Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:23 AM GMT

PDB ID	:	2AAI
Title	:	Crystallographic refinement of ricin to 2.5 Angstroms
Authors	:	Rutenber, E.; Katzin, B.J.; Montfort, W.; Villafranca, J.E.; Ernst, S.R.; Collins, E.J.; Mlsna, D.; Monzingo, A.F.; Ready, M.P.; Robertus, J.D.
Deposited on	:	1993-09-07
Resolution	:	2.50 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

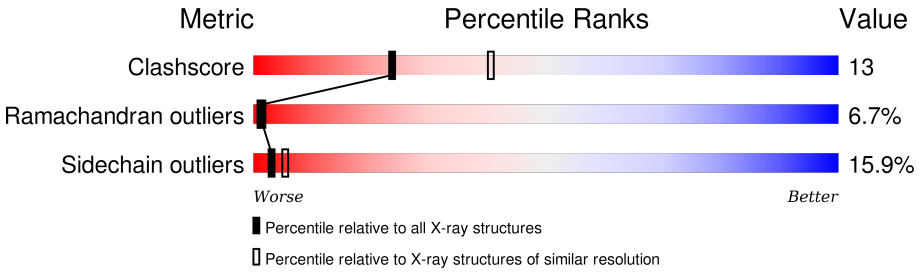
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 >=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 <=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	267	51% 30% 14% 5%
2	B	262	53% 31% 14% .

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	NDG	B	270	X	-	-	-
4	NDG	B	280	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4440 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 RICIN (A CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2114	1342	372	395	5			

- Molecule 2 is a protein called RICIN (B CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2035	1273	357	393	12			

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			61	34	2	25		
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	62	Total	O	0	0
			62	62		

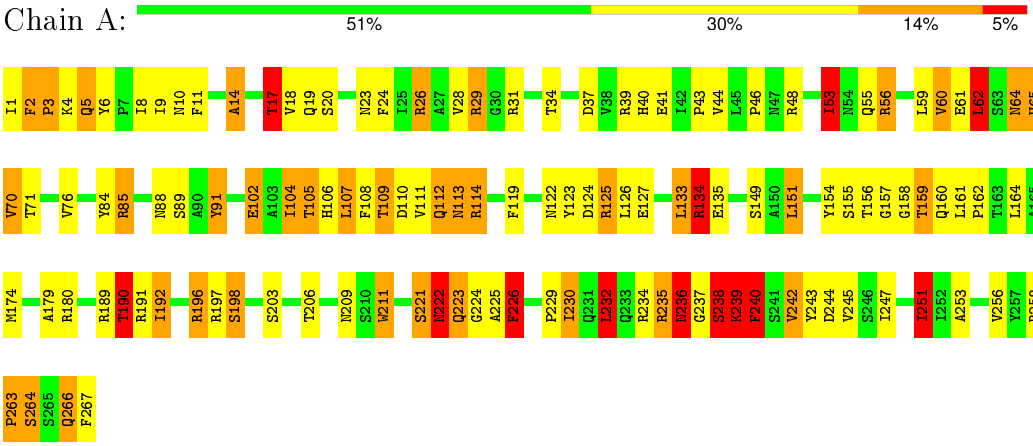
3 Residue-property plots (i)

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.

Note EDS was not executed.

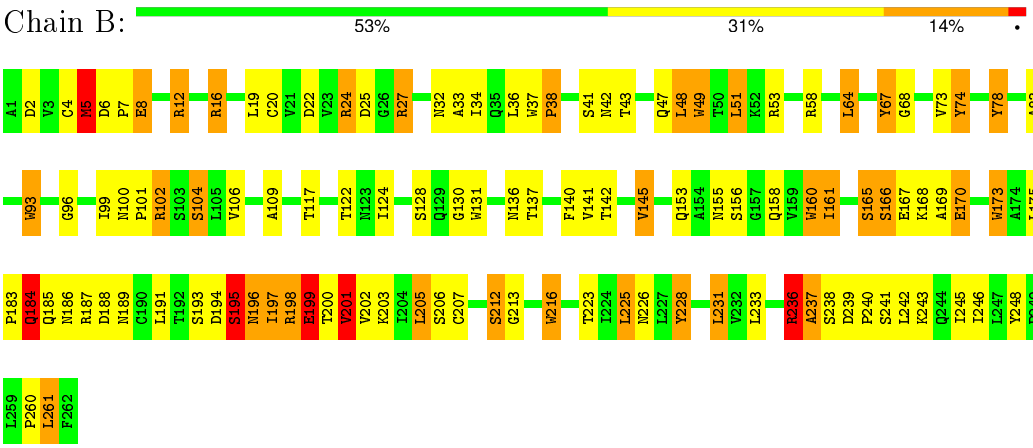
- Molecule 1: RICIN (A CHAIN)

Chain A:



- Molecule 2: RICIN (B CHAIN)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.74Å 78.49Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: BGC, NAG, NDG, GAL, BMA, MAN

