



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 07:50 AM GMT

PDB ID : 1PC8  
Title : Crystal Structure of a novel form of mistletoe lectin from Himalayan Viscum album L. at 3.8Å resolution  
Authors : Mishra, V.; Ethayathulla, A.S.; Paramasivam, M.; Singh, G.; Yadav, S.; Kaur, P.; Sharma, R.S.; Babu, C.R.; Singh, T.P.  
Deposited on : 2003-05-16  
Resolution : 3.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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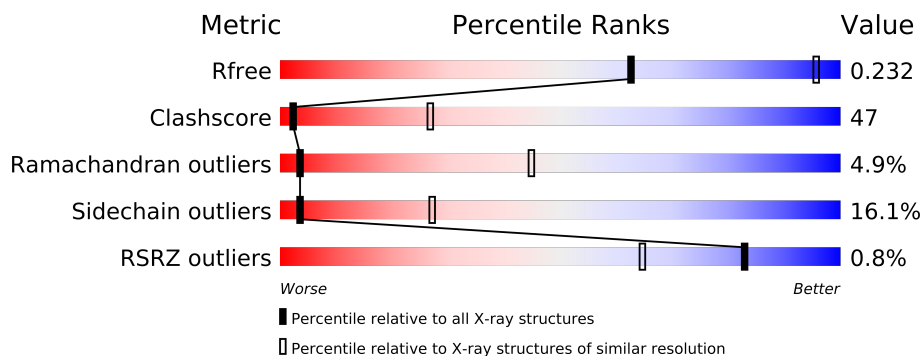
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.80 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))
$R_{free}$	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	1002	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3935 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Himalayan mistletoe ribosome-inactivatingprotein.

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-inactivatingprotein.

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 (3-MER).

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

- 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 (2-MER).

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

- Molecule 7 is water.

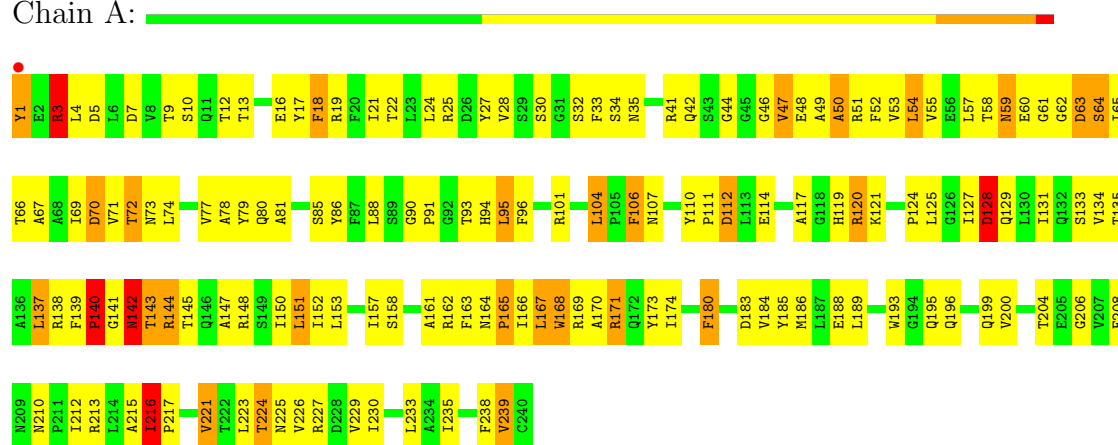
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

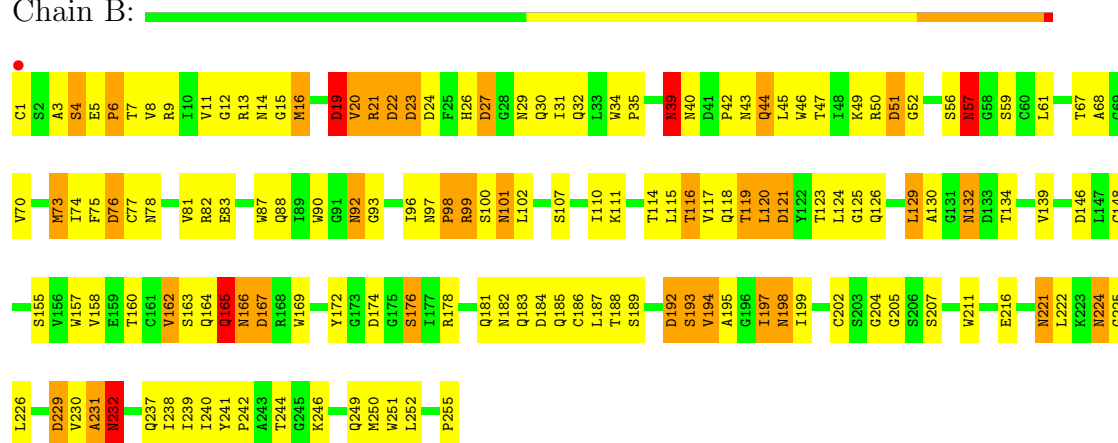
- Molecule 1: Himalayan mistletoe ribosome-inactivatingprotein

Chain A:



- Molecule 2: Himalayan mistletoe ribosome-inactivatingprotein

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.18Å 109.18Å 309.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 32.44 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.80) 99.6 (32.44-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.228 , 0.271 0.223 , 0.232	Depositor DCC
$R_{free}$ test set	584 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 11420 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG

