



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 2MLL / pdb_00002mll
Title : MISTLETOE LECTIN I FROM VISCUM ALBUM
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Mikailova, I.; Stoeva, S.; Wacker, R.; Maier, T.; Singh, T.P.; Mikhailov, A.;
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Deposited on : 1999-03-16
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

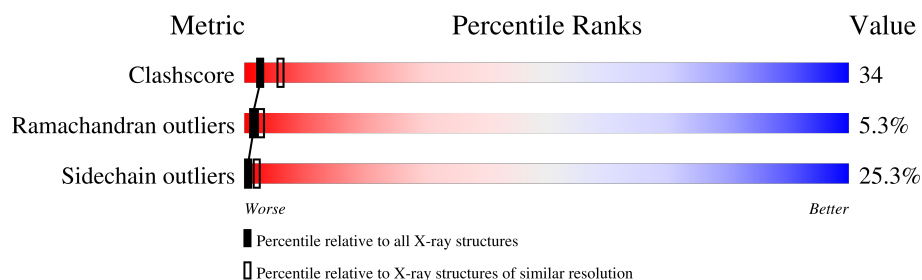
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	241	
2	B	255	

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.

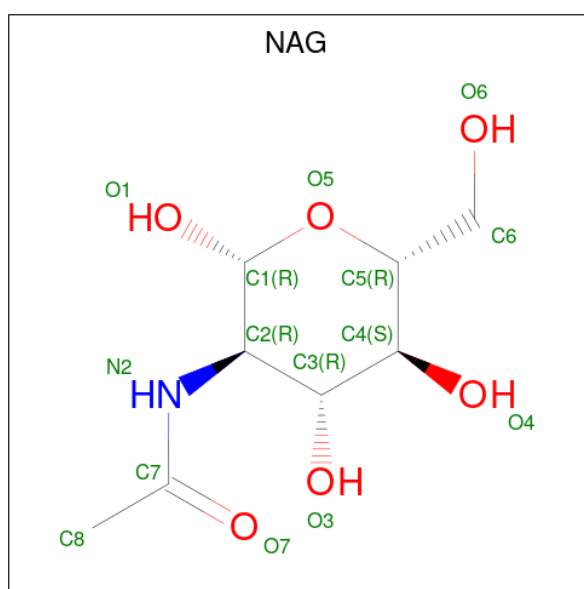
- Molecule 1 is a protein called PROTEIN (RIBOSOME-INACTIVATING PROTEIN TYPE II).

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

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

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 4 is water.

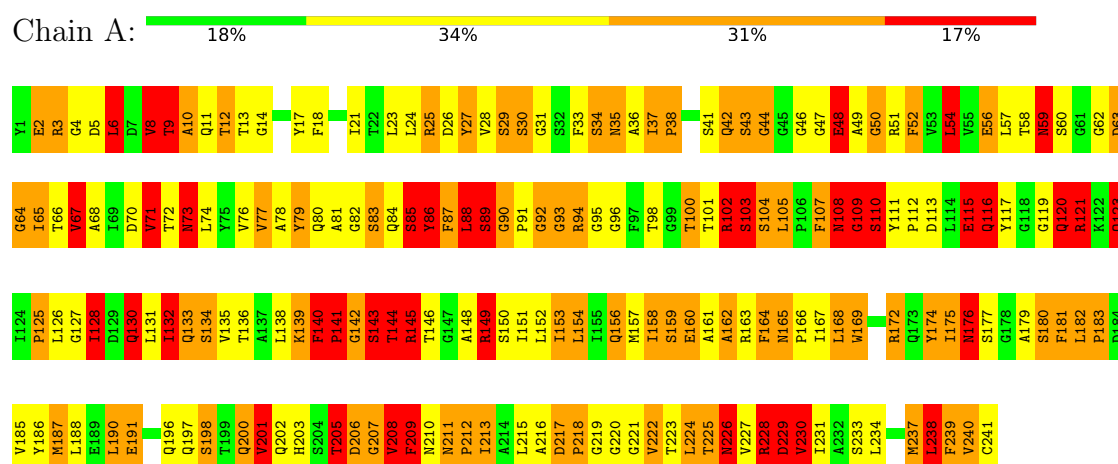
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	107	Total	O	0	0
			107	107		

3 Residue-property plots

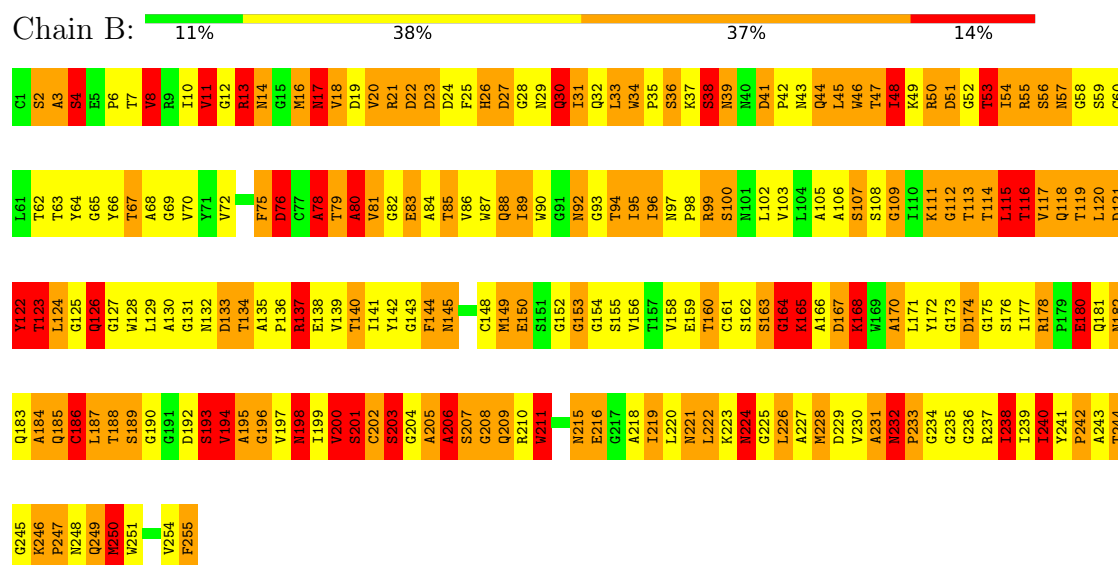
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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



4 Data and refinement statistics

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

5.1 Standard geometry

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	1.08	0/1845	3.57	298/2508 (11.9%)
2	B	1.18	2/1935 (0.1%)	3.54	351/2637 (13.3%)
All	All	1.14	2/3780 (0.1%)	3.55	649/5145 (12.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	THR	N-CA	-7.57	1.36	1.46
2	B	7	THR	N-CA	-6.18	1.39	1.46