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	1.04	0/2162	2.00	89/2941 (3.0%)
2	B	1.04	2/2080 (0.1%)	2.12	86/2842 (3.0%)
All	All	1.04	2/4242 (0.0%)	2.06	175/5783 (3.0%)

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	3
2	B	0	3
4	B	2	0
All	All	2	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	131	TRP	CD1-NE1	-5.74	1.28	1.38
2	B	195	SER	CA-CB	5.14	1.60	1.52

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	200	THR	CA-C-N	-13.18	88.21	117.20
1	A	234	ARG	NE-CZ-NH2	-13.11	113.74	120.30
1	A	234	ARG	NE-CZ-NH1	11.23	125.91	120.30
2	B	37	TRP	CD1-CG-CD2	10.77	114.92	106.30
1	A	258	ARG	NE-CZ-NH1	10.62	125.61	120.30
2	B	170	GLU	CA-C-N	-10.60	93.88	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	258	TRP	CD1-CG-CD2	10.53	114.72	106.30
2	B	216	TRP	CD1-CG-CD2	10.32	114.56	106.30
2	B	258	TRP	CG-CD2-CE3	10.12	143.01	133.90
1	A	236	ASN	CA-C-N	10.08	136.35	116.20
1	A	125	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	258	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	B	212	SER	CA-C-N	9.67	135.54	116.20
2	B	258	TRP	CB-CG-CD1	-9.46	114.70	127.00
2	B	131	TRP	CD1-CG-CD2	9.46	113.86	106.30
2	B	187	ARG	NE-CZ-NH1	9.29	124.94	120.30
2	B	198	ARG	CA-CB-CG	9.13	133.48	113.40
2	B	131	TRP	CE2-CD2-CG	-8.96	100.13	107.30
2	B	160	TRP	CD1-CG-CD2	8.88	113.41	106.30
2	B	90	TRP	CG-CD2-CE3	8.72	141.75	133.90
2	B	258	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	A	114	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	B	200	THR	O-C-N	8.44	136.21	122.70
1	A	235	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	125	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	B	37	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	A	196	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	65	HIS	N-CA-CB	8.16	125.29	110.60
1	A	226	PHE	CB-CG-CD2	-7.95	115.23	120.80
2	B	212	SER	O-C-N	-7.93	109.72	123.20
1	A	29	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	B	27	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	240	PHE	N-CA-C	7.89	132.30	111.00
2	B	90	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	A	65	HIS	CA-C-N	-7.82	99.99	117.20
1	A	197	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	17	THR	N-CA-CB	-7.77	95.54	110.30
2	B	216	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	A	6	TYR	CB-CG-CD2	-7.70	116.38	121.00
2	B	43	THR	CA-CB-CG2	7.69	123.17	112.40
1	A	159	THR	CA-CB-CG2	7.69	123.17	112.40
2	B	173	TRP	CD1-CG-CD2	7.57	112.35	106.30
2	B	24	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	B	16	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	A	133	LEU	CA-CB-CG	7.48	132.51	115.30
2	B	248	TYR	CB-CG-CD1	-7.44	116.54	121.00
2	B	202	VAL	CG1-CB-CG2	-7.39	99.07	110.90
2	B	216	TRP	CG-CD1-NE1	-7.38	102.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	TRP	CD1-CG-CD2	7.36	112.19	106.30
2	B	90	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	226	PHE	N-CA-C	7.33	130.80	111.00
1	A	245	VAL	CA-C-N	7.30	133.25	117.20
2	B	258	TRP	CG-CD1-NE1	-7.27	102.83	110.10
2	B	104	SER	O-C-N	7.25	134.31	122.70
2	B	53	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	B	43	THR	N-CA-CB	-7.15	96.71	110.30
1	A	174	MET	CG-SD-CE	7.13	111.62	100.20
1	A	192	ILE	CG1-CB-CG2	-7.09	95.79	111.40
1	A	242	VAL	CG1-CB-CG2	-7.07	99.58	110.90
2	B	198	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	114	ARG	NE-CZ-NH2	-7.03	116.78	120.30
2	B	173	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	B	236	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	A	28	VAL	CG1-CB-CG2	-6.99	99.72	110.90
2	B	160	TRP	CE2-CD2-CG	-6.93	101.75	107.30
2	B	37	TRP	CG-CD1-NE1	-6.90	103.20	110.10
1	A	266	GLN	N-CA-C	6.84	129.48	111.00
2	B	74	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	64	ASN	CA-C-N	6.74	132.03	117.20
2	B	102	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	251	ILE	CG1-CB-CG2	-6.68	96.71	111.40
1	A	65	HIS	O-C-N	6.65	133.34	122.70
2	B	93	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	A	223	GLN	N-CA-C	-6.61	93.16	111.00
1	A	226	PHE	CB-CA-C	-6.54	97.31	110.40
2	B	49	TRP	CE2-CD2-CG	-6.53	102.08	107.30
2	B	49	TRP	CD1-CG-CD2	6.52	111.51	106.30
1	A	226	PHE	CA-C-N	-6.50	102.89	117.20
1	A	180	ARG	NE-CZ-NH2	-6.49	117.05	120.30
2	B	58	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	60	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	A	232	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	211	TRP	CE2-CD2-CG	-6.38	102.19	107.30
