Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 08:44 AM EDT

PDB ID	:	1CE7
Title	:	MISTLETOE LECTIN I FROM VISCUM ALBUM
Authors	:	Krauspenhaar, R.; Eschenburg, S.; Perbandt, M.; Kornilov, V.; Konareva, N.; Mikailova, I.; Stoeva, S.; Wacker, R.; Maier, T.; Singh, T.P.; Mikhailov, A.; Voelter, W.; Betzel, C.
Deposited on	:	1999-03-18
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

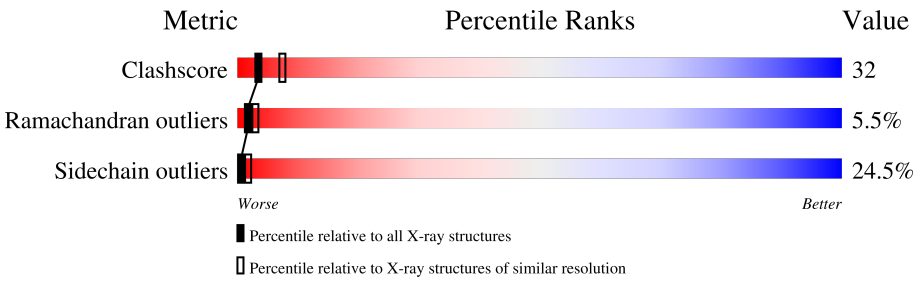
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	241	27% 34% 26% 14%
2	B	255	19% 44% 26% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3963 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.

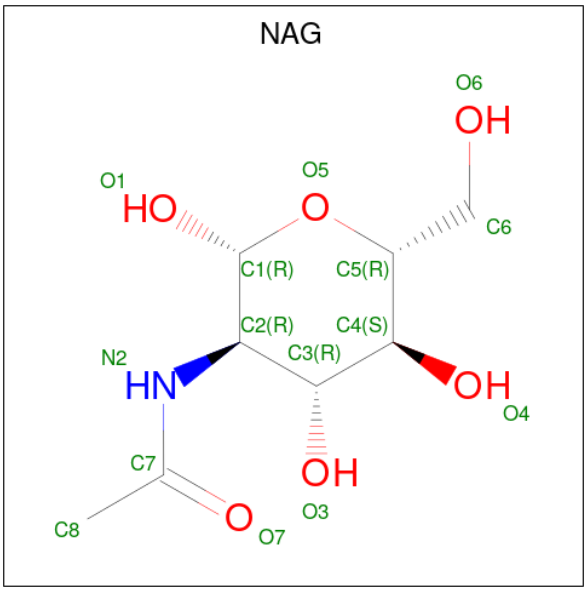
- Molecule 1 is a protein called PROTEIN (RIBOSOME-INACTIVATING PROTEIN TYPE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1809	1145	307	353	4	0	0	0

- Molecule 2 is a protein called PROTEIN (RIBOSOME-INACTIVATING PROTEIN TYPE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	255	1897	1177	332	376	12	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	108	108	108	0	0
			Total	O		
4	B	107	107	107	0	0

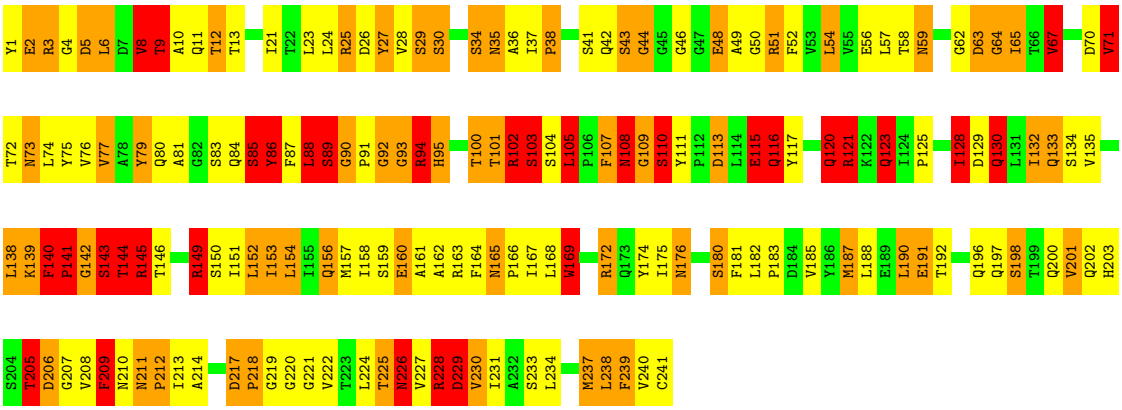
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

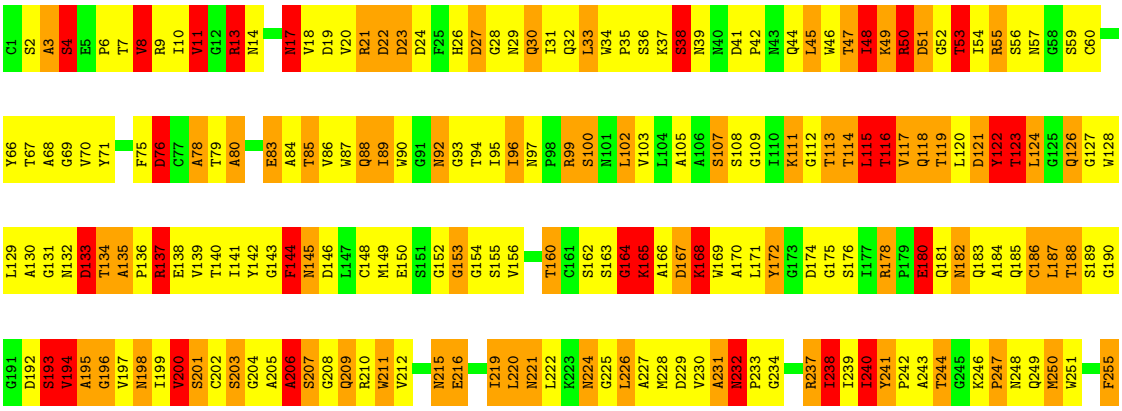
• Molecule 1: PROTEIN (RIBOSOME-INACTIVATING PROTEIN TYPE II)

Chain A: 27% 34% 26% 14%



• Molecule 2: PROTEIN (RIBOSOME-INACTIVATING PROTEIN TYPE II)

Chain B: 19% 44% 26% 11%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.65Å 107.65Å 311.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.1 (8.00-2.70)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.251 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3963	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

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: 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	0.81	0/1845	2.94	161/2508 (6.4%)
2	B	0.88	1/1935 (0.1%)	2.85	180/2637 (6.8%)
All	All	0.85	1/3780 (0.0%)	2.89	341/5145 (6.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	29
2	B	0	50
All	All	0	79

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	186	CYS	CB-SG	-5.46	1.73	1.81