All (649) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	CD-NE-CZ	36.24	175.13	124.40
2	B	196	GLY	CA-C-N	27.58	158.55	120.49
2	B	196	GLY	C-N-CA	27.58	158.55	120.49
2	B	231	ALA	O-C-N	-26.55	88.05	122.83
2	B	17	ASN	OD1-CG-ND2	24.88	147.47	122.60
1	A	149	ARG	CD-NE-CZ	23.55	157.37	124.40
1	A	143	SER	CA-C-N	23.44	166.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	SER	C-N-CA	23.44	166.32	121.54
2	B	164	GLY	O-C-N	-21.66	94.55	122.70
1	A	217	ASP	CA-CB-CG	19.46	132.06	112.60
1	A	11	GLN	OE1-CD-NE2	-17.59	105.01	122.60
1	A	11	GLN	CB-CG-CD	16.73	141.05	112.60
2	B	194	VAL	CA-C-O	16.61	141.55	120.78
2	B	231	ALA	CA-C-O	-14.53	103.03	122.51
1	A	11	GLN	O-C-N	-14.48	107.29	122.64
1	A	145	ARG	NE-CZ-NH2	-14.46	106.19	119.20
1	A	228	ARG	NE-CZ-NH2	-14.28	106.35	119.20
2	B	210	ARG	CD-NE-CZ	14.18	144.25	124.40
1	A	11	GLN	CA-C-O	14.05	139.01	121.58
2	B	116	THR	CA-C-O	-13.41	104.70	121.46
2	B	33	LEU	CA-C-O	-13.05	105.81	120.43
1	A	11	GLN	CB-CA-C	13.00	131.89	111.73
1	A	229	ASP	CA-CB-CG	13.00	125.60	112.60
1	A	123	GLN	OE1-CD-NE2	-12.86	109.74	122.60
2	B	210	ARG	NE-CZ-NH2	12.81	130.73	119.20
1	A	116	GLN	OE1-CD-NE2	-12.78	109.82	122.60
2	B	117	VAL	O-C-N	-12.48	106.53	122.88
1	A	226	ASN	OD1-CG-ND2	-12.31	110.29	122.60
1	A	145	ARG	NE-CZ-NH1	12.27	133.77	121.50
2	B	229	ASP	CA-CB-CG	12.14	124.74	112.60
2	B	175	GLY	CA-C-O	12.13	130.17	118.77
1	A	11	GLN	CA-C-N	12.03	146.21	122.03
1	A	11	GLN	C-N-CA	12.03	146.21	122.03
2	B	10	ILE	O-C-N	-11.96	109.11	123.10
2	B	167	ASP	CA-CB-CG	11.80	124.40	112.60
2	B	182	ASN	OD1-CG-ND2	11.69	134.29	122.60
1	A	237	MET	CA-C-O	11.66	135.11	121.58
2	B	238	ILE	O-C-N	-11.66	109.97	122.68
1	A	142	GLY	CA-C-O	-11.55	100.47	120.57
1	A	9	THR	CA-C-N	11.52	143.55	121.54
1	A	9	THR	C-N-CA	11.52	143.55	121.54
2	B	134	THR	CA-C-O	-11.48	106.16	119.60
2	B	232	ASN	OD1-CG-ND2	11.30	133.90	122.60
1	A	108	ASN	CA-C-N	11.15	132.59	119.99
1	A	108	ASN	C-N-CA	11.15	132.59	119.99
1	A	145	ARG	CD-NE-CZ	11.10	139.94	124.40
2	B	215	ASN	CA-CB-CG	11.04	123.64	112.60
1	A	239	PHE	CA-C-N	10.98	136.91	121.53
1	A	239	PHE	C-N-CA	10.98	136.91	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASN	CA-CB-CG	-10.88	101.72	112.60
1	A	226	ASN	CB-CG-ND2	10.70	132.46	116.40
1	A	128	ILE	N-CA-CB	10.64	124.19	110.57
1	A	88	LEU	CA-C-O	-10.61	109.48	121.89
1	A	116	GLN	CB-CG-CD	10.55	130.54	112.60
1	A	239	PHE	O-C-N	-10.53	109.83	122.89
1	A	38	PRO	CA-C-O	10.52	133.34	121.34
1	A	143	SER	O-C-N	-10.47	108.66	122.59
1	A	220	GLY	N-CA-C	10.44	137.91	113.18
2	B	198	ASN	CA-CB-CG	10.35	122.95	112.60
2	B	168	LYS	O-C-N	-10.33	111.18	123.16
1	A	197	GLN	OE1-CD-NE2	10.30	132.90	122.60
1	A	205	THR	CA-C-N	-10.28	106.69	123.04
1	A	205	THR	C-N-CA	-10.28	106.69	123.04
1	A	153	ILE	O-C-N	-10.22	111.72	121.94
2	B	76	ASP	CA-C-N	10.21	134.98	120.28
2	B	76	ASP	C-N-CA	10.21	134.98	120.28
1	A	159	SER	CA-C-N	10.15	133.88	120.28
1	A	159	SER	C-N-CA	10.15	133.88	120.28
2	B	93	GLY	O-C-N	-10.15	111.60	122.56
1	A	141	PRO	CA-C-N	10.14	141.29	121.41
1	A	141	PRO	C-N-CA	10.14	141.29	121.41
2	B	162	SER	CA-C-O	-10.14	110.38	121.23
1	A	102	ARG	O-C-N	-10.09	110.38	122.89
1	A	89	SER	CA-C-N	10.07	137.67	121.87
1	A	89	SER	C-N-CA	10.07	137.67	121.87
1	A	190	LEU	CA-C-N	10.01	134.70	120.79
1	A	190	LEU	C-N-CA	10.01	134.70	120.79
2	B	190	GLY	O-C-N	-10.01	111.63	122.24
2	B	11	VAL	CA-C-O	-9.95	109.94	120.48
2	B	93	GLY	CA-C-O	9.92	129.29	119.27
2	B	47	THR	CA-C-O	-9.91	109.33	120.43
1	A	143	SER	CA-C-O	9.87	134.62	120.51
1	A	212	PRO	CA-C-N	9.86	136.66	123.06
1	A	212	PRO	C-N-CA	9.86	136.66	123.06
1	A	126	LEU	CA-C-O	-9.85	110.06	121.68
1	A	108	ASN	CB-CG-ND2	-9.73	101.80	116.40
2	B	124	LEU	CA-C-O	-9.68	109.35	120.20
2	B	165	LYS	CA-C-N	9.67	140.43	121.58
2	B	165	LYS	C-N-CA	9.67	140.43	121.58
2	B	96	ILE	CA-C-O	-9.66	108.56	121.32
2	B	215	ASN	O-C-N	-9.61	109.55	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	VAL	O-C-N	-9.60	110.57	122.57
2	B	192	ASP	CA-CB-CG	9.59	122.19	112.60
2	B	55	ARG	NE-CZ-NH2	-9.54	110.61	119.20
2	B	176	SER	CA-C-N	9.46	135.97	123.11
2	B	176	SER	C-N-CA	9.46	135.97	123.11
2	B	194	VAL	CA-C-N	9.45	139.58	121.54
2	B	194	VAL	C-N-CA	9.45	139.58	121.54
2	B	95	ILE	O-C-N	-9.43	111.44	122.94
2	B	121	ASP	O-C-N	-9.43	111.94	121.93
1	A	128	ILE	CB-CA-C	-9.42	99.68	112.02
2	B	163	SER	N-CA-C	9.40	123.72	109.62
2	B	128	TRP	CA-C-N	9.37	135.99	122.77
2	B	128	TRP	C-N-CA	9.37	135.99	122.77
2	B	178	ARG	CD-NE-CZ	-9.36	111.29	124.40