2	B	225	LEU	CA-CB-CG	6.36	129.92	115.30
2	B	90	TRP	CB-CG-CD1	-6.34	118.76	127.00
2	B	24	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	71	THR	CA-CB-CG2	6.30	121.23	112.40
1	A	226	PHE	CA-CB-CG	6.30	129.03	113.90
1	A	62	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	222	ASN	OD1-CG-ND2	-6.26	107.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	237	ALA	CB-CA-C	-6.25	100.72	110.10
1	A	85	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	113	ASN	CA-C-N	-6.21	103.53	117.20
1	A	197	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	64	ASN	CB-CG-ND2	6.13	131.42	116.70
1	A	245	VAL	O-C-N	-6.12	112.91	122.70
2	B	131	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	B	43	THR	CA-CB-OG1	-6.05	96.29	109.00
1	A	238	SER	CA-C-N	-6.04	103.90	117.20
2	B	137	THR	N-CA-CB	-6.04	98.83	110.30
1	A	236	ASN	O-C-N	-6.02	112.96	123.20
2	B	131	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	A	14	ALA	CA-C-N	6.01	128.22	116.20
2	B	22	ASP	O-C-N	-6.00	113.10	122.70
1	A	44	VAL	CG1-CB-CG2	-5.95	101.37	110.90
1	A	238	SER	C-N-CA	5.94	136.55	121.70
1	A	67	GLU	N-CA-C	5.91	126.97	111.00
1	A	91	TYR	CB-CG-CD2	-5.89	117.47	121.00
2	B	160	TRP	CG-CD1-NE1	-5.87	104.23	110.10
2	B	90	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	A	53	ILE	CB-CA-C	-5.81	99.99	111.60
2	B	145	VAL	CG1-CB-CG2	-5.80	101.62	110.90
2	B	173	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	A	56	ARG	N-CA-C	5.76	126.56	111.00
2	B	102	ARG	CA-C-N	-5.76	104.53	117.20
2	B	93	TRP	CD1-CG-CD2	5.75	110.90	106.30
1	A	56	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	B	67	TYR	CB-CG-CD1	-5.72	117.57	121.00
2	B	198	ARG	CA-C-N	-5.70	104.67	117.20
2	B	250	LEU	CA-CB-CG	5.70	128.40	115.30
2	B	48	LEU	CA-CB-CG	5.66	128.33	115.30
2	B	106	VAL	N-CA-CB	-5.66	99.05	111.50
1	A	84	TYR	CB-CG-CD2	-5.64	117.62	121.00
2	B	200	THR	CA-C-O	5.61	131.87	120.10
2	B	165	SER	N-CA-C	-5.59	95.91	111.00
1	A	238	SER	O-C-N	5.59	131.64	122.70
1	A	197	ARG	N-CA-C	-5.55	96.01	111.00
1	A	239	LYS	N-CA-C	5.54	125.95	111.00
2	B	169	ALA	N-CA-C	-5.54	96.05	111.00
1	A	113	ASN	O-C-N	5.52	131.54	122.70
1	A	180	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	155	ASN	CA-C-N	-5.50	105.10	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ASN	O-C-N	-5.49	113.92	122.70
1	A	65	HIS	CB-CA-C	-5.47	99.46	110.40
1	A	71	THR	CA-CB-OG1	-5.47	97.52	109.00
1	A	127	GLU	CA-CB-CG	5.45	125.38	113.40
2	B	22	ASP	N-CA-CB	-5.44	100.80	110.60
1	A	159	THR	OG1-CB-CG2	-5.42	97.54	110.00
1	A	123	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	235	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	29	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	B	184	GLN	CA-CB-CG	-5.37	101.59	113.40
1	A	134	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	37	ASP	CB-CG-OD1	5.34	123.10	118.30
2	B	173	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	26	ARG	CD-NE-CZ	-5.33	116.14	123.60
2	B	239	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	76	VAL	N-CA-CB	-5.33	99.78	111.50
1	A	2	PHE	N-CA-CB	-5.26	101.13	110.60
1	A	190	THR	CA-CB-CG2	5.25	119.75	112.40
1	A	192	ILE	CA-CB-CG1	5.23	120.94	111.00
2	B	131	TRP	CB-CG-CD1	-5.22	120.21	127.00
2	B	216	TRP	CG-CD2-CE3	5.22	138.60	133.90
2	B	22	ASP	CA-C-N	5.21	128.66	117.20
2	B	205	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	221	SER	CA-CB-OG	5.18	125.18	111.20
2	B	176	TYR	CB-CG-CD2	-5.18	117.89	121.00
2	B	104	SER	CA-C-N	-5.17	105.82	117.20
1	A	89	SER	N-CA-CB	-5.16	102.76	110.50
2	B	161	ILE	CA-CB-CG1	-5.16	101.20	111.00
1	A	230	ILE	CG1-CB-CG2	-5.14	100.10	111.40
2	B	102	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	B	109	ALA	CA-C-N	5.09	128.40	117.20
2	B	184	GLN	N-CA-C	5.09	124.75	111.00
1	A	113	ASN	CA-CB-CG	-5.09	102.21	113.40
1	A	240	PHE	CB-CG-CD2	-5.08	117.25	120.80
2	B	41	SER	CA-C-N	-5.06	106.06	117.20
1	A	211	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	238	SER	N-CA-C	5.05	124.65	111.00
1	A	104	ILE	N-CA-CB	-5.04	99.21	110.80
1	A	109	THR	CA-CB-CG2	5.04	119.45	112.40
2	B	231	LEU	CA-CB-CG	5.03	126.88	115.30
2	B	68	GLY	O-C-N	-5.03	114.65	122.70
2	B	201	VAL	N-CA-C	-5.03	97.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	TRP	CG-CD2-CE3	5.03	138.43	133.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	270	NDG	C1
4	B	280	NDG	C1