All (341) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ARG	CD-NE-CZ	36.81	175.13	123.60
1	A	145	ARG	NE-CZ-NH2	-28.22	106.19	120.30
1	A	228	ARG	NE-CZ-NH2	-27.90	106.35	120.30
1	A	145	ARG	NE-CZ-NH1	26.94	133.77	120.30
1	A	149	ARG	CD-NE-CZ	24.12	157.37	123.60
2	B	231	ALA	O-C-N	-21.66	88.05	122.70
2	B	210	ARG	NE-CZ-NH2	20.86	130.73	120.30
2	B	55	ARG	NE-CZ-NH2	-19.38	110.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	167	ASP	CB-CG-OD2	18.16	134.64	118.30
1	A	143	SER	C-N-CA	17.85	166.32	121.70
2	B	164	GLY	O-C-N	-17.60	94.55	122.70
1	A	172	ARG	NE-CZ-NH1	16.23	128.42	120.30
1	A	228	ARG	NE-CZ-NH1	16.20	128.40	120.30
2	B	210	ARG	NE-CZ-NH1	-14.75	112.92	120.30
2	B	210	ARG	CD-NE-CZ	14.75	144.25	123.60
2	B	196	GLY	C-N-CA	14.74	158.55	121.70
2	B	51	ASP	CB-CG-OD2	-13.41	106.23	118.30
2	B	83	GLU	OE1-CD-OE2	-12.92	107.80	123.30
2	B	167	ASP	CB-CG-OD1	-12.69	106.88	118.30
2	B	137	ARG	NE-CZ-NH1	-12.34	114.13	120.30
2	B	23	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	A	145	ARG	CD-NE-CZ	11.68	139.94	123.60
2	B	71	TYR	CB-CG-CD1	11.67	128.00	121.00
2	B	178	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	A	11	GLN	CB-CG-CD	11.32	141.05	111.60
1	A	142	GLY	CA-C-O	-11.18	100.47	120.60
2	B	17	ASN	OD1-CG-ND2	11.12	147.47	121.90
1	A	11	GLN	CB-CA-C	10.74	131.89	110.40
1	A	5	ASP	CB-CG-OD2	-10.74	108.63	118.30
1	A	3	ARG	NE-CZ-NH1	10.50	125.55	120.30
2	B	231	ALA	CA-C-N	10.40	140.08	117.20
2	B	121	ASP	CB-CG-OD1	10.25	127.53	118.30
2	B	194	VAL	CA-C-O	10.21	141.55	120.10
2	B	21	ARG	NE-CZ-NH2	10.14	125.37	120.30
1	A	142	GLY	CA-C-N	10.11	139.45	117.20
2	B	117	VAL	O-C-N	-10.10	106.53	122.70
1	A	220	GLY	N-CA-C	9.93	137.91	113.10
1	A	11	GLN	C-N-CA	9.80	146.21	121.70
1	A	149	ARG	CG-CD-NE	9.78	132.33	111.80
1	A	172	ARG	CG-CD-NE	9.75	132.27	111.80
1	A	11	GLN	O-C-N	-9.63	107.29	122.70
1	A	237	MET	CA-CB-CG	9.59	129.60	113.30
1	A	163	ARG	NE-CZ-NH2	-9.51	115.55	120.30
2	B	172	TYR	CB-CG-CD1	-9.39	115.36	121.00
2	B	11	VAL	CA-CB-CG1	9.13	124.59	110.90
2	B	227	ALA	N-CA-CB	-9.11	97.35	110.10
1	A	94	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	141	PRO	C-N-CA	9.04	141.29	122.30
1	A	121	ARG	CD-NE-CZ	9.01	136.21	123.60
2	B	13	ARG	NE-CZ-NH1	-9.01	115.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	GLN	CA-C-O	9.00	139.01	120.10
1	A	120	GLN	CG-CD-OE1	8.96	139.52	121.60
2	B	11	VAL	CG1-CB-CG2	-8.96	96.57	110.90
2	B	71	TYR	CB-CG-CD2	-8.92	115.65	121.00
2	B	164	GLY	CA-C-N	8.82	136.61	117.20
2	B	178	ARG	CD-NE-CZ	-8.79	111.29	123.60
1	A	143	SER	O-C-N	-8.78	108.66	122.70
1	A	75	TYR	CB-CG-CD2	8.77	126.26	121.00
1	A	9	THR	C-N-CA	8.74	143.55	121.70
2	B	237	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	197	GLN	CG-CD-OE1	-8.68	104.25	121.60
2	B	51	ASP	OD1-CG-OD2	8.59	139.62	123.30
2	B	10	ILE	O-C-N	-8.49	109.11	122.70
1	A	187	MET	CG-SD-CE	8.48	113.77	100.20
1	A	217	ASP	CA-CB-CG	8.48	132.06	113.40
1	A	100	THR	CA-CB-CG2	8.41	124.17	112.40
2	B	133	ASP	CB-CG-OD1	8.25	125.72	118.30
2	B	215	ASN	O-C-N	-8.22	109.55	122.70
1	A	3	ARG	CD-NE-CZ	8.17	135.04	123.60
2	B	194	VAL	CA-CB-CG2	8.17	123.15	110.90
2	B	231	ALA	CA-C-O	-8.13	103.03	120.10
1	A	239	PHE	O-C-N	-8.04	109.83	122.70
2	B	237	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	B	17	ASN	CB-CG-OD1	-8.00	105.61	121.60
2	B	8	VAL	N-CA-CB	-7.97	93.97	111.50
2	B	238	ILE	O-C-N	-7.96	109.97	122.70
2	B	126	GLN	CA-CB-CG	7.86	130.68	113.40
2	B	192	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	102	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	B	117	VAL	CA-C-N	7.74	134.24	117.20
1	A	79	TYR	CB-CG-CD1	7.70	125.62	121.00
1	A	102	ARG	O-C-N	-7.70	110.38	122.70
2	B	99	ARG	CD-NE-CZ	7.68	134.36	123.60
1	A	116	GLN	CG-CD-OE1	7.63	136.87	121.60
2	B	21	ARG	NE-CZ-NH1	-7.61	116.49	120.30
1	A	129	ASP	CB-CG-OD2	-7.60	111.46	118.30
2	B	194	VAL	O-C-N	-7.58	110.57	122.70
1	A	2	GLU	CB-CA-C	7.51	125.42	110.40
1	A	105	LEU	CA-CB-CG	7.51	132.57	115.30
2	B	165	LYS	C-N-CA	7.49	140.43	121.70
2	B	60	CYS	CA-CB-SG	7.49	127.48	114.00
2	B	121	ASP	CB-CG-OD2	-7.47	111.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	255	PHE	CB-CA-C	7.45	125.29	110.40
1	A	108	ASN	CB-CG-OD1	7.44	136.49	121.60
1	A	89	SER	O-C-N	-7.39	110.63	123.20
1	A	11	GLN	OE1-CD-NE2	-7.34	105.01	121.90
2	B	116	THR	CA-C-O	-7.33	104.70	120.10
1	A	89	SER	C-N-CA	7.32	137.67	122.30
1	A	229	ASP	CB-CG-OD2	7.31	124.88	118.30
2	B	11	VAL	CA-CB-CG2	-7.29	99.96	110.90
1	A	116	GLN	CB-CG-CD	7.29	130.54	111.60
1	A	64	GLY	O-C-N	-7.25	111.10	122.70
2	B	102	LEU	CA-CB-CG	7.22	131.91	115.30
1	A	51	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	B	168	LYS	O-C-N	-7.20	111.18	122.70
2	B	188	THR	O-C-N	7.20	134.21	122.70
2	B	99	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	9	THR	O-C-N	-7.18	111.21	122.70
2	B	194	VAL	C-N-CA	7.15	139.58	121.70
1	A	237	MET	CA-C-O	7.15	135.11	120.10
1	A	206	ASP	N-CA-CB	7.14	123.45	110.60
1	A	169	TRP	CA-CB-CG	7.11	127.21	113.70
1	A	89	SER	N-CA-CB	-7.06	99.91	110.50
2	B	95	ILE	O-C-N	-7.04	111.44	122.70
2	B	23	ASP	OD1-CG-OD2	7.04	136.67	123.30
2	B	13	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	A	92	GLY	C-N-CA	7.03	137.07	122.30
1	A	67	VAL	CB-CA-C	7.03	124.75	111.40
1	A	2	GLU	OE1-CD-OE2	-7.01	114.88	123.30
2	B	146	ASP	CB-CG-OD1	7.00	124.60	118.30
2	B	116	THR	CA-CB-CG2	-6.95	102.67	112.40
2	B	83	GLU	O-C-N	-6.95	111.58	122.70
2	B	93	GLY	O-C-N	-6.94	111.60	122.70
1	A	143	SER	CA-C-O	6.92	134.62	120.10
1	A	88	LEU	CA-C-N	6.90	132.38	117.20
1	A	143	SER	N-CA-C	6.88	129.59	111.00
