER:N	2.35	0.41
1:A:76:VAL:HG23	1:A:154:ILE:HD13	2.02	0.41
1:A:204:THR:C	1:A:206:GLY:H	2.23	0.41
2:B:13:ARG:C	2:B:15:GLY:N	2.73	0.41
2:B:76:ASP:OD1	2:B:78:ASN:N	2.52	0.41
2:B:133:ASP:CG	2:B:137:ARG:NH1	2.74	0.41
1:A:209:ASN:ND2	2:B:4:SER:HB2	2.35	0.41
2:B:133:ASP:HB3	2:B:137:ARG:NH2	2.35	0.41
1:A:129:GLN:HB3	1:A:152:ILE:HD13	2.02	0.41
2:B:50:ARG:HA	2:B:50:ARG:HD2	1.55	0.41
2:B:151:SER:HB3	2:B:169:TRP:CH2	2.55	0.41
2:B:34:TRP:CZ3	8:B:267:GAL:H5	2.56	0.41
2:B:172:TYR:CD1	2:B:178:ARG:HD2	2.56	0.41
2:B:21:ARG:NH2	2:B:112:GLY:O	2.53	0.41
1:A:46:GLY:HA3	1:A:51:ARG:HH11	1.85	0.41
1:A:4:LEU:HD23	1:A:54:LEU:HB3	2.03	0.41
1:A:53:VAL:CG1	1:A:69:ILE:CG1	2.95	0.41
1:A:7:ASP:HB2	1:A:20:PHE:CD1	2.56	0.40
1:A:10:SER:HB2	1:A:60:GLU:HG2	2.03	0.40
1:A:150:ILE:HD13	1:A:150:ILE:HA	1.85	0.40
1:A:109:SER:O	1:A:110:TYR:C	2.60	0.40
1:A:107:ASN:HB2	5:A:241:NAG:H82	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASN:HD21	1:A:63:ASP:HB2	1.86	0.40
1:A:124:PRO:O	1:A:125:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

## 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	238/240 (99%)	191 (80%)	37 (16%)	10 (4%)	3	11
2	B	253/255 (99%)	219 (87%)	25 (10%)	9 (4%)	4	14
All	All	491/495 (99%)	410 (84%)	62 (13%)	19 (4%)	4	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	110	TYR
1	A	143	THR
1	A	204	THR
1	A	217	PRO
1	A	221	VAL
2	B	165	GLN
1	A	97	THR
1	A	235	ILE
2	B	144	PHE
2	B	39	ASN
2	B	57	ASN
2	B	194	VAL
2	B	197	ILE
2	B	207	SER
1	A	140	PRO

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Mol	Chain	Res	Type
2	B	233	PRO
1	A	139	PHE
2	B	190	GLY

### 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	205/205 (100%)	154 (75%)	51 (25%)	1	2
2	B	211/211 (100%)	173 (82%)	38 (18%)	2	6
All	All	416/416 (100%)	327 (79%)	89 (21%)	1	3

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	6	LEU
1	A	12	THR
1	A	15	GLU
1	A	23	LEU
1	A	24	LEU
1	A	25	ARG
1	A	32	SER
1	A	42	GLN
1	A	47	VAL
1	A	48	GLU
1	A	53	VAL
1	A	54	LEU
1	A	57	LEU
1	A	59	ASN
1	A	60	GLU
1	A	64	SER
1	A	69	ILE
1	A	72	THR
1	A	74	LEU

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Mol	Chain	Res	Type
1	A	80	GLN
1	A	83	SER
1	A	85	SER
1	A	88	LEU
1	A	93	THR
1	A	101	ARG
1	A	103	SER
1	A	104	LEU
1	A	114	GLU
1	A	120	ARG
1	A	127	ILE
1	A	130	LEU
1	A	132	GLN
1	A	133	SER
1	A	145	THR
1	A	148	ARG
1	A	150	ILE
1	A	151	LEU
1	A	159	GLU
1	A	167	LEU
1	A	168	TRP
1	A	171	ARG
1	A	172	GLN
1	A	181	LEU
1	A	213	ARG
1	A	216	ILE
1	A	219	ASN
1	A	220	PHE
1	A	221	VAL
1	A	235	ILE
1	A	240	CYS
2	B	1	CYS
2	B	8	VAL
2	B	17	ASN
2	B	20	VAL
2	B	23	ASP
2	B	36	SER
2	B	38	SER
2	B	45	LEU
2	B	50	ARG
2	B	83	GLU
2	B	96	ILE