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLY	Mainchain
1	A	262	PRO	Peptide
1	A	56	ARG	Sidechain
2	B	170	GLU	Mainchain
2	B	199	GLU	Mainchain
2	B	74	TYR	Sidechain

5.2 Too-close contacts (i)

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	2114	0	2083	63	0
2	B	2035	0	1974	51	0
3	B	46	0	42	0	0
4	B	122	0	104	1	0
5	A	61	0	0	2	0
5	B	62	0	0	4	0
All	All	4440	0	4203	112	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 13.

All (112) 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:1:ILE:HG23	1:A:2:PHE:H	1.51	0.76
1:A:236:ASN:HD21	1:A:238:SER:HB2	1.53	0.73
2:B:193:SER:HA	2:B:201:VAL:O	1.94	0.67
1:A:225:ALA:HB1	1:A:226:PHE:CD1	2.29	0.67
2:B:198:ARG:HB3	2:B:199:GLU:OE1	1.94	0.67
1:A:224:GLY:HA2	5:A:625:HOH:O	1.94	0.67
1:A:1:ILE:HG12	1:A:53:ILE:HD11	1.76	0.66
2:B:102:ARG:HB2	5:B:671:HOH:O	1.95	0.66
1:A:1:ILE:HG23	1:A:2:PHE:N	2.13	0.62
1:A:225:ALA:HB3	1:A:244:ASP:HA	1.81	0.62
2:B:165:SER:HB3	2:B:168:LYS:HB2	1.82	0.62
2:B:201:VAL:HG12	2:B:203:LYS:NZ	2.15	0.61
1:A:260:ALA:O	2:B:4:CYS:SG	2.58	0.61
1:A:266:GLN:HG3	1:A:267:PHE:N	2.15	0.61
2:B:12:ARG:HD3	2:B:20:CYS:SG	2.42	0.60
1:A:229:PRO:HB3	1:A:243:TYR:CE2	2.37	0.59
1:A:53:ILE:HG21	1:A:106:HIS:CD2	2.37	0.58
2:B:16:ARG:HH11	2:B:128:SER:HB3	1.67	0.58
1:A:91:TYR:OH	1:A:155:SER:HA	2.04	0.58
2:B:78:TYR:HD2	2:B:83:ALA:HB2	1.69	0.57
1:A:154:TYR:CE1	1:A:159:THR:HG23	2.39	0.57
1:A:236:ASN:ND2	1:A:238:SER:HB2	2.18	0.56
1:A:119:PHE:HB2	1:A:125:ARG:HG2	1.86	0.56
2:B:182:ARG:NE	2:B:207:CYS:SG	2.78	0.56
2:B:236:ARG:HD3	2:B:242:LEU:HD13	1.87	0.55
1:A:40:HIS:H	1:A:267:PHE:HB3	1.72	0.55
2:B:67:TYR:HB3	2:B:73:VAL:HB	1.89	0.55
1:A:9:ILE:HD11	1:A:31:ARG:HG2	1.87	0.54
2:B:145:VAL:HG21	2:B:261:LEU:HD12	1.90	0.54
1:A:66:ALA:O	1:A:67:GLU:HB2	2.07	0.54
2:B:141:VAL:HA	2:B:173:TRP:O	2.07	0.53
2:B:153:GLN:HG2	5:B:651:HOH:O	2.08	0.53
1:A:221:SER:O	1:A:222:ASN:HB2	2.08	0.53
1:A:39:ARG:HA	1:A:267:PHE:HB2	1.90	0.53
1:A:88:ASN:HB2	1:A:112:GLN:OE1	2.09	0.52
1:A:206:THR:HG22	1:A:232:LEU:HD12	1.90	0.52
1:A:266:GLN:HG3	1:A:267:PHE:CG	2.45	0.52
1:A:102:GLU:O	1:A:105:THR:HB	2.10	0.52
1:A:53:ILE:HG21	1:A:106:HIS:HD2	1.75	0.52
2:B:99:ILE:HD11	2:B:104:SER:HA	1.92	0.52
2:B:90:TRP:CZ3	2:B:100:ASN:HB2	2.45	0.51
1:A:60:VAL:HG12	1:A:62:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ARG:O	2:B:32:ASN:ND2	2.43	0.51
1:A:29:ARG:HD2	1:A:179:ALA:O	2.10	0.51
1:A:39:ARG:HA	1:A:267:PHE:CB	2.42	0.49
1:A:23:ASN:HA	1:A:26:ARG:HD3	1.93	0.49
2:B:90:TRP:CE3	2:B:100:ASN:HB2	2.47	0.49
2:B:78:TYR:CD2	2:B:83:ALA:HB2	2.48	0.48
1:A:64:ASN:HB3	1:A:66:ALA:HB3	1.95	0.48
2:B:201:VAL:HG12	2:B:203:LYS:HZ2	1.78	0.47
2:B:238:SER:O	2:B:240:PRO:HD3	2.14	0.47
1:A:229:PRO:HA	1:A:242:VAL:O	2.14	0.47
2:B:161:ILE:HD12	2:B:258:TRP:CZ3	2.50	0.47
2:B:34:ILE:HD12	2:B:49:TRP:HH2	1.79	0.47
2:B:12:ARG:HH11	2:B:12:ARG:CG	2.28	0.47
2:B:8:GLU:HA	2:B:51:LEU:O	2.15	0.47
2:B:93:TRP:CZ2	4:B:271:NAG:H83	2.49	0.47
1:A:224:GLY:O	1:A:225:ALA:HB2	2.15	0.47