2	B	86	VAL	O-C-N	-6.87	111.71	122.70
1	A	153	ILE	O-C-N	-6.86	111.72	122.70
2	B	111	LYS	C-N-CA	6.82	136.62	122.30
2	B	22	ASP	CB-CG-OD1	-6.81	112.17	118.30
2	B	190	GLY	O-C-N	-6.80	111.63	123.20
2	B	33	LEU	CA-C-O	-6.80	105.81	120.10
1	A	1	TYR	CB-CG-CD1	-6.79	116.93	121.00
2	B	86	VAL	C-N-CA	6.74	138.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	121	ASP	O-C-N	-6.72	111.94	122.70
1	A	121	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	93	GLY	C-N-CA	6.71	138.48	121.70
1	A	95	HIS	N-CA-C	6.71	129.12	111.00
2	B	200	VAL	CA-CB-CG2	-6.69	100.87	110.90
2	B	84	ALA	N-CA-CB	-6.68	100.75	110.10
1	A	205	THR	CA-C-N	6.67	131.88	117.20
1	A	144	THR	N-CA-CB	6.67	122.97	110.30
1	A	165	ASN	N-CA-CB	-6.65	98.63	110.60
2	B	134	THR	CA-C-O	-6.64	106.16	120.10
2	B	216	GLU	OE1-CD-OE2	-6.62	115.35	123.30
1	A	226	ASN	CB-CG-ND2	6.56	132.46	116.70
2	B	210	ARG	CG-CD-NE	6.51	125.47	111.80
2	B	160	THR	N-CA-CB	6.49	122.63	110.30
2	B	66	TYR	CB-CA-C	6.48	123.36	110.40
2	B	193	SER	CA-C-N	6.48	131.45	117.20
1	A	86	TYR	CB-CA-C	6.48	123.35	110.40
2	B	13	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	144	THR	CA-CB-CG2	6.47	121.46	112.40
1	A	217	ASP	N-CA-CB	6.45	122.22	110.60
2	B	133	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	B	167	ASP	N-CA-CB	6.39	122.11	110.60
2	B	178	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	A	43	SER	CB-CA-C	6.35	122.16	110.10
2	B	153	GLY	CA-C-N	6.31	128.82	116.20
2	B	30	GLN	N-CA-CB	-6.30	99.27	110.60
1	A	121	ARG	CB-CA-C	-6.29	97.81	110.40
2	B	226	LEU	O-C-N	-6.28	112.66	122.70
2	B	55	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	B	86	VAL	CA-C-N	6.27	130.99	117.20
2	B	28	GLY	CA-C-O	-6.26	109.33	120.60
2	B	142	TYR	CB-CG-CD1	6.26	124.75	121.00
2	B	240	ILE	CA-CB-CG2	6.24	123.38	110.90
2	B	118	GLN	O-C-N	-6.24	112.72	122.70
2	B	122	TYR	O-C-N	-6.23	112.74	122.70
1	A	214	ALA	N-CA-CB	-6.23	101.38	110.10
1	A	108	ASN	CB-CG-ND2	-6.21	101.80	116.70
1	A	156	GLN	CA-CB-CG	-6.20	99.75	113.40
1	A	146	THR	O-C-N	-6.20	112.66	123.20
1	A	172	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	211	ASN	N-CA-CB	6.19	121.74	110.60
2	B	51	ASP	CB-CA-C	-6.19	98.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	164	GLY	CA-C-O	-6.18	109.48	120.60
2	B	168	LYS	CB-CA-C	6.17	122.74	110.40
1	A	9	THR	CA-C-O	6.17	133.05	120.10
1	A	181	PHE	N-CA-CB	-6.15	99.54	110.60
1	A	34	SER	N-CA-CB	6.13	119.69	110.50
1	A	79	TYR	CG-CD2-CE2	6.12	126.19	121.30
2	B	28	GLY	CA-C-N	6.09	130.60	117.20
1	A	239	PHE	C-N-CA	6.08	136.91	121.70
2	B	95	ILE	CA-C-N	6.07	130.56	117.20
2	B	219	ILE	CA-CB-CG2	-6.06	98.79	110.90
1	A	144	THR	OG1-CB-CG2	-6.06	96.07	110.00
1	A	79	TYR	CZ-CE2-CD2	-6.00	114.40	119.80
1	A	205	THR	C-N-CA	-6.00	106.69	121.70
1	A	212	PRO	C-N-CA	5.98	136.66	121.70
2	B	13	ARG	CG-CD-NE	5.97	124.34	111.80
2	B	19	ASP	N-CA-CB	-5.97	99.85	110.60
2	B	162	SER	CA-C-N	5.96	130.32	117.20
1	A	128	ILE	CB-CA-C	-5.96	99.68	111.60
2	B	212	VAL	CG1-CB-CG2	-5.95	101.39	110.90
1	A	13	THR	CA-CB-OG1	5.94	121.47	109.00
1	A	192	THR	CA-C-N	5.94	130.26	117.20
2	B	85	THR	O-C-N	-5.93	113.21	122.70
1	A	8	VAL	CA-CB-CG1	5.93	119.80	110.90
1	A	115	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	A	140	PHE	N-CA-CB	-5.92	99.94	110.60
2	B	139	VAL	CG1-CB-CG2	5.92	120.37	110.90
2	B	248	ASN	C-N-CA	5.91	136.47	121.70
2	B	55	ARG	NH1-CZ-NH2	5.90	125.89	119.40
2	B	50	ARG	N-CA-CB	-5.89	100.00	110.60
1	A	81	ALA	C-N-CA	-5.87	109.97	122.30
1	A	62	GLY	CA-C-O	-5.86	110.05	120.60
2	B	33	LEU	CA-C-N	5.86	130.10	117.20
2	B	107	SER	CB-CA-C	-5.86	98.96	110.10
2	B	135	ALA	N-CA-CB	5.86	118.30	110.10
1	A	209	PHE	CB-CG-CD2	-5.85	116.71	120.80
2	B	153	GLY	O-C-N	-5.84	113.27	123.20
1	A	41	SER	CA-CB-OG	5.83	126.95	111.20
1	A	89	SER	CA-C-O	5.83	132.35	120.10
1	A	128	ILE	N-CA-CB	5.82	124.19	110.80
1	A	138	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	146	THR	CA-CB-CG2	5.78	120.50	112.40
2	B	137	ARG	NH1-CZ-NH2	5.76	125.74	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	SER	CA-C-O	5.76	132.19	120.10
2	B	255	PHE	N-CA-CB	-5.75	100.24	110.60
1	A	35	ASN	CB-CG-OD1	-5.74	110.12	121.60
2	B	180	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	A	102	ARG	CD-NE-CZ	5.72	131.61	123.60
2	B	42	PRO	O-C-N	-5.72	113.54	122.70
2	B	128	TRP	C-N-CA	5.71	135.99	121.70
2	B	24	ASP	CB-CG-OD2	-5.71	113.16	118.30
2	B	176	SER	C-N-CA	5.71	135.97	121.70
2	B	19	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	B	188	THR	CB-CA-C	-5.69	96.24	111.60
1	A	133	GLN	CB-CG-CD	5.68	126.38	111.60
1	A	35	ASN	N-CA-CB	5.66	120.80	110.60
1	A	9	THR	N-CA-CB	-5.66	99.54	110.30
2	B	194	VAL	CG1-CB-CG2	-5.66	101.85	110.90
1	A	95	HIS	CA-C-N	-5.65	104.89	116.20
2	B	3	ALA	CB-CA-C	5.65	118.58	110.10
2	B	7	THR	N-CA-CB	5.65	121.04	110.30
1	A	169	TRP	CD1-NE1-CE2	-5.63	103.93	109.00
2	B	207	SER	O-C-N	-5.61	113.66	123.20
2	B	53	THR	C-N-CA	5.61	135.72	121.70
2	B	241	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	A	172	ARG	CB-CG-CD	5.60	126.16	111.60
1	A	217	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	88	LEU	CA-CB-CG	5.57	128.10	115.30
2	B	115	LEU	O-C-N	5.57	131.60	122.70
2	B	2	SER	CA-C-O	5.55	131.76	120.10
2	B	33	LEU	N-CA-CB	-5.55	99.30	110.40
1	A	222	VAL	CA-CB-CG1	5.54	119.22	110.90
1	A	229	ASP	CA-CB-CG	5.54	125.60	113.40
1	A	151	ILE	CB-CA-C	5.54	122.67	111.60
2	B	83	GLU	CG-CD-OE1	5.53	129.36	118.30
1	A	25	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	152	LEU	CB-CG-CD2	5.51	120.37	111.00
2	B	89	ILE	O-C-N	-5.51	113.89	122.70