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Mol	Chain	Res	Type
2	B	101	ASN
2	B	114	THR
2	B	115	LEU
2	B	119	THR
2	B	120	LEU
2	B	129	LEU
2	B	146	ASP
2	B	158	VAL
2	B	160	THR
2	B	163	SER
2	B	164	GLN
2	B	166	ASN
2	B	167	ASP
2	B	182	ASN
2	B	191	ARG
2	B	192	ASP
2	B	193	SER
2	B	197	ILE
2	B	198	ASN
2	B	212	VAL
2	B	224	ASN
2	B	228	MET
2	B	235	LEU
2	B	237	GLN
2	B	238	ILE
2	B	240	ILE
2	B	250	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	59	ASN
1	A	94	HIS
1	A	119	HIS
1	A	196	GLN
1	A	225	ASN
2	B	14	ASN
2	B	17	ASN
2	B	30	GLN
2	B	145	ASN
2	B	164	GLN

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Mol	Chain	Res	Type
2	B	165	GLN
2	B	166	ASN
2	B	198	ASN
2	B	221	ASN
2	B	224	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 ⓘ

11 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	$\# Z  > 2$
3	NAG	B	256	3,2	14,14,15	0.72	0	15,19,21	2.65	7 (46%)
3	NAG	B	257	3	14,14,15	0.69	0	15,19,21	1.52	2 (13%)
4	NAG	B	258	2,4	14,14,15	0.44	0	15,19,21	1.59	4 (26%)
4	NAG	B	259	4	14,14,15	0.48	0	15,19,21	1.64	5 (33%)
4	BMA	B	260	4	11,11,12	0.61	0	14,15,17	2.17	4 (28%)
4	BMA	B	261	4	11,11,12	0.51	0	14,15,17	1.24	3 (21%)
6	NAG	B	262	2,6	14,14,15	0.54	0	15,19,21	1.73	3 (20%)
6	NAG	B	263	6	14,14,15	0.64	0	15,19,21	1.61	3 (20%)
6	BMA	B	264	6	11,11,12	0.47	0	14,15,17	1.54	3 (21%)
7	BGC	B	265	7	12,12,12	0.51	0	17,17,17	1.74	5 (29%)
7	GAL	B	266	7	11,11,12	0.53	0	14,15,17	1.94	4 (28%)