2:B:186:ASN:OD1	2:B:189:ASN:ND2	2.48	0.47
1:A:222:ASN:HB3	1:A:223:GLN:O	2.15	0.46
1:A:40:HIS:O	1:A:41:GLU:HB2	2.15	0.46
2:B:191:LEU:HD23	2:B:216:TRP:CE2	2.50	0.46
1:A:70:VAL:HG11	1:A:151:LEU:HD23	1.97	0.46
2:B:161:ILE:HD12	2:B:258:TRP:HZ3	1.80	0.45
2:B:124:ILE:O	2:B:212:SER:HB3	2.16	0.45
1:A:154:TYR:CD1	1:A:159:THR:HA	2.52	0.45
2:B:201:VAL:HA	2:B:203:LYS:HZ2	1.81	0.45
2:B:213:GLY:HA2	2:B:226:ASN:HD21	1.82	0.45
2:B:175:LEU:HD22	2:B:181:ILE:HG12	1.99	0.45
2:B:233:LEU:HD22	2:B:245:ILE:HG21	1.99	0.45
1:A:191:ARG:NH2	1:A:198:SER:HB3	2.31	0.45
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.63	0.45
2:B:160:TRP:CD2	2:B:243:LYS:HD3	2.52	0.45
1:A:18:VAL:HB	1:A:189:ARG:HG3	1.98	0.45
2:B:223:THR:HG21	2:B:250:LEU:HD23	1.99	0.44
1:A:251:ILE:HD13	2:B:260:PRO:HG2	2.00	0.44
1:A:11:PHE:HB2	1:A:24:PHE:CD1	2.53	0.44
2:B:199:GLU:HA	2:B:246:ILE:HB	2.00	0.43
2:B:228:TYR:N	5:B:675:HOH:O	2.45	0.43
1:A:43:PRO:HD2	1:A:253:ALA:O	2.18	0.43
2:B:183:PRO:O	2:B:185:GLN:N	2.51	0.43
1:A:191:ARG:HH21	1:A:198:SER:HB3	1.83	0.43
1:A:4:LYS:NZ	1:A:55:GLN:HE22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLY:O	2:B:130:GLY:HA2	2.19	0.43
1:A:211:TRP:CH2	1:A:256:VAL:HB	2.53	0.43
2:B:19:LEU:HB2	2:B:36:LEU:HG	2.01	0.43
1:A:190:THR:HG23	1:A:196:ARG:HH12	1.84	0.42
1:A:122:ASN:HD22	1:A:124:ASP:HB2	1.84	0.42
2:B:100:ASN:ND2	5:B:671:HOH:O	2.52	0.42
1:A:4:LYS:O	1:A:5:GLN:HG2	2.19	0.42
2:B:64:LEU:HD23	2:B:90:TRP:NE1	2.34	0.42
2:B:233:LEU:HD22	2:B:245:ILE:CG2	2.49	0.42
1:A:236:ASN:O	1:A:236:ASN:ND2	2.52	0.42
1:A:154:TYR:HD1	1:A:159:THR:HA	1.84	0.41
2:B:213:GLY:CA	2:B:226:ASN:HD21	2.32	0.41
1:A:39:ARG:HG2	1:A:267:PHE:HD2	1.84	0.41
1:A:161:LEU:HB3	1:A:162:PRO:HD3	2.02	0.41
1:A:10:ASN:HB3	1:A:61:GLU:HB3	2.03	0.41
1:A:8:ILE:HA	1:A:59:LEU:O	2.21	0.41
1:A:1:ILE:CG2	1:A:2:PHE:H	2.27	0.41
2:B:140:PHE:CD2	2:B:142:THR:HG23	2.56	0.41
1:A:166:ARG:O	1:A:170:ILE:HG13	2.21	0.41
1:A:238:SER:OG	1:A:239:LYS:HD3	2.20	0.41
1:A:267:PHE:HE2	5:A:310:HOH:O	2.02	0.41
2:B:195:SER:O	2:B:197:ILE:N	2.53	0.41
1:A:108:PHE:O	1:A:111:VAL:HG22	2.21	0.41
1:A:68:LEU:HD12	1:A:149:SER:HA	2.02	0.41
1:A:17:THR:HG22	1:A:20:SER:H	1.85	0.41
1:A:107:LEU:HA	1:A:107:LEU:HD13	1.91	0.41
1:A:119:PHE:HA	1:A:125:ARG:NH1	2.36	0.41
2:B:33:ALA:HB1	2:B:117:THR:HG23	2.03	0.41
2:B:2:ASP:HB3	2:B:5:MET:SD	2.62	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	265/267 (99%)	231 (87%)	17 (6%)	17 (6%)	2 1
2	B	260/262 (99%)	222 (85%)	20 (8%)	18 (7%)	1 1
All	All	525/529 (99%)	453 (86%)	37 (7%)	35 (7%)	1 1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	14	ALA
1	A	66	ALA
1	A	67	GLU
1	A	222	ASN
1	A	226	PHE
1	A	239	LYS
1	A	240	PHE
1	A	263	PRO
2	B	42	ASN
2	B	166	SER
2	B	184	GLN
2	B	195	SER
2	B	199	GLU
2	B	228	TYR
1	A	105	THR
1	A	134	ARG
1	A	237	GLY
1	A	264	SER
2	B	5	MET
2	B	25	ASP
2	B	196	ASN
2	B	201	VAL
2	B	206	SER
1	A	5	GLN
1	A	112	GLN
1	A	157	GLY
2	B	197	ILE
2	B	237	ALA
1	A	156	THR
2	B	7	PRO
2	B	84	ALA
2	B	85	THR
2	B	38	PRO
2	B	101	PRO