2	B	8	VAL	CA-CB-CG1	5.50	119.16	110.90
2	B	231	ALA	CB-CA-C	5.50	118.35	110.10
2	B	96	ILE	CA-C-O	-5.49	108.56	120.10
1	A	198	SER	N-CA-CB	-5.49	102.26	110.50
1	A	38	PRO	CA-C-O	5.47	133.34	120.20
2	B	200	VAL	CA-CB-CG1	5.47	119.10	110.90
2	B	138	GLU	O-C-N	-5.47	113.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	ILE	O-C-N	-5.46	113.95	122.70
2	B	180	GLU	CA-CB-CG	5.46	125.42	113.40
1	A	103	SER	N-CA-CB	5.46	118.69	110.50
2	B	220	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	115	GLU	CA-CB-CG	5.45	125.38	113.40
1	A	187	MET	CA-CB-CG	5.44	122.55	113.30
2	B	27	ASP	CA-C-O	5.41	131.45	120.10
2	B	200	VAL	CB-CA-C	5.40	121.66	111.40
1	A	27	TYR	CA-C-N	5.39	129.07	117.20
2	B	115	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	225	THR	CA-CB-CG2	5.39	119.94	112.40
2	B	182	ASN	OD1-CG-ND2	5.39	134.29	121.90
2	B	45	LEU	O-C-N	-5.38	114.09	122.70
1	A	180	SER	N-CA-CB	5.38	118.57	110.50
1	A	222	VAL	CA-CB-CG2	-5.38	102.84	110.90
2	B	103	VAL	O-C-N	-5.37	114.10	122.70
2	B	248	ASN	CB-CG-OD1	5.37	132.35	121.60
1	A	101	THR	CA-CB-CG2	-5.36	104.89	112.40
1	A	205	THR	CA-C-O	-5.36	108.84	120.10
2	B	134	THR	OG1-CB-CG2	5.36	122.32	110.00
1	A	121	ARG	CA-CB-CG	5.34	125.15	113.40
2	B	59	SER	O-C-N	5.34	131.24	122.70
1	A	123	GLN	CB-CG-CD	5.34	125.48	111.60
1	A	8	VAL	CG1-CB-CG2	-5.33	102.37	110.90
2	B	206	ALA	N-CA-CB	-5.33	102.64	110.10
1	A	210	ASN	CA-C-N	5.32	128.91	117.20
2	B	175	GLY	CA-C-O	5.32	130.17	120.60
1	A	228	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	A	102	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	B	76	ASP	C-N-CA	5.31	134.98	121.70
1	A	210	ASN	CA-CB-CG	-5.31	101.72	113.40
1	A	89	SER	N-CA-C	5.30	125.32	111.00
1	A	123	GLN	OE1-CD-NE2	-5.29	109.74	121.90
2	B	148	CYS	O-C-N	-5.28	114.25	122.70
2	B	6	PRO	O-C-N	-5.28	114.26	122.70
1	A	128	ILE	CG1-CB-CG2	5.27	123.00	111.40
1	A	113	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	116	GLN	OE1-CD-NE2	-5.25	109.82	121.90
2	B	132	ASN	CB-CG-OD1	-5.25	111.09	121.60
2	B	87	TRP	CA-CB-CG	-5.24	103.74	113.70
2	B	124	LEU	CA-C-N	5.24	126.69	116.20
1	A	145	ARG	CA-C-N	5.23	128.71	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	232	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	A	117	TYR	CB-CA-C	-5.21	99.98	110.40
2	B	141	ILE	N-CA-CB	5.21	122.78	110.80
2	B	221	ASN	CB-CG-OD1	-5.21	111.19	121.60
1	A	190	LEU	C-N-CA	5.20	134.70	121.70
2	B	209	GLN	CB-CA-C	5.20	120.80	110.40
2	B	197	VAL	CG1-CB-CG2	-5.19	102.60	110.90
2	B	92	ASN	O-C-N	-5.18	114.39	123.20
2	B	232	ASN	CB-CG-ND2	-5.18	104.26	116.70
1	A	163	ARG	CD-NE-CZ	5.17	130.84	123.60
2	B	49	LYS	CA-CB-CG	-5.17	102.02	113.40
2	B	76	ASP	N-CA-CB	-5.16	101.31	110.60
2	B	229	ASP	CA-CB-CG	5.15	124.74	113.40
2	B	24	ASP	CB-CG-OD1	5.15	122.93	118.30
2	B	6	PRO	C-N-CA	5.14	134.55	121.70
2	B	9	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	66	TYR	CA-C-N	5.13	128.49	117.20
1	A	130	GLN	CG-CD-NE2	5.13	129.01	116.70
2	B	47	THR	CA-C-O	-5.13	109.33	120.10
2	B	165	LYS	O-C-N	-5.12	114.50	122.70
2	B	124	LEU	CA-C-O	-5.12	109.35	120.10
1	A	71	VAL	N-CA-CB	-5.11	100.26	111.50
2	B	92	ASN	N-CA-CB	5.11	119.79	110.60
2	B	84	ALA	O-C-N	-5.10	114.54	122.70
1	A	206	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	24	ASP	CB-CA-C	5.09	120.58	110.40
1	A	191	GLU	C-N-CA	-5.09	108.98	121.70
1	A	237	MET	O-C-N	-5.08	114.57	122.70
2	B	220	LEU	CB-CG-CD2	5.08	119.63	111.00
2	B	113	THR	O-C-N	-5.08	114.58	122.70
1	A	181	PHE	C-N-CA	5.06	134.36	121.70
1	A	88	LEU	CA-C-O	-5.06	109.48	120.10
1	A	226	ASN	OD1-CG-ND2	-5.05	110.29	121.90
2	B	128	TRP	O-C-N	-5.04	114.63	122.70
1	A	35	ASN	CB-CG-ND2	5.04	128.79	116.70
1	A	29	SER	O-C-N	-5.04	114.64	122.70
1	A	70	ASP	O-C-N	-5.02	114.66	122.70
1	A	202	GLN	O-C-N	-5.02	114.66	122.70
1	A	63	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Mainchain
1	A	104	SER	Mainchain
1	A	107	PHE	Mainchain,Peptide
1	A	109	GLY	Mainchain
1	A	110	SER	Mainchain
1	A	123	GLN	Mainchain
1	A	125	PRO	Mainchain
1	A	130	GLN	Mainchain
1	A	132	ILE	Mainchain
1	A	134	SER	Mainchain
1	A	140	PHE	Mainchain
1	A	141	PRO	Peptide
1	A	145	ARG	Mainchain
1	A	164	PHE	Mainchain
1	A	2	GLU	Mainchain
1	A	205	THR	Mainchain
1	A	209	PHE	Mainchain
1	A	213	ILE	Mainchain
1	A	221	GLY	Peptide
1	A	23	LEU	Mainchain
1	A	230	VAL	Mainchain
1	A	239	PHE	Mainchain
1	A	30	SER	Mainchain
1	A	44	GLY	Mainchain
1	A	50	GLY	Mainchain
1	A	64	GLY	Mainchain
1	A	86	TYR	Mainchain
1	A	89	SER	Mainchain
2	B	100	SER	Mainchain
2	B	11	VAL	Mainchain
2	B	114	THR	Mainchain
2	B	116	THR	Mainchain
2	B	117	VAL	Mainchain
2	B	122	TYR	Mainchain
2	B	123	THR	Mainchain
2	B	131	GLY	Mainchain
2	B	133	ASP	Mainchain
2	B	140	THR	Mainchain
2	B	152	GLY	Mainchain
2	B	163	SER	Mainchain
2	B	164	GLY	Mainchain,Peptide
2	B	165	LYS	Mainchain
2	B	166	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	B	168	LYS	Mainchain
2	B	170	ALA	Mainchain
2	B	181	GLN	Mainchain
2	B	184	ALA	Mainchain
2	B	186	CYS	Mainchain
2	B	196	GLY	Mainchain,Peptide
2	B	206	ALA	Mainchain,Peptide
2	B	211	TRP	Mainchain
2	B	215	ASN	Mainchain
2	B	220	LEU	Mainchain
2	B	231	ALA	Mainchain,Peptide
2	B	232	ASN	Peptide
2	B	238	ILE	Mainchain
2	B	240	ILE	Mainchain
2	B	244	THR	Mainchain
2	B	247	PRO	Mainchain
2	B	250	MET	Mainchain
2	B	251	TRP	Mainchain
2	B	33	LEU	Mainchain
2	B	4	SER	Mainchain
2	B	44	GLN	Mainchain
2	B	47	THR	Mainchain
2	B	53	THR	Mainchain
2	B	54	ILE	Mainchain
2	B	56	SER	Mainchain
2	B	76	ASP	Mainchain
2	B	78	ALA	Mainchain
2	B	85	THR	Mainchain
2	B	89	ILE	Mainchain
2	B	92	ASN	Mainchain
2	B	94	THR	Mainchain