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	1.08	1/1913 (0.1%)	1.10	11/2602 (0.4%)
2	B	1.22	2/1978 (0.1%)	1.20	21/2697 (0.8%)
All	All	1.15	3/3891 (0.1%)	1.15	32/5299 (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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	GLN	N-CA	7.79	1.61	1.46
2	B	57	ASN	C-N	6.74	1.45	1.33
1	A	221	VAL	CB-CG2	-5.11	1.42	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	ASN	CB-CA-C	-12.72	84.97	110.40
2	B	21	ARG	NE-CZ-NH1	-11.22	114.69	120.30
2	B	44	GLN	N-CA-C	9.38	136.32	111.00
2	B	57	ASN	CA-C-N	-8.46	99.28	116.20
2	B	21	ARG	NE-CZ-NH2	8.38	124.49	120.30
2	B	57	ASN	O-C-N	7.70	136.29	123.20
2	B	167	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	142	ASN	CB-CA-C	7.65	125.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	140	PRO	N-CA-C	7.49	131.56	112.10
2	B	24	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	3	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	B	19	ASP	CB-CG-OD2	7.30	124.87	118.30
2	B	44	GLN	N-CA-CB	-7.14	97.74	110.60
1	A	7	ASP	CB-CG-OD2	7.02	124.62	118.30
2	B	22	ASP	CB-CG-OD2	6.79	124.42	118.30
1	A	63	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	5	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	70	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	128	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	112	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	192	ASP	CB-CG-OD2	6.15	123.83	118.30
2	B	146	ASP	CB-CG-OD2	6.13	123.82	118.30
2	B	40	ASN	N-CA-C	6.00	127.19	111.00
2	B	13	ARG	CA-C-N	-5.88	104.27	117.20
2	B	184	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	3	ARG	CG-CD-NE	-5.55	100.14	111.80
2	B	13	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	B	121	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	229	ASP	CB-CG-OD2	5.43	123.19	118.30
2	B	21	ARG	CG-CD-NE	5.22	122.77	111.80
2	B	165	GLN	O-C-N	-5.09	114.56	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	ASN	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1850	195	0
2	B	1938	0	1851	166	0
3	B	28	0	25	3	0
4	B	39	0	34	5	0
5	A	14	0	13	0	0
6	B	28	0	25	2	0
7	A	8	0	0	1	0
7	B	5	0	0	0	0
All	All	3935	0	3798	360	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