1	A	120	GLN	CG-CD-OE1	9.36	139.52	120.80
2	B	83	GLU	O-C-N	-9.31	111.58	122.20
1	A	149	ARG	CG-CD-NE	9.24	132.33	112.00
2	B	27	ASP	CA-C-O	9.24	131.45	120.92
1	A	172	ARG	CG-CD-NE	9.21	132.27	112.00
2	B	86	VAL	O-C-N	-9.21	111.71	122.94
1	A	151	ILE	N-CA-C	-9.20	101.90	110.82
1	A	181	PHE	CA-CB-CG	9.16	122.96	113.80
1	A	205	THR	CA-C-O	-9.15	108.84	120.00
2	B	39	ASN	CA-CB-CG	9.14	121.74	112.60
2	B	53	THR	CA-C-N	9.14	135.72	123.11
2	B	53	THR	C-N-CA	9.14	135.72	123.11
2	B	118	GLN	O-C-N	-9.02	112.72	123.10
2	B	188	THR	O-C-N	8.99	134.21	123.33
1	A	89	SER	O-C-N	-8.99	110.63	122.59
2	B	111	LYS	CA-C-N	8.99	136.62	122.51
2	B	111	LYS	C-N-CA	8.99	136.62	122.51
2	B	255	PHE	CA-CB-CG	-8.94	104.86	113.80
1	A	86	TYR	CA-C-O	-8.93	111.24	120.71
1	A	64	GLY	O-C-N	-8.92	111.10	122.70
2	B	200	VAL	CA-C-O	-8.92	109.63	120.78
1	A	93	GLY	CA-C-N	8.87	138.48	121.54
1	A	93	GLY	C-N-CA	8.87	138.48	121.54
2	B	4	SER	CA-C-N	8.87	133.88	123.15
2	B	4	SER	C-N-CA	8.87	133.88	123.15
1	A	143	SER	N-CA-C	8.82	129.59	110.80
2	B	141	ILE	N-CA-CB	8.82	122.78	111.67
2	B	8	VAL	N-CA-CB	-8.79	93.97	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	SER	CA-C-O	8.79	132.19	120.15
1	A	206	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	2	GLU	CB-CA-C	8.67	125.42	109.46
2	B	86	VAL	CA-C-N	8.67	138.56	123.03
2	B	86	VAL	C-N-CA	8.67	138.56	123.03
2	B	123	THR	CA-C-O	-8.66	111.46	121.68
2	B	210	ARG	NE-CZ-NH1	-8.58	112.92	121.50
1	A	67	VAL	CB-CA-C	8.57	124.75	110.95
2	B	2	SER	CA-C-O	8.54	131.76	121.94
2	B	28	GLY	CA-C-O	-8.51	109.33	119.03
1	A	164	PHE	N-CA-C	8.50	122.28	108.34
2	B	103	VAL	O-C-N	-8.50	114.10	123.03
1	A	156	GLN	OE1-CD-NE2	8.49	131.09	122.60
1	A	200	GLN	CA-C-O	-8.49	111.91	120.82
1	A	62	GLY	CA-C-O	-8.48	110.05	119.04
2	B	160	THR	N-CA-CB	8.48	122.63	109.48
2	B	17	ASN	N-CA-C	8.48	122.66	109.52
1	A	121	ARG	CD-NE-CZ	8.44	136.21	124.40
1	A	131	LEU	N-CA-C	-8.44	101.11	111.40
1	A	130	GLN	CG-CD-NE2	8.41	129.01	116.40
2	B	248	ASN	CA-C-N	8.39	136.47	122.79
2	B	248	ASN	C-N-CA	8.39	136.47	122.79
1	A	151	ILE	CA-C-O	-8.39	110.98	120.96
1	A	103	SER	CA-C-O	-8.38	111.34	121.06
1	A	146	THR	O-C-N	-8.37	112.66	122.20
1	A	156	GLN	N-CA-C	8.36	120.02	111.07
2	B	11	VAL	CA-CB-CG1	8.35	124.59	110.40
2	B	126	GLN	CA-CB-CG	8.29	130.68	114.10
2	B	250	MET	CA-C-O	-8.29	111.12	120.32
1	A	89	SER	CA-C-O	8.28	132.35	120.51
1	A	197	GLN	CG-CD-OE1	-8.28	104.25	120.80
1	A	35	ASN	CB-CG-ND2	8.26	128.79	116.40
1	A	217	ASP	N-CA-CB	8.26	122.22	111.40
2	B	6	PRO	CA-C-N	8.23	134.55	122.86
2	B	6	PRO	C-N-CA	8.23	134.55	122.86
1	A	151	ILE	CB-CA-C	8.12	122.67	112.04
1	A	133	GLN	CB-CG-CD	8.10	126.38	112.60
2	B	232	ASN	CB-CG-ND2	-8.09	104.26	116.40
2	B	140	THR	CA-C-O	-8.08	111.35	120.32
1	A	100	THR	CA-CB-CG2	8.04	124.17	110.50
1	A	120	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	A	116	GLN	CG-CD-OE1	8.03	136.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	LYS	CB-CA-C	8.01	122.74	109.53
2	B	255	PHE	CB-CA-C	8.00	125.29	110.10
1	A	92	GLY	CA-C-N	7.99	137.07	121.41
1	A	92	GLY	C-N-CA	7.99	137.07	121.41
2	B	66	TYR	CB-CA-C	7.97	123.36	111.17
1	A	41	SER	CA-CB-OG	7.93	126.95	111.10
1	A	13	THR	CA-CB-OG1	7.92	121.47	109.60
1	A	73	ASN	CA-CB-CG	7.91	120.51	112.60
2	B	45	LEU	O-C-N	-7.91	114.09	123.27
1	A	108	ASN	CB-CG-OD1	7.84	136.49	120.80
1	A	162	ALA	N-CA-C	-7.81	104.64	114.56
2	B	67	THR	CA-C-N	-7.77	109.51	121.02
2	B	67	THR	C-N-CA	-7.77	109.51	121.02
1	A	86	TYR	CB-CA-C	7.76	123.35	109.38
1	A	174	TYR	CA-C-O	-7.76	112.33	120.55
2	B	54	ILE	CA-C-O	-7.75	112.71	120.31
1	A	237	MET	CA-CB-CG	7.75	129.60	114.10
1	A	181	PHE	N-CA-CB	-7.74	99.54	111.46
1	A	206	ASP	N-CA-CB	7.72	123.45	111.64
1	A	165	ASN	CA-C-O	7.71	125.72	118.63
2	B	148	CYS	O-C-N	-7.71	114.25	122.96
1	A	103	SER	CA-C-N	7.70	133.83	123.05
1	A	103	SER	C-N-CA	7.70	133.83	123.05
2	B	227	ALA	N-CA-CB	-7.70	97.35	111.13
2	B	95	ILE	N-CA-CB	-7.70	102.23	111.00
2	B	188	THR	CA-C-O	-7.70	111.36	120.60
2	B	139	VAL	N-CA-C	7.67	117.89	108.53
2	B	210	ARG	CA-C-O	7.65	128.43	120.40
1	A	9	THR	N-CA-CB	-7.64	99.54	111.23
2	B	115	LEU	O-C-N	7.63	131.60	123.06
2	B	85	THR	O-C-N	-7.61	113.21	122.34
1	A	3	ARG	CD-NE-CZ	7.60	135.04	124.40
1	A	145	ARG	CA-C-O	-7.60	109.64	120.51
2	B	17	ASN	CB-CG-OD1	-7.60	105.61	120.80
2	B	167	ASP	N-CA-CB	7.59	122.11	110.80
2	B	41	ASP	CA-C-O	7.58	128.05	120.17
2	B	240	ILE	CA-CB-CG2	7.58	123.38	110.50
1	A	123	GLN	CB-CG-CD	7.57	125.48	112.60
2	B	8	VAL	CA-C-O	7.56	129.01	121.45
2	B	238	ILE	CB-CA-C	7.55	119.39	111.23