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	1809	0	1775	113	0
2	B	1897	0	1821	128	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	4	0
3	B	28	0	26	0	0
4	A	108	0	0	9	2
4	B	107	0	0	9	3
All	All	3963	0	3635	238	5

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 32.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASN:ND2	2:B:30:GLN:H	1.52	1.05
2:B:121:ASP:H	2:B:126:GLN:NE2	1.56	1.01
1:A:108:ASN:HD21	3:A:303:NAG:C1	1.75	0.98
1:A:102:ARG:NH2	4:A:361:HOH:O	1.94	0.97
1:A:102:ARG:NE	4:A:361:HOH:O	1.82	0.97
4:A:396:HOH:O	2:B:250:MET:HE3	1.66	0.94
1:A:102:ARG:NH2	4:A:377:HOH:O	1.84	0.92
2:B:205:ALA:CB	4:B:316:HOH:O	2.19	0.91
2:B:21:ARG:HH12	2:B:30:GLN:HE21	1.17	0.88
2:B:168:LYS:HB3	2:B:180:GLU:HG3	1.57	0.86
2:B:221:ASN:HD22	2:B:224:ASN:H	1.23	0.86
2:B:29:ASN:ND2	2:B:30:GLN:N	2.24	0.85
2:B:205:ALA:HB3	4:B:316:HOH:O	1.76	0.82
2:B:121:ASP:H	2:B:126:GLN:HE22	1.28	0.81
2:B:57:ASN:OD1	4:B:334:HOH:O	1.99	0.80
2:B:244:THR:HB	2:B:246:LYS:HG3	1.63	0.79
2:B:83:GLU:HG2	2:B:99:ARG:HH11	1.47	0.78
2:B:29:ASN:HD22	2:B:30:GLN:H	1.30	0.77
2:B:135:ALA:HB1	2:B:136:PRO:HD2	1.67	0.76
2:B:219:ILE:HB	2:B:228:MET:HG3	1.68	0.75
1:A:240:VAL:O	1:A:241:CYS:HB3	1.85	0.74
1:A:77:VAL:HG11	1:A:91:PRO:HD3	1.70	0.72
1:A:115:GLU:OE1	1:A:152:LEU:HD11	1.89	0.71
1:A:234:LEU:HD21	1:A:237:MET:HG2	1.71	0.71
2:B:21:ARG:HH12	2:B:30:GLN:NE2	1.88	0.71
2:B:14:ASN:HD22	2:B:178:ARG:HH22	1.36	0.70
2:B:224:ASN:HD22	2:B:226:LEU:H	1.39	0.68
2:B:32:GLN:NE2	2:B:112:GLY:HA2	2.08	0.68
1:A:67:VAL:HG23	1:A:76:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HG12	1:A:187:MET:HG3	1.74	0.68
4:A:396:HOH:O	2:B:250:MET:CE	2.31	0.67
2:B:145:ASN:N	2:B:145:ASN:HD22	1.92	0.67
2:B:205:ALA:HB1	4:B:316:HOH:O	1.87	0.67
2:B:188:THR:HA	2:B:208:GLY:O	1.95	0.67
2:B:189:SER:HB3	2:B:240:ILE:HD13	1.78	0.66
2:B:224:ASN:ND2	2:B:226:LEU:H	1.93	0.66
2:B:149:MET:HE1	2:B:187:LEU:HD21	1.78	0.65
1:A:238:LEU:O	1:A:240:VAL:HG23	1.95	0.65
2:B:29:ASN:HD22	2:B:30:GLN:N	1.92	0.65
1:A:206:ASP:H	1:A:208:VAL:HG23	1.61	0.65
1:A:217:ASP:O	1:A:218:PRO:C	2.35	0.65
1:A:200:GLN:NE2	1:A:211:ASN:H	1.95	0.65
1:A:8:VAL:HG21	4:A:389:HOH:O	1.96	0.65
1:A:35:ASN:O	1:A:36:ALA:HB3	1.97	0.64
1:A:149:ARG:O	1:A:153:ILE:HD12	1.97	0.64
2:B:195:ALA:HA	2:B:239:ILE:HB	1.77	0.64
2:B:133:ASP:OD2	2:B:137:ARG:NH1	2.31	0.64
1:A:59:ASN:ND2	1:A:63:ASP:H	1.95	0.64
1:A:9:THR:O	1:A:132:ILE:HG12	1.97	0.63
1:A:224:LEU:HD13	1:A:230:VAL:HG12	1.80	0.63
1:A:160:GLU:OE1	1:A:160:GLU:HA	1.97	0.63
2:B:200:VAL:CG1	2:B:201:SER:H	2.11	0.63
1:A:226:ASN:HD22	1:A:228:ARG:H	1.45	0.63
1:A:84:GLN:NE2	1:A:101:THR:HB	2.14	0.62
2:B:121:ASP:N	2:B:126:GLN:HE22	1.96	0.62
2:B:195:ALA:HB1	4:B:398:HOH:O	1.99	0.62
2:B:224:ASN:HD22	2:B:224:ASN:C	2.03	0.62
1:A:85:SER:HG	1:A:87:PHE:HE1	1.48	0.61
2:B:246:LYS:HB3	2:B:247:PRO:CD	2.30	0.61
1:A:156:GLN:HA	1:A:160:GLU:HB2	1.82	0.61
2:B:203:SER:O	2:B:204:GLY:C	2.38	0.61
1:A:59:ASN:HD21	1:A:63:ASP:H	1.50	0.60
1:A:141:PRO:HA	4:A:326:HOH:O	2.01	0.60
1:A:109:GLY:O	1:A:110:SER:C	2.40	0.60
2:B:221:ASN:ND2	2:B:224:ASN:H	1.97	0.60
2:B:145:ASN:HD22	2:B:145:ASN:H	1.49	0.60
2:B:135:ALA:HB1	2:B:136:PRO:CD	2.31	0.60
1:A:77:VAL:CG1	1:A:91:PRO:HD3	2.31	0.59
1:A:113:ASP:O	1:A:116:GLN:HB2	2.02	0.59
2:B:83:GLU:HB3	2:B:99:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:LEU:HA	2:B:126:GLN:HE22	1.66	0.59
2:B:34:TRP:CD1	2:B:35:PRO:HD2	2.38	0.59
2:B:100:SER:OG	2:B:102:LEU:HB2	2.03	0.59
1:A:88:LEU:O	1:A:90:GLY:N	2.34	0.59
2:B:172:TYR:CE1	2:B:178:ARG:HD2	2.37	0.59
1:A:79:TYR:CZ	1:A:138:LEU:HD22	2.38	0.59