All (360) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:ILE:CG2	1:A:217:PRO:HD2	1.51	1.40
1:A:216:ILE:HG22	1:A:217:PRO:CD	1.56	1.35
1:A:52:PHE:CD2	1:A:95:LEU:HD11	1.79	1.18
1:A:216:ILE:HD11	1:A:221:VAL:CG2	1.74	1.16
2:B:189:SER:HB2	2:B:240:ILE:HD11	1.25	1.13
1:A:93:THR:HG22	1:A:94:HIS:H	1.13	1.09
1:A:70:ASP:OD1	1:A:72:THR:HG23	1.53	1.08
1:A:139:PHE:HB3	1:A:140:PRO:HD2	1.38	1.04
2:B:198:ASN:N	2:B:198:ASN:HD22	1.51	1.04
1:A:225:ASN:HD22	1:A:227:ARG:H	1.04	0.99
1:A:25:ARG:HG3	1:A:235:ILE:HD11	1.43	0.99
1:A:86:TYR:HB3	1:A:104:LEU:HD21	1.45	0.98
2:B:224:ASN:HD22	2:B:225:GLY:N	1.61	0.98
1:A:59:ASN:OD1	1:A:63:ASP:HB2	1.64	0.98
2:B:198:ASN:H	2:B:198:ASN:ND2	1.59	0.98
1:A:48:GLU:HG2	1:A:49:ALA:H	1.28	0.97
2:B:121:ASP:OD1	2:B:123:THR:HG23	1.63	0.97
2:B:20:VAL:HG21	2:B:74:ILE:HD12	1.44	0.97
1:A:52:PHE:CE2	1:A:95:LEU:HD11	2.02	0.95
1:A:215:ALA:O	1:A:216:ILE:HG12	1.68	0.92
1:A:215:ALA:C	1:A:216:ILE:HG12	1.90	0.91
2:B:194:VAL:HG12	2:B:194:VAL:O	1.70	0.90
1:A:110:TYR:HB3	1:A:111:PRO:HD3	1.55	0.88
1:A:93:THR:CG2	1:A:94:HIS:H	1.81	0.88
2:B:226:LEU:HD12	2:B:226:LEU:N	1.89	0.88
2:B:224:ASN:HD22	2:B:225:GLY:H	1.22	0.88
2:B:195:ALA:HA	2:B:239:ILE:HG23	1.57	0.86
1:A:216:ILE:HD11	1:A:221:VAL:HG23	1.55	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:121:ASP:H	2:B:126:GLN:HE22	0.91	0.86
1:A:225:ASN:ND2	1:A:227:ARG:H	1.73	0.86
2:B:166:ASN:N	2:B:166:ASN:HD22	1.74	0.85
2:B:189:SER:CB	2:B:240:ILE:HD11	2.06	0.85
1:A:94:HIS:O	1:A:95:LEU:HB2	1.75	0.84
2:B:121:ASP:H	2:B:126:GLN:NE2	1.76	0.83
1:A:141:GLY:O	1:A:142:ASN:HB3	1.81	0.81
1:A:32:SER:C	1:A:33:PHE:HD1	1.84	0.81
1:A:216:ILE:HD11	1:A:221:VAL:HG21	1.62	0.81
2:B:244:THR:HG23	2:B:246:LYS:H	1.44	0.79
2:B:21:ARG:HD3	2:B:32:GLN:NE2	1.97	0.79
4:B:259:NAG:H3	4:B:259:NAG:H83	1.65	0.78
2:B:166:ASN:HD22	2:B:166:ASN:H	1.30	0.78
1:A:93:THR:HG22	1:A:94:HIS:N	1.97	0.76
1:A:52:PHE:CE2	1:A:95:LEU:CD1	2.68	0.76
2:B:121:ASP:N	2:B:126:GLN:HE22	1.76	0.75
1:A:139:PHE:CB	1:A:140:PRO:HD2	2.11	0.75
1:A:110:TYR:O	1:A:114:GLU:HG2	1.86	0.75
1:A:61:GLY:O	1:A:63:ASP:N	2.20	0.75
2:B:117:VAL:HG23	2:B:117:VAL:O	1.88	0.74
1:A:27:TYR:O	1:A:27:TYR:CD1	2.40	0.73
2:B:139:VAL:HG12	2:B:255:PRO:HA	1.71	0.73
2:B:5:GLU:OE2	2:B:49:LYS:HD3	1.89	0.72
2:B:224:ASN:HB2	2:B:226:LEU:HD13	1.70	0.72
2:B:92:ASN:N	2:B:92:ASN:OD1	2.19	0.72
2:B:98:PRO:O	2:B:99:ARG:C	2.28	0.72
1:A:212:ILE:HB	1:A:223:LEU:HD12	1.71	0.72
1:A:65:ILE:HD11	1:A:137:LEU:HB3	1.70	0.71
1:A:138:ARG:HG3	1:A:139:PHE:CE1	2.26	0.71
1:A:94:HIS:O	1:A:95:LEU:CB	2.37	0.71
1:A:180:PHE:HD1	1:A:180:PHE:H	1.37	0.71
2:B:221:ASN:HB3	2:B:224:ASN:HD21	1.56	0.70
2:B:76:ASP:OD1	2:B:76:ASP:C	2.29	0.70
2:B:57:ASN:C	2:B:57:ASN:OD1	2.30	0.70
2:B:31:ILE:HD13	2:B:61:LEU:HD12	1.74	0.70
2:B:100:SER:OG	2:B:102:LEU:HG	1.91	0.69
1:A:188:GLU:OE1	1:A:215:ALA:N	2.22	0.69
1:A:59:ASN:HD21	1:A:63:ASP:N	1.90	0.69
2:B:231:ALA:O	2:B:232:ASN:HB2	1.93	0.69
2:B:76:ASP:OD1	2:B:78:ASN:N	2.26	0.69
1:A:117:ALA:HB2	1:A:147:ALA:HB1	1.73	0.68
1:A:158:SER:O	1:A:161:ALA:HB3	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:67:THR:O	2:B:70:VAL:HG22	1.93	0.68
2:B:3:ALA:O	2:B:4:SER:HB2	1.94	0.68
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.29	0.68
2:B:8:VAL:HG12	2:B:9:ARG:N	2.09	0.67
1:A:53:VAL:HG12	1:A:69:ILE:HB	1.77	0.67
2:B:90:TRP:CH2	2:B:96:ILE:HD12	2.29	0.67
1:A:164:ASN:O	1:A:168:TRP:HB2	1.94	0.66
2:B:226:LEU:CD1	2:B:226:LEU:N	2.57	0.66
1:A:77:VAL:O	1:A:88:LEU:HG	1.95	0.66
1:A:104:LEU:HD22	1:A:104:LEU:N	2.10	0.66
2:B:198:ASN:N	2:B:198:ASN:ND2	2.22	0.66
2:B:222:LEU:HD11	3:B:256:NDG:H8C3	1.79	0.65
2:B:57:ASN:O	2:B:57:ASN:OD1	2.15	0.65
2:B:193:SER:O	2:B:194:VAL:HG23	1.96	0.65
2:B:8:VAL:HG12	2:B:9:ARG:O	1.96	0.65
1:A:34:SER:O	1:A:35:ASN:HB2	1.97	0.65
1:A:19:ARG:O	1:A:22:THR:HB	1.95	0.65
2:B:20:VAL:CG2	2:B:74:ILE:HD12	2.22	0.65
2:B:198:ASN:H	2:B:198:ASN:HD22	0.75	0.64
1:A:120:ARG:H	1:A:120:ARG:HD3	1.61	0.64
2:B:222:LEU:CD1	3:B:256:NDG:H8C3	2.28	0.64
2:B:124:LEU:HD12	2:B:205:GLY:HA2	1.79	0.64
1:A:158:SER:O	1:A:161:ALA:N	2.30	0.64
1:A:33:PHE:HD1	1:A:33:PHE:N	1.96	0.64
1:A:33:PHE:CD1	1:A:33:PHE:N	2.62	0.64
1:A:79:TYR:CZ	1:A:137:LEU:HD22	2.32	0.64
1:A:95:LEU:O	1:A:96:PHE:CD1	2.50	0.64
1:A:48:GLU:HG2	1:A:49:ALA:N	2.08	0.64
2:B:101:ASN:O	2:B:102:LEU:HD23	1.98	0.64
1:A:21:ILE:HG21	1:A:167:LEU:HD23	1.80	0.64
1:A:216:ILE:CB	1:A:217:PRO:HD2	2.24	0.63
4:B:258:NAG:O3	4:B:259:NAG:N2	2.32	0.63
1:A:59:ASN:HB3	1:A:134:VAL:HG21	1.81	0.63
2:B:96:ILE:HG22	2:B:97:ASN:N	2.13	0.63
1:A:208:PHE:HB2	1:A:224:THR:O	1.98	0.63
2:B:224:ASN:CB	2:B:226:LEU:HD13	2.28	0.63
2:B:121:ASP:C	2:B:121:ASP:OD1	2.37	0.63
1:A:141:GLY:O	1:A:142:ASN:CB	2.45	0.63
1:A:18:PHE:HD1	1:A:171:ARG:CZ	2.11	0.63
1:A:110:TYR:CB	1:A:111:PRO:HD3	2.29	0.62
2:B:244:THR:HG22	2:B:249:GLN:CD	2.20	0.62
1:A:162:ARG:HD3	1:A:193:TRP:CE2	2.34	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:166:ASN:ND2	2:B:166:ASN:H	1.98	0.61
1:A:12:THR:OG1	1:A:13:THR:N	2.31	0.61
2:B:51:ASP:OD1	2:B:52:GLY:N	2.33	0.61
1:A:125:LEU:HB2	1:A:180:PHE:CE1	2.36	0.61
1:A:49:ALA:O	1:A:51:ARG:N	2.32	0.61
1:A:225:ASN:HD22	1:A:227:ARG:N	1.87	0.61
1:A:58:THR:HG23	1:A:64:SER:OG	2.00	0.61