1	A	176	ASN	OD1-CG-ND2	7.55	130.15	122.60
1	A	190	LEU	CA-C-O	7.53	128.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	17	ASN	CA-CB-CG	7.50	120.11	112.60
2	B	44	GLN	CA-C-O	-7.50	111.09	119.95
2	B	194	VAL	CA-CB-CG2	7.50	123.15	110.40
1	A	104	SER	N-CA-C	7.46	120.68	108.52
2	B	227	ALA	CA-C-O	-7.45	111.66	120.60
1	A	127	GLY	CA-C-O	-7.43	114.62	122.05
1	A	87	PHE	CA-C-O	-7.42	112.31	120.33
2	B	122	TYR	O-C-N	-7.41	112.74	122.59
1	A	186	TYR	CA-C-O	-7.40	113.23	121.00
1	A	9	THR	O-C-N	-7.40	111.21	122.61
1	A	144	THR	N-CA-CB	7.39	122.97	110.49
2	B	26	HIS	CA-C-N	-7.38	110.42	120.82
2	B	26	HIS	C-N-CA	-7.38	110.42	120.82
2	B	137	ARG	NE-CZ-NH1	-7.37	114.13	121.50
2	B	138	GLU	O-C-N	-7.37	113.95	123.02
1	A	228	ARG	CA-C-O	-7.37	110.58	119.49
1	A	176	ASN	CA-C-O	-7.36	113.10	120.82
1	A	79	TYR	CA-C-N	7.35	133.53	122.95
1	A	79	TYR	C-N-CA	7.35	133.53	122.95
2	B	228	MET	CA-C-O	-7.34	113.12	121.19
1	A	102	ARG	CB-CA-C	7.32	118.80	109.80
2	B	42	PRO	CA-C-N	7.31	132.29	120.60
2	B	42	PRO	C-N-CA	7.31	132.29	120.60
2	B	249	GLN	CA-C-N	-7.30	111.50	122.74
2	B	249	GLN	C-N-CA	-7.30	111.50	122.74
2	B	153	GLY	O-C-N	-7.25	113.27	122.70
1	A	216	ALA	N-CA-C	7.25	120.21	110.35
2	B	226	LEU	O-C-N	-7.24	112.66	122.36
2	B	30	GLN	N-CA-CB	-7.24	99.27	110.56
2	B	42	PRO	O-C-N	-7.24	113.54	122.23
1	A	226	ASN	O-C-N	-7.23	115.89	123.56
1	A	164	PHE	CA-C-O	7.22	127.90	120.24
1	A	223	THR	CA-C-N	-7.19	112.98	123.05
1	A	223	THR	C-N-CA	-7.19	112.98	123.05
1	A	2	GLU	N-CA-C	-7.18	99.85	110.48
1	A	156	GLN	CA-CB-CG	-7.17	99.75	114.10
2	B	50	ARG	N-CA-CB	-7.17	100.00	110.47
2	B	231	ALA	CA-C-N	7.17	132.34	120.86
2	B	231	ALA	C-N-CA	7.17	132.34	120.86
1	A	169	TRP	CA-CB-CG	7.17	127.21	113.60
2	B	170	ALA	O-C-N	-7.15	115.07	123.22
1	A	82	GLY	CA-C-N	7.11	131.12	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	GLY	C-N-CA	7.11	131.12	120.17
2	B	83	GLU	CA-C-O	7.11	128.16	120.20
2	B	99	ARG	CD-NE-CZ	7.11	134.36	124.40
2	B	56	SER	O-C-N	-7.10	115.00	123.31
1	A	9	THR	CB-CA-C	7.08	122.26	111.85
1	A	183	PRO	CB-CA-C	7.08	120.59	111.46
1	A	164	PHE	O-C-N	-7.06	115.01	123.27
2	B	167	ASP	CB-CG-OD2	7.06	134.64	118.40
2	B	229	ASP	CA-C-O	-7.04	111.38	120.25
2	B	6	PRO	O-C-N	-7.04	114.26	122.71
2	B	142	TYR	N-CA-C	-7.04	99.12	110.32
1	A	162	ALA	CA-C-O	7.01	126.54	118.55
1	A	226	ASN	CA-CB-CG	7.00	119.60	112.60
2	B	174	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	120	GLN	CG-CD-NE2	-6.99	105.92	116.40
2	B	221	ASN	OD1-CG-ND2	6.98	129.58	122.60
2	B	178	ARG	NE-CZ-NH1	-6.98	114.52	121.50
2	B	98	PRO	N-CA-C	-6.97	104.06	113.40
2	B	51	ASP	OD1-CG-OD2	6.97	139.62	122.90
2	B	89	ILE	O-C-N	-6.94	113.89	122.57
1	A	210	ASN	CA-C-O	-6.94	111.99	119.97
2	B	53	THR	CA-C-O	-6.92	113.51	121.47
1	A	172	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	A	228	ARG	NE-CZ-NH1	6.90	128.40	121.50
2	B	12	GLY	O-C-N	6.89	130.27	123.31
2	B	48	ILE	O-C-N	-6.89	113.95	122.57
1	A	177	SER	CA-C-O	6.89	127.38	119.18
2	B	219	ILE	CA-CB-CG2	-6.89	98.79	110.50
1	A	66	THR	CA-C-N	-6.86	112.39	122.68
1	A	66	THR	C-N-CA	-6.86	112.39	122.68
2	B	21	ARG	NE-CZ-NH2	6.86	125.37	119.20
1	A	43	SER	CB-CA-C	6.85	122.16	110.86
2	B	16	MET	CA-C-N	-6.83	111.86	122.59
2	B	16	MET	C-N-CA	-6.83	111.86	122.59
1	A	89	SER	N-CA-C	6.82	125.32	110.80
2	B	205	ALA	N-CA-C	-6.79	102.82	111.92
1	A	18	PHE	CA-CB-CG	-6.77	107.03	113.80
2	B	39	ASN	OD1-CG-ND2	-6.75	115.85	122.60
2	B	202	CYS	CA-C-O	-6.74	111.38	119.27
2	B	19	ASP	N-CA-CB	-6.74	99.85	110.69
2	B	207	SER	O-C-N	-6.71	113.66	122.59
2	B	85	THR	CA-CB-OG1	-6.71	99.53	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	THR	N-CA-CB	6.71	121.04	110.84
2	B	34	TRP	O-C-N	-6.70	117.12	121.88
2	B	57	ASN	CA-CB-CG	-6.70	105.90	112.60
2	B	92	ASN	N-CA-CB	6.69	119.79	110.56
1	A	191	GLU	CA-C-N	-6.68	108.98	122.55
1	A	191	GLU	C-N-CA	-6.68	108.98	122.55
1	A	179	ALA	CA-C-N	-6.68	111.07	123.03
1	A	179	ALA	C-N-CA	-6.68	111.07	123.03
2	B	84	ALA	O-C-N	-6.68	114.54	122.15
2	B	134	THR	CA-CB-OG1	-6.66	99.61	109.60
2	B	185	GLN	O-C-N	-6.65	115.52	123.03
2	B	248	ASN	CA-CB-CG	6.65	119.25	112.60
2	B	36	SER	CA-C-O	-6.62	113.37	120.92
1	A	144	THR	OG1-CB-CG2	-6.61	96.07	109.30
1	A	31	GLY	CA-C-O	-6.61	112.60	119.27
2	B	95	ILE	CA-C-N	6.60	133.76	122.67
2	B	95	ILE	C-N-CA	6.60	133.76	122.67
1	A	29	SER	O-C-N	-6.60	114.64	122.96
2	B	186	CYS	O-C-N	-6.58	115.34	123.44
1	A	180	SER	N-CA-C	-6.58	99.75	109.81
1	A	148	ALA	O-C-N	-6.57	115.30	122.07
2	B	24	ASP	CB-CA-C	6.56	120.58	109.75