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	226/226 (100%)	184 (81%)	42 (19%)	2 3
2	B	227/227 (100%)	197 (87%)	30 (13%)	5 9
All	All	453/453 (100%)	381 (84%)	72 (16%)	3 5

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	17	THR
1	A	19	GLN
1	A	34	THR
1	A	46	PRO
1	A	48	ARG
1	A	53	ILE
1	A	62	LEU
1	A	65	HIS
1	A	67	GLU
1	A	70	VAL
1	A	85	ARG
1	A	102	GLU
1	A	104	ILE
1	A	107	LEU
1	A	109	THR
1	A	110	ASP
1	A	113	ASN
1	A	114	ARG
1	A	126	LEU
1	A	133	LEU
1	A	135	GLU
1	A	151	LEU
1	A	160	GLN
1	A	164	LEU
1	A	190	THR
1	A	192	ILE

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Mol	Chain	Res	Type
1	A	198	SER
1	A	203	SER
1	A	222	ASN
1	A	226	PHE
1	A	230	ILE
1	A	232	LEU
1	A	235	ARG
1	A	236	ASN
1	A	238	SER
1	A	239	LYS
1	A	240	PHE
1	A	247	ILE
1	A	251	ILE
1	A	263	PRO
1	A	264	SER
2	B	5	MET
2	B	6	ASP
2	B	8	GLU
2	B	12	ARG
2	B	24	ARG
2	B	38	PRO
2	B	47	GLN
2	B	48	LEU
2	B	51	LEU
2	B	64	LEU
2	B	78	TYR
2	B	122	THR
2	B	136	ASN
2	B	156	SER
2	B	158	GLN
2	B	166	SER
2	B	167	GLU
2	B	184	GLN
2	B	188	ASP
2	B	194	ASP
2	B	196	ASN
2	B	199	GLU
2	B	201	VAL
2	B	205	LEU
2	B	225	LEU
2	B	231	LEU
2	B	236	ARG

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Mol	Chain	Res	Type
2	B	241	SER
2	B	251	HIS
2	B	261	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	98	GLN
1	A	128	GLN
1	A	132	ASN
1	A	173	GLN
1	A	209	ASN
1	A	233	GLN
1	A	236	ASN
2	B	55	ASN
2	B	186	ASN
2	B	189	ASN
2	B	196	ASN
2	B	220	ASN
2	B	226	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