1:A:215:ALA:C	1:A:216:ILE:CG1	2.68	0.61
1:A:165:PRO:O	1:A:166:ILE:C	2.38	0.61
2:B:34:TRP:CG	2:B:35:PRO:HD2	2.35	0.60
1:A:58:THR:HG23	1:A:64:SER:CB	2.32	0.60
1:A:46:GLY:HA3	1:A:51:ARG:HH11	1.67	0.60
2:B:193:SER:O	2:B:194:VAL:CG2	2.49	0.60
2:B:224:ASN:HB2	2:B:226:LEU:CD1	2.32	0.60
1:A:85:SER:C	1:A:86:TYR:CD1	2.75	0.60
2:B:120:LEU:HD12	2:B:121:ASP:N	2.17	0.60
1:A:55:VAL:CG1	1:A:67:ALA:HB3	2.32	0.59
2:B:26:HIS:O	2:B:27:ASP:C	2.39	0.59
1:A:17:TYR:CZ	1:A:21:ILE:HD11	2.38	0.59
2:B:129:LEU:C	2:B:129:LEU:CD1	2.71	0.59
1:A:199:GLN:OE1	1:A:210:ASN:HB2	2.03	0.59
2:B:241:TYR:CD2	2:B:242:PRO:HD2	2.38	0.58
2:B:157:TRP:HZ3	2:B:237:GLN:HG2	1.68	0.58
2:B:21:ARG:HH21	2:B:32:GLN:HE21	1.52	0.58
2:B:221:ASN:HD22	2:B:221:ASN:C	2.07	0.58
1:A:49:ALA:C	1:A:51:ARG:H	2.07	0.58
2:B:172:TYR:HB3	2:B:174:ASP:OD1	2.03	0.58
2:B:189:SER:HB2	2:B:240:ILE:CD1	2.17	0.58
2:B:96:ILE:CG2	2:B:97:ASN:N	2.66	0.58
2:B:11:VAL:HG12	2:B:12:GLY:N	2.18	0.58
1:A:52:PHE:CD2	1:A:95:LEU:CD1	2.71	0.58
1:A:27:TYR:C	1:A:27:TYR:CD1	2.77	0.58
1:A:59:ASN:HD21	1:A:63:ASP:H	1.50	0.57
1:A:4:LEU:HD23	1:A:54:LEU:HB3	1.86	0.57
2:B:34:TRP:CG	2:B:35:PRO:CD	2.86	0.57
2:B:194:VAL:CG1	2:B:194:VAL:O	2.45	0.57
1:A:226:VAL:O	1:A:230:ILE:HG13	2.04	0.57
2:B:98:PRO:O	2:B:100:SER:N	2.38	0.57
2:B:224:ASN:CG	2:B:226:LEU:HD13	2.25	0.57
2:B:225:GLY:C	2:B:226:LEU:HD12	2.24	0.57
2:B:34:TRP:CD1	2:B:35:PRO:HD2	2.39	0.57
2:B:221:ASN:ND2	2:B:221:ASN:C	2.58	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:121:ASP:CG	2:B:123:THR:HG23	2.25	0.56
1:A:55:VAL:HG13	1:A:67:ALA:HB3	1.86	0.56
1:A:65:ILE:CD1	1:A:137:LEU:HB3	2.35	0.56
1:A:142:ASN:O	1:A:145:THR:N	2.38	0.56
1:A:117:ALA:HB2	1:A:147:ALA:CB	2.35	0.56
1:A:163:PHE:CE1	1:A:189:LEU:HB3	2.40	0.56
1:A:1:TYR:HE2	1:A:4:LEU:HG	1.71	0.56
2:B:12:GLY:O	2:B:15:GLY:N	2.30	0.55
2:B:67:THR:O	2:B:68:ALA:C	2.45	0.55
1:A:10:SER:HA	1:A:131:ILE:HD11	1.88	0.55
1:A:148:ARG:O	1:A:151:LEU:HB3	2.07	0.55
1:A:46:GLY:HA3	1:A:51:ARG:NH1	2.22	0.55
1:A:133:SER:O	1:A:137:LEU:HB2	2.06	0.55
2:B:197:ILE:HD12	2:B:238:ILE:HG22	1.88	0.55
1:A:79:TYR:CE1	1:A:86:TYR:HB2	2.42	0.55
1:A:138:ARG:O	1:A:139:PHE:CD1	2.60	0.55
1:A:52:PHE:CG	1:A:95:LEU:HD11	2.36	0.54
2:B:76:ASP:OD1	2:B:77:CYS:N	2.40	0.54
2:B:229:ASP:OD1	2:B:230:VAL:N	2.41	0.54
2:B:42:PRO:HG2	6:B:261:NAG:O7	2.08	0.54
2:B:56:SER:O	2:B:57:ASN:HB3	2.06	0.54
1:A:170:ALA:O	1:A:173:TYR:N	2.40	0.54
2:B:20:VAL:O	2:B:20:VAL:HG22	2.08	0.54
1:A:142:ASN:O	1:A:143:THR:C	2.45	0.54
2:B:197:ILE:CD1	2:B:238:ILE:HG22	2.38	0.54
1:A:238:PHE:CD1	1:A:239:VAL:N	2.76	0.54
2:B:11:VAL:CG1	2:B:12:GLY:N	2.72	0.53
2:B:158:VAL:HG23	2:B:158:VAL:O	2.07	0.53
1:A:106:PHE:HB2	1:A:112:ASP:OD2	2.08	0.53
1:A:18:PHE:O	1:A:19:ARG:C	2.46	0.53
1:A:204:THR:HG21	2:B:6:PRO:HD3	1.90	0.53
2:B:45:LEU:CD1	2:B:45:LEU:N	2.71	0.53
2:B:181:GLN:OE1	2:B:181:GLN:HA	2.08	0.53
1:A:129:GLN:HB3	1:A:152:ILE:HD13	1.90	0.53
1:A:53:VAL:CG1	1:A:69:ILE:HB	2.39	0.53
2:B:129:LEU:HD13	2:B:129:LEU:C	2.29	0.52
1:A:199:GLN:HE21	1:A:199:GLN:HA	1.75	0.52
2:B:20:VAL:HB	2:B:74:ILE:HD11	1.91	0.52
1:A:162:ARG:HB2	1:A:163:PHE:CD2	2.44	0.52
1:A:46:GLY:HA2	1:A:48:GLU:OE1	2.10	0.52
1:A:77:VAL:HG23	1:A:78:ALA:N	2.25	0.52
1:A:65:ILE:HG22	1:A:66:THR:N	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:14:ASN:HD22	2:B:178:ARG:HH22	1.58	0.51
1:A:199:GLN:NE2	1:A:199:GLN:HA	2.26	0.51
1:A:164:ASN:N	1:A:165:PRO:CD	2.73	0.51
2:B:30:GLN:NE2	2:B:114:THR:HG21	2.26	0.51
2:B:117:VAL:CG2	2:B:117:VAL:O	2.57	0.51
2:B:20:VAL:HG13	2:B:43:ASN:CB	2.41	0.51
1:A:124:PRO:O	1:A:129:GLN:HG2	2.11	0.51
1:A:157:ILE:HG22	1:A:158:SER:N	2.25	0.51
2:B:148:CYS:O	2:B:158:VAL:HA	2.10	0.51
1:A:104:LEU:H	1:A:104:LEU:HD22	1.76	0.51
1:A:59:ASN:C	1:A:59:ASN:HD22	2.14	0.51
2:B:44:GLN:C	2:B:45:LEU:HD12	2.31	0.51
2:B:211:TRP:CZ3	2:B:221:ASN:HB2	2.46	0.50
1:A:48:GLU:CG	1:A:49:ALA:H	2.07	0.50
1:A:106:PHE:CA	1:A:112:ASP:OD2	2.60	0.50
1:A:227:ARG:HH22	2:B:93:GLY:HA2	1.76	0.50
2:B:174:ASP:OD1	2:B:176:SER:OG	2.29	0.50
1:A:104:LEU:CD2	1:A:104:LEU:N	2.74	0.50
1:A:106:PHE:CB	1:A:112:ASP:OD2	2.60	0.50
1:A:17:TYR:CD2	1:A:174:ILE:HD12	2.45	0.50
2:B:42:PRO:CG	6:B:261:NAG:O7	2.60	0.50
1:A:143:THR:O	1:A:144:ARG:C	2.48	0.49
1:A:184:VAL:O	1:A:185:TYR:C	2.50	0.49
2:B:29:ASN:O	2:B:73:MET:HB2	2.12	0.49
1:A:188:GLU:OE1	1:A:215:ALA:HB3	2.13	0.49
1:A:104:LEU:H	1:A:104:LEU:CD2	2.26	0.49
2:B:185:GLN:HB3	2:B:199:ILE:CG2	2.42	0.49
2:B:189:SER:O	2:B:189:SER:OG	2.19	0.49
1:A:79:TYR:CZ	1:A:137:LEU:CD2	2.95	0.49
2:B:20:VAL:CG1	2:B:43:ASN:HA	2.43	0.49
1:A:13:THR:HG23	1:A:16:GLU:OE2	2.12	0.49
1:A:79:TYR:CE2	1:A:137:LEU:HD22	2.48	0.48
1:A:142:ASN:O	1:A:145:THR:HG22	2.13	0.48
2:B:124:LEU:CD1	2:B:205:GLY:HA2	2.42	0.48
2:B:115:LEU:HD22	2:B:115:LEU:N	2.28	0.48
2:B:7:THR:C	2:B:8:VAL:HG23	2.33	0.48
1:A:58:THR:HG23	1:A:64:SER:HB2	1.96	0.48
1:A:150:ILE:O	1:A:153:LEU:HB2	2.14	0.48
1:A:195:GLN:O	1:A:196:GLN:C	2.52	0.48
1:A:1:TYR:CE2	1:A:4:LEU:HG	2.48	0.48
1:A:124:PRO:O	1:A:125:LEU:HD23	2.14	0.48
1:A:128:ASP:O	1:A:131:ILE:N	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:ARG:HD2	1:A:51:ARG:O	2.13	0.48
2:B:75:PHE:CD1	2:B:76:ASP:N	2.82	0.48