1	A	212	PRO	CB-CA-C	6.56	121.50	111.40
1	A	209	PHE	CA-C-O	-6.56	113.44	120.92
1	A	200	GLN	OE1-CD-NE2	-6.53	116.08	122.60
2	B	245	GLY	N-CA-C	-6.52	106.73	115.21
2	B	134	THR	OG1-CB-CG2	6.51	122.32	109.30
2	B	65	GLY	O-C-N	-6.51	114.72	123.64
2	B	33	LEU	N-CA-CB	-6.47	99.30	110.17
2	B	188	THR	CB-CA-C	-6.47	96.24	109.38
2	B	161	CYS	O-C-N	-6.47	115.18	122.75
2	B	11	VAL	CG1-CB-CG2	-6.47	96.57	110.80
2	B	98	PRO	CB-CA-C	6.47	122.25	112.55
1	A	172	ARG	CB-CG-CD	6.46	126.16	111.30
1	A	27	TYR	CA-C-O	-6.46	113.66	120.63
2	B	25	PHE	CA-CB-CG	-6.45	107.35	113.80
1	A	130	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	A	144	THR	CA-CB-CG2	6.45	121.46	110.50
1	A	149	ARG	CA-C-O	-6.43	111.71	119.49
1	A	207	GLY	N-CA-C	-6.42	106.82	115.36
2	B	45	LEU	CA-C-O	6.42	127.16	120.30
2	B	223	LYS	CA-C-O	-6.42	112.29	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	SER	O-C-N	6.41	131.24	123.16
2	B	138	GLU	N-CA-C	6.41	119.06	109.25
1	A	109	GLY	O-C-N	-6.41	115.79	122.13
2	B	164	GLY	CA-C-O	-6.37	109.48	120.57
1	A	168	LEU	CA-C-N	6.36	128.71	120.44
1	A	168	LEU	C-N-CA	6.36	128.71	120.44
2	B	84	ALA	N-CA-CB	-6.36	100.75	110.16
1	A	136	THR	O-C-N	-6.36	115.52	122.07
2	B	14	ASN	N-CA-C	6.35	120.34	112.47
2	B	17	ASN	CB-CG-ND2	-6.34	106.89	116.40
1	A	165	ASN	O-C-N	-6.33	114.53	120.55
2	B	128	TRP	O-C-N	-6.33	114.63	123.11
2	B	200	VAL	CB-CA-C	6.32	121.66	111.29
2	B	4	SER	O-C-N	-6.32	114.94	123.15
2	B	103	VAL	N-CA-C	6.32	118.58	108.85
2	B	193	SER	N-CA-C	6.31	124.24	110.80
2	B	83	GLU	OE1-CD-OE2	-6.29	107.80	122.90
2	B	117	VAL	CA-C-N	6.28	133.32	122.64
2	B	117	VAL	C-N-CA	6.28	133.32	122.64
2	B	44	GLN	CG-CD-NE2	6.28	125.82	116.40
1	A	125	PRO	N-CA-C	6.27	121.06	111.15
1	A	89	SER	N-CA-CB	-6.26	99.91	110.49
1	A	112	PRO	O-C-N	6.24	130.03	122.23
1	A	132	ILE	O-C-N	-6.24	115.40	121.83
2	B	66	TYR	CA-C-O	-6.24	111.44	119.80
2	B	79	THR	CA-CB-OG1	-6.23	100.25	109.60
2	B	92	ASN	O-C-N	-6.23	114.39	122.37
2	B	94	THR	N-CA-C	6.23	118.13	109.15
2	B	72	VAL	CB-CA-C	6.22	120.05	110.96
2	B	209	GLN	CB-CA-C	6.21	120.80	109.99
2	B	113	THR	O-C-N	-6.20	114.58	123.07
1	A	10	ALA	CA-C-O	6.19	129.36	120.51
1	A	226	ASN	CA-C-O	6.17	127.67	120.75
1	A	43	SER	N-CA-C	-6.17	103.28	111.24
2	B	23	ASP	CA-CB-CG	-6.17	106.43	112.60
2	B	93	GLY	CA-C-N	6.17	131.28	121.66
2	B	93	GLY	C-N-CA	6.17	131.28	121.66
1	A	71	VAL	O-C-N	-6.16	115.04	122.06
1	A	213	ILE	O-C-N	-6.15	116.54	123.18
2	B	208	GLY	O-C-N	-6.15	114.70	122.70
2	B	192	ASP	CA-C-N	6.14	133.28	121.54
2	B	192	ASP	C-N-CA	6.14	133.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	VAL	CA-CB-CG2	-6.14	99.96	110.40
2	B	21	ARG	N-CA-CB	6.14	119.08	109.69
1	A	48	GLU	CB-CG-CD	6.14	123.03	112.60
2	B	163	SER	O-C-N	-6.12	115.05	122.71
2	B	210	ARG	CG-CD-NE	6.12	125.47	112.00
1	A	59	ASN	CB-CG-ND2	6.12	125.58	116.40
1	A	93	GLY	O-C-N	-6.12	114.75	122.70
2	B	63	THR	O-C-N	-6.11	115.65	122.86
2	B	177	ILE	CA-C-O	6.11	127.81	120.66
1	A	237	MET	O-C-N	-6.11	114.57	122.94
2	B	106	ALA	CA-C-N	6.10	133.19	121.54
2	B	106	ALA	C-N-CA	6.10	133.19	121.54
1	A	34	SER	CA-C-O	6.10	127.78	120.28
1	A	182	LEU	CA-C-O	6.09	127.05	120.05
1	A	211	ASN	N-CA-CB	6.09	121.74	111.39
2	B	161	CYS	CA-C-N	6.08	132.75	121.62
2	B	161	CYS	C-N-CA	6.08	132.75	121.62
2	B	141	ILE	N-CA-C	-6.08	98.37	107.37
2	B	165	LYS	O-C-N	-6.08	114.50	122.59
1	A	34	SER	CA-C-N	6.08	130.76	122.07
1	A	34	SER	C-N-CA	6.08	130.76	122.07
1	A	165	ASN	N-CA-CB	-6.06	98.63	110.08
2	B	14	ASN	CB-CA-C	-6.06	101.85	111.48
2	B	10	ILE	CA-C-O	6.05	127.01	120.53
2	B	81	VAL	N-CA-C	-6.05	99.64	108.11
2	B	163	SER	N-CA-CB	-6.04	103.16	110.53
2	B	49	LYS	CA-CB-CG	-6.04	102.02	114.10
2	B	255	PHE	N-CA-CB	-6.03	100.24	110.50
2	B	13	ARG	NH1-CZ-NH2	6.03	127.14	119.30
2	B	189	SER	CA-CB-OG	6.02	123.14	111.10
1	A	54	LEU	CA-C-N	-6.02	115.73	123.19
1	A	54	LEU	C-N-CA	-6.02	115.73	123.19
1	A	35	ASN	N-CA-CB	6.01	120.80	111.84
1	A	70	ASP	O-C-N	-6.01	114.66	122.77
1	A	224	LEU	CA-C-O	-6.01	113.71	120.32
2	B	233	PRO	CA-C-O	-6.00	110.60	119.18
2	B	189	SER	O-C-N	-5.98	115.33	122.63
2	B	72	VAL	CA-C-O	5.98	126.93	120.53
1	A	104	SER	O-C-N	-5.98	116.22	123.27
1	A	9	THR	CA-C-O	5.97	133.05	121.35
1	A	175	ILE	CA-C-O	-5.97	114.85	121.05
1	A	202	GLN	O-C-N	-5.96	114.66	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	N-CA-C	5.96	129.12	111.07
1	A	14	GLY	CA-C-N	-5.96	111.83	120.29
1	A	14	GLY	C-N-CA	-5.96	111.83	120.29
2	B	8	VAL	N-CA-C	5.96	117.67	108.44
1	A	134	SER	CA-C-N	-5.95	111.97	120.42