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	B	256	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	257	3	-	0/6/23/26	0/1/1/1
4	NAG	B	258	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	259	4	-	0/6/23/26	0/1/1/1
4	BMA	B	260	4	1/1/4/5	0/2/19/22	0/1/1/1
4	BMA	B	261	4	-	0/2/19/22	0/1/1/1
6	NAG	B	262	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	263	6	-	0/6/23/26	0/1/1/1
6	BMA	B	264	6	-	0/2/19/22	1/1/1/1
7	BGC	B	265	7	-	0/2/22/22	0/1/1/1
7	GAL	B	266	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	258	NAG	C3-C4-C5	-3.54	104.02	110.20
6	B	263	NAG	C1-O5-C5	-3.26	108.11	112.25
3	B	256	NAG	O7-C7-C8	-3.18	116.22	122.06
4	B	259	NAG	C3-C4-C5	-2.93	105.09	110.20
3	B	256	NAG	C3-C4-C5	-2.74	105.42	110.20
4	B	258	NAG	O4-C4-C3	-2.74	104.17	110.34
6	B	264	BMA	C2-C3-C4	-2.66	106.52	111.04
4	B	259	NAG	C1-O5-C5	-2.59	108.96	112.25
6	B	264	BMA	O5-C1-C2	-2.55	106.73	110.86
3	B	256	NAG	C4-C3-C2	-2.53	107.30	111.23
6	B	262	NAG	C2-N2-C7	-2.23	120.17	123.04
4	B	258	NAG	C6-C5-C4	-2.18	107.64	113.02
7	B	265	BGC	C4-C3-C2	2.02	114.56	110.79
4	B	259	NAG	O4-C4-C5	2.08	114.75	109.24
4	B	261	BMA	O2-C2-C1	2.11	113.43	109.21
7	B	266	GAL	C2-C3-C4	2.22	114.81	111.04
4	B	258	NAG	C1-O5-C5	2.23	115.07	112.25
4	B	259	NAG	C6-C5-C4	2.28	118.65	113.02
3	B	256	NAG	C8-C7-N2	2.31	120.52	116.11
4	B	260	BMA	O5-C5-C6	2.33	112.39	107.35
6	B	263	NAG	O4-C4-C5	2.44	115.71	109.24
6	B	262	NAG	C4-C3-C2	2.52	115.15	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	261	BMA	C1-C2-C3	2.58	112.59	109.54
6	B	264	BMA	O2-C2-C1	2.59	114.40	109.21
3	B	257	NAG	O3-C3-C2	2.71	114.47	109.11
4	B	261	BMA	O5-C5-C6	2.81	113.43	107.35
3	B	256	NAG	O3-C3-C2	2.83	114.72	109.11
4	B	259	NAG	O5-C5-C6	2.87	113.56	107.35
7	B	265	BGC	O5-C1-C2	2.96	114.52	109.80
7	B	266	GAL	C3-C4-C5	3.01	115.45	110.20
7	B	265	BGC	C1-C2-C3	3.28	115.31	110.43
7	B	265	BGC	C1-O5-C5	3.38	119.72	113.47
7	B	266	GAL	C1-C2-C3	3.54	113.73	109.54
7	B	265	BGC	O5-C5-C4	3.56	116.37	109.68
4	B	260	BMA	O3-C3-C4	3.73	118.73	110.34
6	B	262	NAG	C1-O5-C5	3.94	117.25	112.25
3	B	257	NAG	C4-C3-C2	4.20	117.76	111.23
6	B	263	NAG	C4-C3-C2	4.29	117.90	111.23
3	B	256	NAG	C3-C2-N2	4.30	120.86	110.56
7	B	266	GAL	C1-O5-C5	4.36	117.78	112.25
4	B	260	BMA	C2-C3-C4	4.36	118.45	111.04
4	B	260	BMA	O3-C3-C2	4.43	118.00	110.00
3	B	256	NAG	C1-O5-C5	6.44	120.42	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	260	BMA	C3

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	264	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	256	NAG	3	0
3	B	257	NAG	3	0
4	B	258	NAG	3	0
4	B	259	NAG	7	0
4	B	260	BMA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	261	BMA	1	0
6	B	263	NAG	3	0
6	B	264	BMA	3	0

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
5	NAG	A	241	1	14,14,15	0.49	0	15,19,21	1.54	3 (20%)
9	P6C	A	242	-	14,18,18	2.36	2 (14%)	16,26,26	3.85	9 (56%)
8	GAL	B	267	-	11,11,12	1.11	1 (9%)	14,15,17	1.89	4 (28%)

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
5	NAG	A	241	1	1/1/5/7	0/6/23/26	0/1/1/1
9	P6C	A	242	-	-	0/4/8/8	0/2/2/2
8	GAL	B	267	-	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	242	P6C	C14-N13	-2.03	1.33	1.37
8	B	267	GAL	O5-C1	2.92	1.48	1.43
9	A	242	P6C	C8-C5	7.43	1.61	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	267	GAL	C1-O5-C5	-3.49	107.82	112.25
9	A	242	P6C	C11-C12-N13	-3.34	120.49	123.65
5	A	241	NAG	C4-C3-C2	-3.34	106.04	111.23
9	A	242	P6C	C12-C11-N10	-2.88	118.66	120.83
9	A	242	P6C	C9-C14-N13	-2.54	117.19	121.81
9	A	242	P6C	C9-C14-N15	-2.28	118.43	122.11
8	B	267	GAL	C2-C3-C4	2.06	114.54	111.04
5	A	241	NAG	O3-C3-C2	2.23	113.52	109.11
9	A	242	P6C	C6-C5-C8	2.80	116.30	111.26
8	B	267	GAL	O2-C2-C1	3.11	115.45	109.21
5	A	241	NAG	C1-O5-C5	3.36	116.51	112.25
8	B	267	GAL	C3-C4-C5	3.57	116.42	110.20
9	A	242	P6C	C12-N13-C14	4.73	122.51	116.93
9	A	242	P6C	N13-C14-N15	5.75	124.36	116.14
9	A	242	P6C	C11-N10-C9	7.90	123.20	118.33
9	A	242	P6C	C4-C5-C8	8.42	126.43	111.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	241	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	241	NAG	1	0
8	B	267	GAL	7	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.