1:A:158:SER:O	1:A:161:ALA:CB	2.62	0.48
1:A:9:THR:O	1:A:9:THR:HG23	2.14	0.48
1:A:25:ARG:HG3	1:A:235:ILE:CD1	2.30	0.47
1:A:106:PHE:HA	1:A:112:ASP:OD2	2.14	0.47
2:B:88:GLN:HE21	2:B:98:PRO:HG3	1.79	0.47
2:B:8:VAL:CG1	2:B:9:ARG:N	2.76	0.47
1:A:226:VAL:HG12	1:A:226:VAL:O	2.14	0.47
1:A:57:LEU:HD12	1:A:57:LEU:N	2.29	0.47
1:A:127:ILE:O	1:A:128:ASP:C	2.53	0.47
1:A:238:PHE:CD1	1:A:238:PHE:C	2.88	0.47
1:A:238:PHE:HD1	1:A:239:VAL:N	2.12	0.47
2:B:226:LEU:HB2	2:B:240:ILE:CG2	2.45	0.47
1:A:151:LEU:C	1:A:151:LEU:HD13	2.35	0.47
2:B:241:TYR:CD2	2:B:242:PRO:CD	2.97	0.47
1:A:167:LEU:O	1:A:168:TRP:C	2.53	0.47
2:B:29:ASN:HD22	2:B:30:GLN:H	1.61	0.47
1:A:88:LEU:N	1:A:88:LEU:HD23	2.29	0.47
2:B:16:MET:CE	2:B:35:PRO:HG3	2.44	0.46
2:B:90:TRP:CZ2	2:B:96:ILE:HD12	2.50	0.46
2:B:29:ASN:ND2	2:B:30:GLN:H	2.12	0.46
1:A:81:ALA:HB1	1:A:138:ARG:HD2	1.97	0.46
1:A:78:ALA:HB1	1:A:86:TYR:O	2.15	0.46
1:A:165:PRO:O	1:A:167:LEU:N	2.48	0.46
2:B:34:TRP:CD2	2:B:35:PRO:HD2	2.50	0.46
1:A:3:ARG:CZ	7:A:1010:HOH:O	2.64	0.46
1:A:85:SER:O	1:A:86:TYR:CD1	2.68	0.46
2:B:241:TYR:CD2	2:B:242:PRO:HG2	2.51	0.46
2:B:90:TRP:CH2	2:B:96:ILE:CD1	2.98	0.46
1:A:10:SER:H	1:A:12:THR:CG2	2.29	0.46
2:B:119:THR:O	2:B:120:LEU:C	2.50	0.46
1:A:21:ILE:HD12	1:A:167:LEU:HD22	1.98	0.46
1:A:61:GLY:C	1:A:63:ASP:H	2.17	0.46
2:B:57:ASN:C	2:B:59:SER:H	2.19	0.46
2:B:46:TRP:N	2:B:46:TRP:CD1	2.83	0.45
2:B:202:CYS:C	2:B:204:GLY:N	2.69	0.45
1:A:216:ILE:HG22	1:A:217:PRO:HD2	0.64	0.45
2:B:239:ILE:HG22	2:B:240:ILE:N	2.32	0.45
2:B:129:LEU:HD13	2:B:130:ALA:N	2.32	0.45
2:B:224:ASN:ND2	2:B:225:GLY:H	2.02	0.45
2:B:250:MET:C	2:B:251:TRP:CD1	2.89	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:244:THR:HG22	2:B:249:GLN:NE2	2.31	0.45
2:B:3:ALA:O	2:B:4:SER:CB	2.65	0.45
1:A:199:GLN:CA	1:A:199:GLN:HE21	2.28	0.45
1:A:119:HIS:ND1	1:A:121:LYS:HE2	2.31	0.45
2:B:188:THR:CG2	2:B:189:SER:N	2.78	0.45
2:B:101:ASN:C	2:B:102:LEU:HD23	2.37	0.45
1:A:124:PRO:C	1:A:125:LEU:HD23	2.37	0.45
1:A:170:ALA:O	1:A:171:ARG:C	2.54	0.45
1:A:10:SER:HB2	1:A:60:GLU:HG2	1.99	0.45
1:A:107:ASN:N	1:A:112:ASP:OD2	2.44	0.45
2:B:81:VAL:O	2:B:82:ARG:C	2.55	0.45
1:A:230:ILE:O	1:A:230:ILE:HG22	2.17	0.45
1:A:142:ASN:C	1:A:144:ARG:N	2.68	0.44
1:A:24:LEU:O	1:A:28:VAL:HG22	2.17	0.44
2:B:185:GLN:C	2:B:202:CYS:SG	2.96	0.44
1:A:150:ILE:O	1:A:153:LEU:N	2.50	0.44
1:A:133:SER:O	1:A:134:VAL:C	2.54	0.44
2:B:124:LEU:O	2:B:125:GLY:C	2.54	0.44
4:B:258:NAG:O3	4:B:259:NAG:C7	2.65	0.44
1:A:21:ILE:HG21	1:A:167:LEU:CD2	2.47	0.44
2:B:21:ARG:HH21	2:B:32:GLN:NE2	2.16	0.44
1:A:18:PHE:CD1	1:A:171:ARG:CZ	2.97	0.44
2:B:124:LEU:HD12	2:B:205:GLY:CA	2.45	0.44
1:A:50:ALA:O	1:A:71:VAL:HG21	2.18	0.44
1:A:183:ASP:O	1:A:184:VAL:C	2.53	0.44
2:B:139:VAL:HG12	2:B:255:PRO:CA	2.46	0.44
2:B:162:VAL:HG12	2:B:163:SER:H	1.80	0.44
1:A:95:LEU:O	1:A:96:PHE:CG	2.71	0.44
2:B:61:LEU:HD23	2:B:87:TRP:CE2	2.53	0.44
2:B:92:ASN:OD1	3:B:256:NDG:O	2.32	0.43
1:A:213:ARG:HG3	1:A:213:ARG:O	2.18	0.43
1:A:21:ILE:O	1:A:22:THR:C	2.57	0.43
2:B:45:LEU:N	2:B:45:LEU:HD12	2.33	0.43
2:B:169:TRP:CZ3	2:B:187:LEU:HD13	2.53	0.43
2:B:19:ASP:C	2:B:19:ASP:OD1	2.57	0.43
2:B:7:THR:C	2:B:8:VAL:CG2	2.87	0.43
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.67	0.43
1:A:169:ARG:O	1:A:170:ALA:C	2.56	0.43
1:A:70:ASP:O	1:A:71:VAL:C	2.57	0.43
2:B:231:ALA:O	2:B:232:ASN:CB	2.64	0.43
1:A:163:PHE:CD1	1:A:189:LEU:HB3	2.53	0.43
2:B:186:CYS:O	2:B:187:LEU:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:226:LEU:CB	2:B:240:ILE:CG2	2.97	0.42
1:A:165:PRO:O	1:A:168:TRP:N	2.52	0.42
1:A:204:THR:HG21	2:B:4:SER:O	2.19	0.42
2:B:98:PRO:C	2:B:100:SER:N	2.72	0.42
2:B:115:LEU:HD22	2:B:115:LEU:H	1.84	0.42
2:B:193:SER:C	2:B:194:VAL:HG23	2.39	0.42
1:A:47:VAL:O	1:A:47:VAL:HG12	2.20	0.42
2:B:226:LEU:HB3	2:B:240:ILE:HG22	2.02	0.42
4:B:259:NAG:H3	4:B:259:NAG:C8	2.43	0.42
1:A:147:ALA:O	1:A:148:ARG:C	2.58	0.42
2:B:22:ASP:O	2:B:23:ASP:C	2.54	0.42
2:B:7:THR:HA	2:B:47:THR:HA	2.00	0.42
1:A:10:SER:O	1:A:12:THR:HG23	2.19	0.42
2:B:165:GLN:HG2	2:B:165:GLN:H	1.58	0.42
2:B:114:THR:O	2:B:116:THR:HG22	2.20	0.42
1:A:65:ILE:CG2	1:A:66:THR:N	2.83	0.42
1:A:49:ALA:C	1:A:51:ARG:N	2.73	0.41
1:A:169:ARG:NH1	1:A:186:MET:HE3	2.35	0.41
1:A:200:VAL:HG12	1:A:200:VAL:O	2.19	0.41
2:B:132:ASN:HD22	4:B:258:NAG:C7	2.32	0.41
1:A:51:ARG:NE	1:A:72:THR:CG2	2.83	0.41
1:A:169:ARG:HE	1:A:173:TYR:HE2	1.69	0.41
1:A:167:LEU:O	1:A:169:ARG:N	2.53	0.41
1:A:167:LEU:C	1:A:169:ARG:N	2.73	0.41
2:B:110:ILE:O	2:B:111:LYS:C	2.57	0.41
1:A:135:THR:O	1:A:138:ARG:N	2.50	0.41
2:B:231:ALA:HB3	2:B:237:GLN:H	1.86	0.41
2:B:20:VAL:HG13	2:B:43:ASN:HB2	2.03	0.41
2:B:202:CYS:O	2:B:204:GLY:N	2.54	0.41
1:A:74:LEU:HD22	1:A:74:LEU:N	2.36	0.41
1:A:227:ARG:CZ	2:B:129:LEU:HD22	2.51	0.41
2:B:20:VAL:HB	2:B:74:ILE:CD1	2.51	0.41
1:A:166:ILE:HD11	1:A:186:MET:HG3	2.03	0.40
1:A:135:THR:C	1:A:137:LEU:N	2.74	0.40
1:A:110:TYR:CB	1:A:111:PRO:CD	2.99	0.40
2:B:99:ARG:HB2	2:B:99:ARG:HH11	1.87	0.40
1:A:164:ASN:HB3	2:B:252:LEU:HD13	2.02	0.40
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/240 (99%)	176 (74%)	49 (21%)	13 (6%)	3	42
2	B	253/255 (99%)	208 (82%)	34 (13%)	11 (4%)	4	49
All	All	491/495 (99%)	384 (78%)	83 (17%)	24 (5%)	3	45