1	A	134	SER	C-N-CA	-5.95	111.97	120.42
2	B	51	ASP	CB-CA-C	-5.95	98.03	110.17
1	A	186	TYR	CB-CA-C	5.94	120.11	110.96
1	A	60	SER	O-C-N	5.93	128.91	122.15
1	A	95	GLY	CA-C-O	5.92	128.48	121.91
1	A	229	ASP	CA-C-N	5.92	128.71	122.14
1	A	229	ASP	C-N-CA	5.92	128.71	122.14
2	B	254	VAL	O-C-N	5.92	129.43	123.10
1	A	238	LEU	CA-C-O	-5.91	114.59	120.98
2	B	218	ALA	CA-C-N	-5.91	115.19	122.93
2	B	218	ALA	C-N-CA	-5.91	115.19	122.93
2	B	46	TRP	O-C-N	-5.90	116.33	123.29
1	A	98	THR	N-CA-C	5.89	117.38	111.07
2	B	173	GLY	O-C-N	-5.89	116.06	122.54
2	B	107	SER	CA-CB-OG	-5.89	99.32	111.10
1	A	87	PHE	CB-CA-C	-5.88	101.73	110.62
2	B	28	GLY	N-CA-C	-5.88	106.40	114.64
1	A	146	THR	CA-CB-CG2	5.88	120.50	110.50
2	B	142	TYR	CB-CA-C	5.88	119.56	109.51
2	B	21	ARG	CA-C-N	5.87	132.45	123.47
2	B	21	ARG	C-N-CA	5.87	132.45	123.47
2	B	41	ASP	N-CA-CB	5.86	119.18	109.98
1	A	187	MET	CG-SD-CE	5.85	113.77	100.90
1	A	81	ALA	CA-C-N	-5.84	109.97	121.41
1	A	81	ALA	C-N-CA	-5.84	109.97	121.41
1	A	70	ASP	CA-C-O	5.83	127.56	120.62
2	B	96	ILE	CB-CG1-CD1	-5.83	101.56	113.80
1	A	102	ARG	CA-C-N	5.83	131.91	122.29
1	A	102	ARG	C-N-CA	5.83	131.91	122.29
1	A	10	ALA	O-C-N	-5.83	114.84	122.59
2	B	64	TYR	O-C-N	5.82	128.78	122.15
1	A	136	THR	N-CA-C	5.81	117.29	111.07
2	B	209	GLN	CB-CG-CD	5.81	122.48	112.60
1	A	117	TYR	CB-CA-C	-5.81	99.98	109.56
2	B	94	THR	CA-C-O	-5.80	113.72	120.62
2	B	182	ASN	CB-CA-C	-5.78	103.84	111.82
2	B	248	ASN	CB-CG-OD1	5.77	132.35	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	SER	CB-CA-C	-5.76	98.96	110.42
2	B	206	ALA	O-C-N	-5.75	115.90	122.68
2	B	23	ASP	OD1-CG-OD2	5.74	136.67	122.90
1	A	70	ASP	CA-C-N	5.73	130.43	120.86
1	A	70	ASP	C-N-CA	5.73	130.43	120.86
2	B	223	LYS	O-C-N	5.73	130.04	122.30
2	B	193	SER	O-C-N	-5.72	114.97	122.59
2	B	190	GLY	CA-C-N	5.72	129.69	122.77
2	B	190	GLY	C-N-CA	5.72	129.69	122.77
2	B	201	SER	O-C-N	-5.71	116.88	123.33
1	A	222	VAL	CA-C-O	-5.70	114.24	121.48
2	B	13	ARG	NE-CZ-NH1	-5.70	115.80	121.50
2	B	60	CYS	CA-CB-SG	5.69	127.48	114.40
1	A	224	LEU	N-CA-C	-5.68	99.27	108.52
2	B	27	ASP	O-C-N	-5.67	115.92	122.95
2	B	43	ASN	CA-C-O	-5.66	112.64	119.49
1	A	121	ARG	CB-CA-C	-5.66	97.81	110.21
2	B	180	GLU	CA-CB-CG	5.66	125.42	114.10
2	B	184	ALA	N-CA-C	-5.66	106.36	113.72
1	A	208	VAL	CA-C-O	5.65	126.75	120.59
1	A	115	GLU	CA-CB-CG	5.64	125.38	114.10
2	B	12	GLY	CA-C-O	-5.63	116.31	121.72
2	B	56	SER	CA-C-N	5.63	132.30	121.54
2	B	56	SER	C-N-CA	5.63	132.30	121.54
2	B	206	ALA	N-CA-CB	-5.63	102.64	110.29
2	B	240	ILE	CB-CG1-CD1	-5.61	102.01	113.80
2	B	13	ARG	CG-CD-NE	5.61	124.34	112.00
2	B	200	VAL	CA-CB-CG2	-5.61	100.87	110.40
2	B	211	TRP	N-CA-C	5.60	118.61	109.59
1	A	225	THR	CA-CB-OG1	-5.60	101.21	109.60
2	B	31	ILE	N-CA-C	-5.60	100.42	108.53
2	B	65	GLY	CA-C-O	5.60	127.20	121.21
2	B	125	GLY	CA-C-N	-5.60	113.70	122.49
2	B	125	GLY	C-N-CA	-5.60	113.70	122.49
1	A	68	ALA	CA-C-N	-5.59	115.88	122.93
1	A	68	ALA	C-N-CA	-5.59	115.88	122.93
2	B	75	PHE	CA-C-O	5.59	127.25	120.99
2	B	177	ILE	CB-CG1-CD1	5.59	125.54	113.80
1	A	153	ILE	CA-C-N	5.58	128.01	120.65
1	A	153	ILE	C-N-CA	5.58	128.01	120.65
1	A	141	PRO	N-CA-C	5.57	119.34	110.21
2	B	233	PRO	N-CA-C	5.57	121.08	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	VAL	N-CA-CB	5.56	118.81	111.25
1	A	225	THR	CA-CB-CG2	5.56	119.94	110.50
2	B	19	ASP	O-C-N	-5.55	116.16	123.21
2	B	186	CYS	N-CA-C	5.54	118.46	108.48
1	A	134	SER	CA-CB-OG	-5.54	100.02	111.10
2	B	109	GLY	CA-C-N	-5.54	113.43	122.57
2	B	109	GLY	C-N-CA	-5.54	113.43	122.57
2	B	196	GLY	O-C-N	-5.54	115.50	122.70
2	B	20	VAL	N-CA-CB	5.54	117.31	111.00
2	B	159	GLU	CB-CG-CD	-5.53	103.19	112.60
1	A	8	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	121	ARG	CA-CB-CG	5.53	125.15	114.10
1	A	159	SER	O-C-N	-5.52	116.13	122.09
1	A	87	PHE	CA-CB-CG	-5.52	108.28	113.80
2	B	59	SER	CA-C-O	-5.52	114.92	121.16
2	B	224	ASN	O-C-N	-5.50	114.87	122.46
1	A	38	PRO	O-C-N	-5.49	116.39	123.03
2	B	76	ASP	O-C-N	-5.48	115.57	123.07
1	A	201	VAL	O-C-N	-5.47	115.73	122.57
2	B	84	ALA	CA-C-O	5.47	126.22	120.42
1	A	125	PRO	CB-CA-C	-5.46	104.63	111.56
2	B	203	SER	CB-CA-C	-5.46	101.68	110.74
1	A	230	VAL	CB-CA-C	-5.45	104.74	110.62
2	B	126	GLN	CB-CA-C	5.44	119.84	111.02
1	A	31	GLY	N-CA-C	-5.44	107.52	114.37
2	B	209	GLN	N-CA-C	-5.44	105.45	113.61
1	A	112	PRO	N-CA-C	-5.43	106.12	113.40
2	B	16	MET	CA-C-O	-5.42	115.00	121.56
2	B	197	VAL	N-CA-CB	5.41	118.86	110.14
2	B	111	LYS	O-C-N	-5.41	116.22	122.87
2	B	20	VAL	CA-C-N	5.41	128.44	120.82