1:A:240:VAL:O	1:A:241:CYS:CB	2.51	0.58
2:B:124:LEU:HB2	2:B:205:ALA:HB1	1.85	0.58
1:A:88:LEU:HB3	1:A:105:LEU:HD23	1.86	0.57
1:A:26:ASP:O	1:A:29:SER:HB2	2.05	0.57
2:B:224:ASN:ND2	2:B:226:LEU:HB2	2.20	0.57
1:A:52:PHE:CE1	1:A:77:VAL:HG21	2.40	0.57
1:A:108:ASN:ND2	3:A:303:NAG:C1	2.58	0.57
1:A:6:LEU:HD13	1:A:56:GLU:O	2.05	0.56
1:A:224:LEU:HD13	1:A:230:VAL:CG1	2.36	0.56
1:A:230:VAL:O	1:A:231:ILE:C	2.41	0.56
2:B:22:ASP:O	2:B:23:ASP:HB2	2.06	0.55
1:A:226:ASN:HD22	1:A:228:ARG:HB2	1.71	0.55
2:B:185:GLN:HE22	2:B:201:SER:HB2	1.70	0.55
2:B:211:TRP:HH2	2:B:240:ILE:HD11	1.71	0.55
2:B:200:VAL:HG12	2:B:201:SER:H	1.72	0.55
1:A:167:ILE:CG1	1:A:187:MET:HG3	2.37	0.54
2:B:178:ARG:HG2	2:B:185:GLN:O	2.07	0.54
1:A:160:GLU:CD	1:A:191:GLU:HG2	2.26	0.54
2:B:241:TYR:CD2	2:B:242:PRO:HD2	2.41	0.54
1:A:111:TYR:CE1	1:A:121:ARG:HD3	2.42	0.54
2:B:243:ALA:HA	2:B:249:GLN:OE1	2.06	0.54
1:A:83:SER:O	1:A:100:THR:HB	2.06	0.54
2:B:211:TRP:CH2	2:B:240:ILE:HD11	2.42	0.54
1:A:120:GLN:CA	1:A:120:GLN:HE21	2.20	0.54
2:B:70:VAL:O	2:B:116:THR:HG22	2.08	0.54
2:B:232:ASN:HB3	2:B:233:PRO:HD2	1.90	0.53
1:A:52:PHE:HE1	1:A:77:VAL:HG21	1.73	0.53
1:A:3:ARG:HG2	1:A:27:TYR:CD2	2.43	0.53
1:A:205:THR:HG21	2:B:4:SER:O	2.08	0.53
1:A:226:ASN:O	1:A:227:VAL:C	2.46	0.53
1:A:198:SER:OG	1:A:237:MET:HB3	2.09	0.53
2:B:119:THR:HG23	4:B:321:HOH:O	2.09	0.52
2:B:11:VAL:HG22	2:B:17:ASN:HB3	1.91	0.52
2:B:154:GLY:O	2:B:198:ASN:HB2	2.10	0.52
1:A:226:ASN:ND2	1:A:228:ARG:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:O	1:A:44:GLY:C	2.48	0.52
1:A:188:LEU:O	1:A:191:GLU:HB2	2.10	0.52
2:B:13:ARG:HD3	2:B:109:GLY:CA	2.40	0.52
2:B:76:ASP:OD1	2:B:78:ALA:HB3	2.09	0.52
1:A:102:ARG:CZ	4:A:361:HOH:O	2.17	0.51
1:A:108:ASN:ND2	3:A:303:NAG:HN2	2.08	0.51
1:A:120:GLN:HE21	1:A:120:GLN:HA	1.74	0.51
1:A:160:GLU:HG3	1:A:191:GLU:OE2	2.11	0.51
1:A:174:TYR:O	1:A:175:ILE:C	2.47	0.51
2:B:168:LYS:HB3	2:B:180:GLU:CG	2.33	0.51
1:A:115:GLU:OE2	1:A:152:LEU:HD21	2.10	0.51
1:A:37:ILE:HB	1:A:237:MET:HE1	1.92	0.51
2:B:121:ASP:N	2:B:126:GLN:NE2	2.40	0.51
2:B:237:ARG:NH2	4:B:398:HOH:O	2.17	0.51
1:A:200:GLN:HE22	1:A:211:ASN:H	1.59	0.50
1:A:65:ILE:HD13	1:A:138:LEU:HD12	1.94	0.50
1:A:140:PHE:O	4:A:326:HOH:O	2.19	0.50
2:B:165:LYS:HA	2:B:165:LYS:HE2	1.93	0.50
2:B:145:ASN:N	2:B:145:ASN:ND2	2.54	0.50
2:B:27:ASP:HB3	2:B:75:PHE:CE2	2.47	0.49
2:B:34:TRP:CG	2:B:35:PRO:HD2	2.47	0.49
1:A:165:ASN:N	1:A:166:PRO:HD2	2.27	0.49
1:A:183:PRO:HB3	1:A:187:MET:SD	2.53	0.49
2:B:14:ASN:HA	2:B:178:ARG:NH2	2.28	0.49
2:B:121:ASP:OD1	2:B:123:THR:OG1	2.25	0.48
1:A:6:LEU:HD22	1:A:56:GLU:HB3	1.96	0.48
1:A:85:SER:OG	1:A:87:PHE:HE1	1.96	0.48
2:B:202:CYS:O	2:B:205:ALA:N	2.46	0.48
2:B:50:ARG:HB3	4:B:332:HOH:O	2.12	0.48
2:B:53:THR:OG1	2:B:55:ARG:NE	2.32	0.48
1:A:28:VAL:HG12	1:A:71:VAL:HG22	1.96	0.47
1:A:84:GLN:HB3	1:A:86:TYR:CZ	2.48	0.47
1:A:25:ARG:HD2	1:A:162:ALA:O	2.14	0.47
2:B:156:VAL:HG13	2:B:238:ILE:HD12	1.96	0.47
2:B:67:THR:HG22	2:B:68:ALA:O	2.14	0.47
1:A:57:LEU:HD21	1:A:158:ILE:HD11	1.96	0.47
1:A:128:ILE:O	1:A:132:ILE:HG13	2.15	0.47
1:A:130:GLN:N	1:A:130:GLN:OE1	2.47	0.47
1:A:200:GLN:HE21	1:A:209:PHE:HB3	1.80	0.47
2:B:143:GLY:O	2:B:144:PHE:C	2.53	0.47
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ALA:HB1	2:B:50:ARG:CD	2.45	0.47
2:B:150:GLU:HG3	2:B:167:ASP:OD1	2.15	0.47
1:A:85:SER:O	1:A:103:SER:N	2.48	0.46
1:A:132:ILE:O	1:A:135:VAL:HG22	2.16	0.46
1:A:139:LYS:O	1:A:139:LYS:HE2	2.16	0.46
2:B:200:VAL:HG12	2:B:209:GLN:NE2	2.31	0.46
2:B:224:ASN:HD21	2:B:226:LEU:HB2	1.80	0.46
1:A:207:GLY:HA2	1:A:227:VAL:HG23	1.98	0.46
1:A:169:TRP:HH2	2:B:250:MET:HG2	1.80	0.46