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	50	ALA
1	A	90	GLY
1	A	91	PRO
1	A	140	PRO
1	A	216	ILE
2	B	165	GLN
2	B	193	SER
2	B	232	ASN
1	A	62	GLY
2	B	4	SER
2	B	39	ASN
1	A	165	PRO
1	A	206	GLY
2	B	162	VAL
2	B	194	VAL
2	B	231	ALA
1	A	44	GLY
2	B	27	ASP
1	A	73	ASN
2	B	98	PRO
2	B	197	ILE
1	A	30	SER
1	A	239	VAL

### 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	205/205 (100%)	177 (86%)	28 (14%)	5	36
2	B	211/211 (100%)	172 (82%)	39 (18%)	2	18
All	All	416/416 (100%)	349 (84%)	67 (16%)	3	27

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TYR
1	A	3	ARG
1	A	18	PHE
1	A	41	ARG
1	A	42	GLN
1	A	54	LEU
1	A	59	ASN
1	A	64	SER
1	A	72	THR
1	A	80	GLN
1	A	95	LEU
1	A	101	ARG
1	A	104	LEU
1	A	106	PHE
1	A	120	ARG
1	A	128	ASP
1	A	137	LEU
1	A	142	ASN
1	A	143	THR
1	A	144	ARG
1	A	151	LEU
1	A	167	LEU
1	A	168	TRP
1	A	171	ARG
1	A	180	PHE
1	A	216	ILE
1	A	224	THR
1	A	229	VAL
2	B	1	CYS