2	B	20	VAL	C-N-CA	5.41	128.44	120.82
2	B	112	GLY	CA-C-N	-5.40	112.68	121.26
2	B	112	GLY	C-N-CA	-5.40	112.68	121.26
1	A	83	SER	N-CA-C	-5.39	104.60	113.50
2	B	120	LEU	CA-C-O	-5.39	114.61	120.81
2	B	222	LEU	N-CA-C	5.39	117.58	111.11
1	A	96	GLY	CA-C-N	-5.38	114.09	122.16
1	A	96	GLY	C-N-CA	-5.38	114.09	122.16
2	B	221	ASN	CA-CB-CG	-5.38	107.22	112.60
2	B	242	PRO	CA-C-O	5.38	127.45	121.43
1	A	14	GLY	N-CA-C	-5.37	106.28	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	PRO	O-C-N	-5.37	117.72	122.93
1	A	156	GLN	CA-C-O	-5.37	115.19	120.82
2	B	115	LEU	CA-C-O	-5.36	114.93	121.36
2	B	226	LEU	N-CA-CB	-5.35	102.97	110.25
1	A	136	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	198	SER	N-CA-CB	-5.34	102.26	110.12
2	B	18	VAL	O-C-N	-5.34	115.89	122.57
1	A	35	ASN	CB-CG-OD1	-5.34	110.12	120.80
2	B	80	ALA	O-C-N	-5.34	115.49	122.59
2	B	246	LYS	CA-C-O	5.33	127.30	121.01
1	A	140	PHE	N-CA-CB	-5.33	99.94	110.70
1	A	63	ASP	CA-C-O	-5.32	115.91	121.55
2	B	58	GLY	CA-C-N	-5.32	114.30	122.87
2	B	58	GLY	C-N-CA	-5.32	114.30	122.87
1	A	37	ILE	CA-C-O	5.32	122.65	119.19
1	A	71	VAL	N-CA-CB	-5.31	100.26	110.78
2	B	198	ASN	CA-C-O	-5.31	115.63	121.31
2	B	51	ASP	CB-CG-OD2	-5.29	106.23	118.40
1	A	34	SER	N-CA-CB	5.29	119.69	110.81
1	A	42	GLN	CA-C-O	5.29	128.00	121.87
2	B	113	THR	CA-C-N	5.28	128.37	120.87
2	B	113	THR	C-N-CA	5.28	128.37	120.87
1	A	164	PHE	CB-CA-C	-5.27	101.71	110.14
1	A	230	VAL	O-C-N	-5.26	115.29	122.03
1	A	50	GLY	N-CA-C	-5.26	100.71	113.18
1	A	56	GLU	CA-C-O	5.26	125.93	120.30
1	A	13	THR	N-CA-C	5.25	118.56	110.42
1	A	158	ILE	N-CA-CB	5.25	119.90	111.23
1	A	156	GLN	CG-CD-NE2	-5.25	108.52	116.40
1	A	33	PHE	CA-C-O	-5.25	115.30	121.44
2	B	240	ILE	CB-CA-C	5.24	117.98	110.33
2	B	123	THR	OG1-CB-CG2	-5.24	98.82	109.30
2	B	132	ASN	CA-C-N	-5.24	113.68	122.17
2	B	132	ASN	C-N-CA	-5.24	113.68	122.17
2	B	177	ILE	O-C-N	-5.24	116.02	122.88
2	B	227	ALA	N-CA-C	5.24	117.96	109.06
2	B	99	ARG	CB-CA-C	-5.24	102.10	110.79
1	A	51	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	B	60	CYS	N-CA-CB	-5.23	101.88	110.41
2	B	198	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	B	78	ALA	N-CA-C	5.23	116.78	111.14
1	A	11	GLN	CG-CD-NE2	5.22	124.23	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	B	30	GLN	N-CA-C	5.21	118.50	110.42
2	B	162	SER	N-CA-C	-5.21	100.82	108.79
1	A	115	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	A	163	ARG	CA-C-O	5.19	126.00	120.24
2	B	87	TRP	CA-CB-CG	-5.19	103.74	113.60
1	A	222	VAL	CA-CB-CG1	5.19	119.22	110.40
2	B	141	ILE	O-C-N	5.18	129.67	122.88
2	B	53	THR	O-C-N	-5.17	117.11	122.96
2	B	112	GLY	N-CA-C	-5.17	108.19	114.92
1	A	100	THR	OG1-CB-CG2	-5.17	98.97	109.30
1	A	102	ARG	CD-NE-CZ	5.15	131.61	124.40
2	B	8	VAL	CA-CB-CG1	5.15	119.16	110.40
1	A	212	PRO	N-CA-C	-5.15	103.97	111.33
2	B	182	ASN	N-CA-C	5.14	118.01	107.37
2	B	22	ASP	CA-C-O	5.14	126.03	120.12
2	B	193	SER	CA-C-O	-5.13	113.18	120.51
1	A	117	TYR	CA-CB-CG	-5.12	104.68	113.90
1	A	205	THR	O-C-N	-5.12	114.75	122.28
2	B	51	ASP	N-CA-C	5.12	119.16	113.01
2	B	60	CYS	O-C-N	-5.12	117.33	123.06
2	B	200	VAL	CA-CB-CG1	5.12	119.10	110.40
1	A	52	PHE	CA-C-N	-5.11	115.01	122.68
1	A	52	PHE	C-N-CA	-5.11	115.01	122.68
2	B	137	ARG	CA-CB-CG	5.11	124.33	114.10
2	B	153	GLY	N-CA-C	5.11	125.28	113.18
2	B	67	THR	O-C-N	5.10	129.49	123.27
1	A	123	GLN	CA-C-O	-5.10	113.78	119.95
2	B	167	ASP	N-CA-C	-5.09	105.97	113.61
1	A	29	SER	CA-C-N	5.09	127.10	120.28
1	A	29	SER	C-N-CA	5.09	127.10	120.28
1	A	133	GLN	N-CA-C	-5.08	105.93	111.82
2	B	94	THR	O-C-N	-5.08	115.92	122.77
2	B	200	VAL	CA-C-N	5.08	130.83	121.85
2	B	200	VAL	C-N-CA	5.08	130.83	121.85
2	B	3	ALA	CB-CA-C	5.07	118.58	110.16
2	B	55	ARG	NH1-CZ-NH2	5.07	125.89	119.30
2	B	185	GLN	N-CA-C	5.07	118.28	110.42
1	A	240	VAL	N-CA-C	-5.07	108.90	113.71
2	B	150	GLU	CA-CB-CG	-5.06	103.97	114.10
1	A	17	TYR	CA-C-N	5.06	127.32	120.44
1	A	17	TYR	C-N-CA	5.06	127.32	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	VAL	CB-CA-C	-5.06	104.05	110.98
1	A	6	LEU	N-CA-C	5.05	117.80	109.72
1	A	119	GLY	N-CA-C	-5.04	106.64	112.29
2	B	62	THR	O-C-N	-5.04	117.30	123.30
1	A	29	SER	CA-C-O	5.04	126.42	120.58
1	A	78	ALA	N-CA-CB	-5.03	103.19	111.69
1	A	59	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	180	SER	N-CA-CB	5.01	118.57	111.05
2	B	86	VAL	CB-CA-C	5.01	117.02	110.96
2	B	167	ASP	CB-CG-OD1	-5.01	106.88	118.40
2	B	21	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	B	249	GLN	CA-C-O	5.00	126.81	120.65