1:A:108:ASN:HD21	3:A:303:NAG:C2	2.27	0.45
2:B:37:LYS:O	2:B:38:SER:C	2.54	0.45
1:A:35:ASN:O	1:A:36:ALA:CB	2.61	0.45
2:B:156:VAL:HG21	2:B:187:LEU:HD11	1.98	0.45
1:A:85:SER:HB3	1:A:100:THR:OG1	2.16	0.45
1:A:183:PRO:CB	1:A:187:MET:SD	3.04	0.45
1:A:185:VAL:HG11	1:A:218:PRO:HD3	1.98	0.45
1:A:229:ASP:OD1	2:B:137:ARG:NH2	2.49	0.45
2:B:48:ILE:HD13	2:B:48:ILE:N	2.31	0.45
2:B:21:ARG:HH11	2:B:21:ARG:HD2	1.60	0.44
2:B:37:LYS:O	2:B:39:ASN:N	2.49	0.44
2:B:206:ALA:HB3	2:B:209:GLN:HG3	1.98	0.44
1:A:200:GLN:HB3	1:A:209:PHE:CG	2.51	0.44
1:A:217:ASP:O	1:A:219:GLY:N	2.51	0.44
2:B:188:THR:OG1	2:B:200:VAL:HB	2.17	0.44
2:B:222:LEU:HD12	2:B:222:LEU:O	2.18	0.44
1:A:142:GLY:O	1:A:143:SER:HB3	2.17	0.44
2:B:195:ALA:CB	4:B:398:HOH:O	2.63	0.44
2:B:246:LYS:CB	2:B:247:PRO:CD	2.95	0.44
2:B:113:THR:HG22	2:B:114:THR:O	2.18	0.44
1:A:21:ILE:HG21	1:A:161:ALA:O	2.17	0.44
1:A:200:GLN:O	1:A:201:VAL:C	2.56	0.44
1:A:67:VAL:HG11	1:A:154:LEU:HD13	2.00	0.44
1:A:176:ASN:HD22	1:A:176:ASN:HA	1.56	0.44
2:B:14:ASN:HA	2:B:178:ARG:HH22	1.83	0.44
2:B:216:GLU:CD	2:B:216:GLU:H	2.21	0.44
1:A:152:LEU:O	1:A:153:ILE:C	2.56	0.43
1:A:165:ASN:O	1:A:166:PRO:C	2.53	0.43
2:B:51:ASP:OD1	2:B:52:GLY:N	2.51	0.43
2:B:127:GLY:O	2:B:174:ASP:HA	2.18	0.43
2:B:224:ASN:HD22	2:B:225:GLY:N	2.16	0.43
2:B:244:THR:HB	2:B:246:LYS:CG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:O	1:A:73:ASN:HB3	2.19	0.43
1:A:86:TYR:CD1	1:A:86:TYR:N	2.85	0.43
2:B:18:VAL:HG12	2:B:46:TRP:CZ2	2.53	0.43
2:B:205:ALA:N	2:B:209:GLN:OE1	2.51	0.43
2:B:13:ARG:HH11	2:B:13:ARG:HD2	1.57	0.43
1:A:203:HIS:CD2	1:A:241:CYS:SG	3.11	0.43
1:A:9:THR:HA	1:A:12:THR:HG21	1.99	0.42
2:B:178:ARG:NH1	2:B:183:GLN:O	2.51	0.42
1:A:144:THR:HG22	1:A:145:ARG:N	2.34	0.42
2:B:193:SER:O	2:B:194:VAL:HG23	2.19	0.42
2:B:105:ALA:HB3	2:B:118:GLN:HG2	2.00	0.42
2:B:122:TYR:H	2:B:126:GLN:HE21	1.68	0.42
1:A:37:ILE:HA	1:A:38:PRO:HD3	1.88	0.42
1:A:105:LEU:HG	1:A:107:PHE:CZ	2.55	0.42
2:B:232:ASN:OD1	2:B:232:ASN:N	2.50	0.42
1:A:43:SER:O	1:A:46:GLY:N	2.53	0.42
2:B:51:ASP:OD1	2:B:51:ASP:C	2.57	0.42
1:A:111:TYR:CD1	1:A:121:ARG:HD3	2.55	0.42
2:B:230:VAL:H	2:B:230:VAL:HG23	1.60	0.42
2:B:246:LYS:HB3	2:B:247:PRO:HD3	2.02	0.41
1:A:121:ARG:HG2	1:A:152:LEU:HD22	2.01	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.77	0.41
2:B:144:PHE:HB2	2:B:230:VAL:HG21	2.02	0.41
1:A:166:PRO:HG2	1:A:190:LEU:CD1	2.50	0.41
2:B:149:MET:HE3	2:B:169:TRP:CZ2	2.56	0.41
1:A:166:PRO:CD	1:A:233:SER:HB2	2.50	0.41
2:B:3:ALA:HB1	2:B:50:ARG:HD2	2.01	0.41
2:B:67:THR:O	2:B:68:ALA:C	2.57	0.41
1:A:4:GLY:HA2	1:A:54:LEU:HB2	2.03	0.41
2:B:8:VAL:CG1	2:B:130:ALA:HB1	2.51	0.41
2:B:31:ILE:HG22	2:B:115:LEU:HD22	2.01	0.41
1:A:57:LEU:HB3	1:A:135:VAL:HG11	2.03	0.41
2:B:26:HIS:O	2:B:27:ASP:C	2.58	0.41
2:B:88:GLN:HG2	2:B:90:TRP:NE1	2.35	0.41
2:B:185:GLN:NE2	2:B:201:SER:HB2	2.35	0.41
2:B:79:THR:O	2:B:80:ALA:O	2.39	0.41
2:B:255:PHE:CD1	2:B:255:PHE:N	2.89	0.41
1:A:142:GLY:O	1:A:143:SER:CB	2.69	0.40
2:B:83:GLU:HG2	2:B:99:ARG:NH1	2.26	0.40
2:B:137:ARG:HB2	2:B:171:LEU:HB2	2.03	0.40
1:A:150:SER:O	1:A:154:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LYS:HB3	2:B:247:PRO:HD2	2.01	0.40
2:B:185:GLN:HB3	2:B:199:ILE:HG22	2.02	0.40
1:A:212:PRO:HB3	1:A:225:THR:HG22	2.04	0.40
2:B:76:ASP:OD1	2:B:78:ALA:N	2.54	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:336:HOH:O	4:A:336:HOH:O[10_665]	0.98	1.22
4:B:409:HOH:O	4:B:409:HOH:O[12_554]	1.13	1.07
4:B:319:HOH:O	4:B:319:HOH:O[12_554]	1.27	0.93
4:A:358:HOH:O	4:A:358:HOH:O[10_665]	1.95	0.25
2:B:69:GLY:O	4:B:319:HOH:O[12_554]	2.11	0.09