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Mol	Chain	Res	Type
2	B	6	PRO
2	B	16	MET
2	B	19	ASP
2	B	20	VAL
2	B	23	ASP
2	B	50	ARG
2	B	51	ASP
2	B	57	ASN
2	B	73	MET
2	B	76	ASP
2	B	83	GLU
2	B	92	ASN
2	B	99	ARG
2	B	101	ASN
2	B	107	SER
2	B	116	THR
2	B	118	GLN
2	B	119	THR
2	B	120	LEU
2	B	129	LEU
2	B	132	ASN
2	B	134	THR
2	B	155	SER
2	B	160	THR
2	B	164	GLN
2	B	165	GLN
2	B	166	ASN
2	B	167	ASP
2	B	176	SER
2	B	182	ASN
2	B	183	GLN
2	B	192	ASP
2	B	198	ASN
2	B	207	SER
2	B	216	GLU
2	B	221	ASN
2	B	224	ASN
2	B	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	59	ASN
1	A	115	GLN
1	A	199	GLN
1	A	225	ASN
2	B	14	ASN
2	B	29	ASN
2	B	30	GLN
2	B	32	GLN
2	B	39	ASN
2	B	101	ASN
2	B	118	GLN
2	B	126	GLN
2	B	145	ASN
2	B	164	GLN
2	B	166	ASN
2	B	182	ASN
2	B	198	ASN
2	B	221	ASN
2	B	224	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