14 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	GAL	B	264	3	11,11,12	1.04	1 (9%)	14,15,17	1.49	2 (14%)
3	BGC	B	265	3	12,12,12	1.27	1 (8%)	17,17,17	1.72	4 (23%)
3	GAL	B	267	3	11,11,12	1.11	1 (9%)	14,15,17	2.04	6 (42%)
3	BGC	B	268	3	12,12,12	1.21	0	17,17,17	2.15	3 (17%)
4	NDG	B	270	2,4	14,14,15	1.26	2 (14%)	15,19,21	1.53	2 (13%)
4	NAG	B	271	4	14,14,15	1.71	6 (42%)	15,19,21	3.35	5 (33%)
4	BMA	B	272	4	11,11,12	1.55	2 (18%)	14,15,17	4.11	8 (57%)
4	MAN	B	273	4	11,11,12	2.18	4 (36%)	14,15,17	2.40	8 (57%)
4	MAN	B	274	4	11,11,12	1.48	1 (9%)	14,15,17	1.08	1 (7%)
4	NDG	B	280	2,4	14,14,15	0.86	0	15,19,21	1.08	2 (13%)
4	NAG	B	281	4	14,14,15	1.06	1 (7%)	15,19,21	2.58	5 (33%)
4	BMA	B	282	4	11,11,12	1.81	2 (18%)	14,15,17	2.08	6 (42%)
4	MAN	B	283	4	11,11,12	1.38	0	14,15,17	4.00	9 (64%)
4	MAN	B	284	4	11,11,12	1.24	1 (9%)	14,15,17	3.12	12 (85%)