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	239/241 (99%)	195 (82%)	29 (12%)	15 (6%)	1 2
2	B	253/255 (99%)	217 (86%)	24 (10%)	12 (5%)	2 4
All	All	492/496 (99%)	412 (84%)	53 (11%)	27 (6%)	2 3

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	94	ARG
1	A	95	HIS
1	A	218	PRO
2	B	80	ALA

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Mol	Chain	Res	Type
2	B	165	LYS
1	A	49	ALA
1	A	143	SER
2	B	38	SER
2	B	153	GLY
2	B	200	VAL
1	A	48	GLU
1	A	110	SER
1	A	144	THR
1	A	201	VAL
2	B	193	SER
2	B	194	VAL
2	B	195	ALA
1	A	92	GLY
1	A	93	GLY
2	B	144	PHE
1	A	10	ALA
1	A	73	ASN
1	A	90	GLY
2	B	13	ARG
2	B	164	GLY
2	B	234	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	193/194 (100%)	136 (70%)	57 (30%)	0 1
2	B	203/203 (100%)	163 (80%)	40 (20%)	1 3
All	All	396/397 (100%)	299 (76%)	97 (24%)	0 2

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP

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Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	VAL
1	A	9	THR
1	A	12	THR
1	A	24	LEU
1	A	30	SER
1	A	34	SER
1	A	42	GLN
1	A	48	GLU
1	A	51	ARG
1	A	54	LEU
1	A	58	THR
1	A	59	ASN
1	A	65	ILE
1	A	67	VAL
1	A	71	VAL
1	A	74	LEU
1	A	77	VAL
1	A	80	GLN
1	A	85	SER
1	A	86	TYR
1	A	88	LEU
1	A	89	SER
1	A	94	ARG
1	A	102	ARG
1	A	103	SER
1	A	105	LEU
1	A	108	ASN
1	A	110	SER
1	A	115	GLU
1	A	116	GLN
1	A	120	GLN
1	A	121	ARG
1	A	123	GLN
1	A	128	ILE
1	A	133	GLN
1	A	139	LYS
1	A	144	THR
1	A	145	ARG
1	A	149	ARG
1	A	154	LEU
1	A	157	MET

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Mol	Chain	Res	Type
1	A	159	SER
1	A	160	GLU
1	A	168	LEU
1	A	169	TRP
1	A	172	ARG
1	A	176	ASN
1	A	180	SER
1	A	182	LEU
1	A	196	GLN
1	A	205	THR
1	A	226	ASN
1	A	228	ARG
1	A	229	ASP
1	A	238	LEU
2	B	4	SER
2	B	8	VAL
2	B	17	ASN
2	B	20	VAL
2	B	36	SER
2	B	38	SER
2	B	41	ASP
2	B	45	LEU
2	B	48	ILE
2	B	49	LYS
2	B	50	ARG
2	B	88	GLN
2	B	96	ILE
2	B	97	ASN
2	B	107	SER
2	B	108	SER
2	B	111	LYS
2	B	115	LEU
2	B	116	THR
2	B	119	THR
2	B	123	THR
2	B	129	LEU
2	B	134	THR
2	B	137	ARG
2	B	144	PHE
2	B	145	ASN
2	B	155	SER
2	B	160	THR

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Mol	Chain	Res	Type
2	B	165	LYS
2	B	168	LYS
2	B	180	GLU
2	B	182	ASN
2	B	187	LEU
2	B	198	ASN
2	B	200	VAL
2	B	201	SER
2	B	203	SER
2	B	207	SER
2	B	224	ASN
2	B	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	84	GLN
1	A	108	ASN
1	A	120	GLN
1	A	173	GLN
1	A	176	ASN
1	A	196	GLN
1	A	200	GLN
1	A	203	HIS
1	A	210	ASN
1	A	226	ASN
2	B	14	ASN
2	B	29	ASN
2	B	30	GLN
2	B	32	GLN
2	B	57	ASN
2	B	126	GLN
2	B	145	ASN
2	B	183	GLN
2	B	185	GLN
2	B	221	ASN
2	B	224	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

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	$\#\|Z\| > 2$
3	NAG	B	302	2	14,14,15	1.26	1 (7%)	17,19,21	2.88	9 (52%)
3	NAG	A	303	-	14,14,15	1.12	1 (7%)	17,19,21	2.75	6 (35%)
3	NAG	B	301	2	14,14,15	1.48	2 (14%)	17,19,21	3.35	4 (23%)

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	302	2	-	2/6/23/26	0/1/1/1
3	NAG	A	303	-	-	6/6/23/26	0/1/1/1
3	NAG	B	301	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	O7-C7	-4.11	1.13	1.23
3	A	303	NAG	O7-C7	-3.27	1.15	1.23
3	B	302	NAG	O7-C7	-3.02	1.16	1.23
3	B	301	NAG	O5-C5	-2.11	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	NAG	C1-O5-C5	12.59	129.25	112.19
3	A	303	NAG	C4-C3-C2	-7.73	99.69	111.02
3	B	302	NAG	C3-C4-C5	-5.46	100.50	110.24
3	B	302	NAG	O3-C3-C4	5.25	122.49	110.35
3	B	302	NAG	O4-C4-C3	5.02	121.96	110.35
3	A	303	NAG	O3-C3-C2	4.12	117.99	109.47
3	A	303	NAG	C1-O5-C5	-4.11	106.63	112.19
3	B	302	NAG	O7-C7-C8	3.49	128.53	122.06
3	B	301	NAG	C4-C3-C2	-3.34	106.12	111.02
3	A	303	NAG	C8-C7-N2	3.30	121.68	116.10
3	B	302	NAG	O5-C1-C2	-3.27	106.12	111.29
3	A	303	NAG	O7-C7-N2	-3.08	116.28	121.95
3	B	301	NAG	O5-C1-C2	-2.94	106.65	111.29
3	B	302	NAG	O7-C7-N2	-2.77	116.86	121.95
3	B	302	NAG	O4-C4-C5	-2.53	103.02	109.30
3	A	303	NAG	O5-C5-C6	-2.42	103.41	107.20
3	B	302	NAG	C1-O5-C5	2.40	115.45	112.19
3	B	301	NAG	C6-C5-C4	-2.31	107.59	113.00
3	B	302	NAG	O3-C3-C2	-2.17	104.98	109.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	NAG	C8-C7-N2-C2
3	A	303	NAG	O7-C7-N2-C2
3	A	303	NAG	O5-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	A	303	NAG	C1-C2-N2-C7
3	B	302	NAG	O5-C5-C6-O6
3	A	303	NAG	C4-C5-C6-O6
3	B	301	NAG	C4-C5-C6-O6
3	B	302	NAG	C4-C5-C6-O6
3	A	303	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.