7 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	NDG	B	256	3,2	12,14,15	1.35	3 (25%)	15,19,21	2.61	5 (33%)
3	NAG	B	257	3	12,14,15	0.50	0	15,19,21	2.10	3 (20%)
4	NAG	B	258	2,4	12,14,15	1.63	2 (16%)	15,19,21	2.71	3 (20%)
4	NAG	B	259	4	12,14,15	1.22	1 (8%)	15,19,21	4.13	9 (60%)
4	BMA	B	260	4	10,11,12	0.64	0	11,15,17	2.44	3 (27%)
6	NAG	B	261	2,6	12,14,15	0.93	0	15,19,21	2.99	6 (40%)
6	NAG	B	262	6	12,14,15	0.78	0	15,19,21	1.03	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	B	256	3,2	-	0/6/23/26	1/1/1/1
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	-	0/2/19/22	0/1/1/1
6	NAG	B	261	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	262	6	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	258	NAG	C3-C2	-3.09	1.46	1.52
4	B	259	NAG	O5-C5	-2.87	1.40	1.45
3	B	256	NDG	C2-N2	-2.72	1.43	1.46
4	B	258	NAG	O5-C5	-2.62	1.40	1.45
3	B	256	NDG	O-C5	-2.49	1.40	1.45
3	B	256	NDG	O4-C4	-2.48	1.37	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	259	NAG	O5-C5-C4	-12.25	95.10	110.65
4	B	258	NAG	O4-C4-C3	-8.88	90.44	110.35
6	B	261	NAG	O4-C4-C3	-7.87	92.70	110.35
3	B	256	NDG	O-C5-C6	6.75	114.07	106.98
4	B	260	BMA	O5-C5-C6	6.36	113.66	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	257	NAG	O5-C5-C6	6.19	113.48	106.98
3	B	256	NDG	O4-C4-C5	-5.58	94.58	109.28
4	B	259	NAG	O5-C5-C6	5.22	112.46	106.98
6	B	261	NAG	O5-C5-C6	4.96	112.19	106.98
4	B	259	NAG	O4-C4-C3	4.68	120.84	110.35
4	B	259	NAG	C3-C2-N2	-3.83	105.93	111.76
4	B	258	NAG	C3-C2-N2	-3.83	105.93	111.76
4	B	260	BMA	O5-C5-C4	3.59	115.21	110.65
4	B	259	NAG	C2-N2-C7	-3.45	117.30	123.09
6	B	261	NAG	O3-C3-C2	3.30	116.02	109.09
6	B	261	NAG	C3-C4-C5	3.14	115.81	110.20
6	B	261	NAG	O4-C4-C5	3.10	117.46	109.28
4	B	260	BMA	C3-C4-C5	2.80	115.21	110.20
4	B	259	NAG	C3-C4-C5	-2.74	105.30	110.20
3	B	256	NDG	C4-C3-C2	-2.66	104.80	111.32
3	B	257	NAG	O5-C5-C4	2.64	114.01	110.65
3	B	256	NDG	C2-N2-C7	-2.54	118.82	123.09
6	B	261	NAG	C6-C5-C4	-2.53	106.88	113.00
4	B	259	NAG	O7-C7-C8	-2.51	117.14	122.04
3	B	257	NAG	C6-C5-C4	-2.45	107.08	113.00
6	B	262	NAG	C2-N2-C7	-2.24	119.32	123.09
4	B	259	NAG	C4-C3-C2	-2.21	105.91	111.32
3	B	256	NDG	O-C5-C4	-2.15	107.93	110.65
4	B	259	NAG	C8-C7-N2	2.08	120.18	116.11
4	B	258	NAG	O5-C5-C4	-2.06	108.04	110.65

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	256	NDG	C1-C2-C3-C4-C5-O

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1002	1	12,14,15	0.56	0	15,19,21	1.38	2 (13%)

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	1002	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	NAG	O5-C5-C6	3.12	110.26	106.98
5	A	1002	NAG	O5-C5-C4	2.23	113.48	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	240/240 (100%)	-0.15	1 (0%) 90 79	27, 62, 100, 127	0
2	B	255/255 (100%)	-0.18	1 (0%) 90 79	27, 50, 91, 115	0
All	All	495/495 (100%)	-0.17	2 (0%) 83 79	27, 55, 97, 127	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	TYR	2.3
2	B	1	CYS	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	B	261	14/15	0.59	4.05	116,130,141,142	0
4	NAG	B	259	14/15	0.39	0.41	109,123,132,133	0
4	NAG	B	258	14/15	0.26	0.23	65,70,79,91	0
3	NDG	B	256	14/15	0.21	0.15	99,114,119,127	0
4	BMA	B	260	11/12	0.39	-	142,146,147,147	0
3	NAG	B	257	14/15	0.45	-	136,141,151,152	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	262	14/15	0.57	-	147,151,155,157	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1002	14/15	0.43	7.51	123,130,134,134	0

## 6.5 Other polymers

There are no such residues in this entry.