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	GAL	B	264	3	-	0/2/19/22	0/1/1/1
3	BGC	B	265	3	-	0/2/22/22	0/1/1/1
3	GAL	B	267	3	-	0/2/19/22	0/1/1/1
3	BGC	B	268	3	-	0/2/22/22	0/1/1/1
4	NDG	B	270	2,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	271	4	-	0/6/23/26	0/1/1/1
4	BMA	B	272	4	-	0/2/19/22	0/1/1/1
4	MAN	B	273	4	-	0/2/19/22	0/1/1/1
4	MAN	B	274	4	-	0/2/19/22	0/1/1/1
4	NDG	B	280	2,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	281	4	-	1/6/23/26	0/1/1/1
4	BMA	B	282	4	-	0/2/19/22	0/1/1/1
4	MAN	B	283	4	-	0/2/19/22	1/1/1/1
4	MAN	B	284	4	-	0/2/19/22	1/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	274	MAN	C2-C3	-4.23	1.46	1.52
3	B	264	GAL	C2-C3	-2.69	1.48	1.52
4	B	270	NDG	O-C1	-2.42	1.39	1.43
4	B	281	NAG	O5-C1	-2.30	1.39	1.43
4	B	270	NDG	C1-C2	-2.17	1.49	1.52
4	B	271	NAG	C4-C3	2.11	1.57	1.52
4	B	271	NAG	O4-C4	2.12	1.48	1.43
4	B	272	BMA	O3-C3	2.13	1.48	1.43
3	B	265	BGC	O1-C1	2.16	1.47	1.39
4	B	271	NAG	O3-C3	2.16	1.48	1.43
3	B	267	GAL	O4-C4	2.27	1.48	1.43
4	B	284	MAN	C2-C3	2.29	1.55	1.52
4	B	273	MAN	O3-C3	2.41	1.48	1.43
4	B	273	MAN	C6-C5	2.43	1.60	1.51
4	B	271	NAG	O5-C5	2.50	1.49	1.43
4	B	273	MAN	C1-C2	2.77	1.58	1.52
4	B	271	NAG	C3-C2	2.85	1.59	1.52
4	B	272	BMA	O2-C2	3.12	1.50	1.43
4	B	271	NAG	C1-C2	3.13	1.56	1.52
4	B	282	BMA	C2-C3	3.41	1.57	1.52
4	B	282	BMA	O5-C5	3.58	1.51	1.43
4	B	273	MAN	C2-C3	4.23	1.58	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	283	MAN	O5-C1-C2	-10.85	93.25	110.86
4	B	272	BMA	C1-C2-C3	-10.63	96.96	109.54
4	B	271	NAG	C1-O5-C5	-8.51	101.44	112.25
4	B	281	NAG	C2-N2-C7	-7.88	112.92	123.04
3	B	268	BGC	C3-C4-C5	-6.74	98.45	110.20
4	B	271	NAG	C3-C4-C5	-6.50	98.86	110.20
4	B	271	NAG	C4-C3-C2	-5.99	101.92	111.23
4	B	284	MAN	O5-C1-C2	-5.56	101.83	110.86
4	B	272	BMA	C6-C5-C4	-5.00	100.69	113.02
4	B	272	BMA	C1-O5-C5	-4.98	105.92	112.25
3	B	265	BGC	C6-C5-C4	-4.06	103.00	113.02
4	B	284	MAN	C1-C2-C3	-3.95	104.87	109.54
4	B	283	MAN	O4-C4-C3	-3.95	101.44	110.34
4	B	283	MAN	C3-C4-C5	-3.93	103.35	110.20
4	B	284	MAN	C2-C3-C4	-3.83	104.53	111.04
4	B	284	MAN	O2-C2-C3	-3.71	102.66	110.12
3	B	267	GAL	O2-C2-C3	-3.67	102.74	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	283	MAN	O3-C3-C4	-3.48	102.49	110.34
4	B	273	MAN	C2-C3-C4	-3.31	105.43	111.04
4	B	282	BMA	O2-C2-C1	-3.17	102.85	109.21
4	B	281	NAG	C1-O5-C5	-3.16	108.23	112.25
4	B	273	MAN	O4-C4-C3	-2.99	103.61	110.34
4	B	282	BMA	C1-O5-C5	-2.98	108.47	112.25
3	B	264	GAL	O5-C1-C2	-2.80	106.31	110.86
4	B	284	MAN	O3-C3-C4	-2.80	104.03	110.34
4	B	281	NAG	O7-C7-N2	-2.78	116.19	121.86
4	B	284	MAN	C6-C5-C4	-2.71	106.32	113.02
4	B	271	NAG	O6-C6-C5	-2.70	102.42	111.33
4	B	273	MAN	C6-C5-C4	-2.65	106.49	113.02
4	B	284	MAN	C3-C4-C5	-2.62	105.62	110.20
4	B	272	BMA	O5-C1-C2	-2.59	106.66	110.86
4	B	282	BMA	C6-C5-C4	-2.46	106.94	113.02
4	B	283	MAN	O2-C2-C1	-2.39	104.42	109.21
4	B	280	NDG	C3-C4-C5	-2.34	106.12	110.20
4	B	270	NDG	C4-C3-C2	-2.34	107.60	111.23
3	B	267	GAL	O3-C3-C4	-2.33	105.10	110.34
4	B	283	MAN	C2-C3-C4	-2.32	107.09	111.04
4	B	284	MAN	O6-C6-C5	-2.32	103.68	111.33
3	B	267	GAL	C6-C5-C4	-2.24	107.48	113.02
4	B	273	MAN	O3-C3-C4	-2.17	105.44	110.34
4	B	284	MAN	C1-O5-C5	-2.04	109.66	112.25
4	B	281	NAG	C4-C3-C2	-2.03	108.07	111.23
4	B	274	MAN	O6-C6-C5	-2.03	104.63	111.33
4	B	272	BMA	O4-C4-C5	-2.01	103.92	109.24
4	B	271	NAG	O4-C4-C5	2.07	114.73	109.24
4	B	273	MAN	O5-C5-C6	2.13	111.96	107.35
4	B	282	BMA	O2-C2-C3	2.14	114.42	110.12
4	B	284	MAN	O5-C5-C6	2.16	112.02	107.35
3	B	265	BGC	O5-C1-C2	2.26	113.41	109.80
3	B	268	BGC	O4-C4-C5	2.29	115.30	109.24
4	B	282	BMA	C3-C4-C5	2.44	114.46	110.20
3	B	267	GAL	C1-O5-C5	2.48	115.39	112.25
4	B	272	BMA	O2-C2-C1	2.52	114.26	109.21
3	B	267	GAL	O2-C2-C1	2.61	114.43	109.21
4	B	280	NDG	C1-O-C5	2.62	115.58	112.25
4	B	273	MAN	O5-C1-C2	2.64	115.14	110.86
4	B	284	MAN	O3-C3-C2	2.81	115.07	110.00
4	B	281	NAG	O7-C7-C8	2.81	127.22	122.06
3	B	267	GAL	C1-C2-C3	2.92	113.00	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	265	BGC	O5-C5-C4	3.01	115.33	109.68
4	B	283	MAN	O3-C3-C2	3.12	115.63	110.00
4	B	270	NDG	C8-C7-N2	3.19	122.22	116.11
3	B	264	GAL	C1-C2-C3	3.21	113.34	109.54
3	B	265	BGC	O5-C5-C6	3.36	114.85	106.36
4	B	273	MAN	O3-C3-C2	3.47	116.27	110.00
4	B	283	MAN	O4-C4-C5	3.80	119.32	109.24
4	B	282	BMA	O6-C6-C5	3.86	124.10	111.33
4	B	284	MAN	O2-C2-C1	3.93	117.09	109.21
4	B	273	MAN	C1-C2-C3	4.02	114.30	109.54
3	B	268	BGC	O5-C1-C2	4.18	116.47	109.80
4	B	283	MAN	C1-O5-C5	4.31	117.72	112.25
4	B	272	BMA	O5-C5-C6	4.88	117.91	107.35
4	B	272	BMA	C3-C4-C5	5.15	119.18	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	280	NDG	C1
4	B	270	NDG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	281	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	283	MAN	C1-C2-C3-C4-C5-O5
4	B	284	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	271	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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