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	1777	118	0
2	B	1897	0	1821	137	1
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	3637	252	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 34.

All (252) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:217:ASP:O	1:A:218:PRO:C	2.35	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
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:224:ASN:HD22	2:B:224:ASN:C	2.03	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:203:SER:O	2:B:204:GLY:C	2.38	0.66
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:109:GLY:O	1:A:110:SER:C	2.40	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: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:37:ILE:HB	1:A:237:MET:HE2	1.79	0.64
1:A:9:THR:O	1:A:132:ILE:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:ASN:O	1:A:36:ALA:HB3	1.97	0.62
1:A:84:GLN:NE2	1:A:101:THR:HB	2.14	0.62
1:A:230:VAL:O	1:A:231:ILE:C	2.41	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:16:MET:HE1	2:B:111:LYS:HB2	1.81	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:219:ILE:HD12	2:B:228:MET:HE2	1.82	0.61
1:A:59:ASN:HD21	1:A:63:ASP:H	1.50	0.60
1:A:160:GLU:CD	1:A:191:GLU:HG2	2.26	0.60
1:A:141:PRO:HA	4:A:326:HOH:O	2.01	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
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:85:SER:HG	1:A:87:PHE:HE1	1.51	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:226:ASN:O	1:A:227:VAL:C	2.46	0.57
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:43:SER:O	1:A:44:GLY:C	2.48	0.56
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
2:B:22:ASP:O	2:B:23:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:O	1:A:175:ILE:C	2.47	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
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:149:MET:SD	2:B:228:MET:HE1	2.49	0.53
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: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
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
2:B:143:GLY:O	2:B:144:PHE:C	2.53	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
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
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
2:B:37:LYS:O	2:B:38:SER:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:200:GLN:O	1:A:201:VAL:C	2.56	0.48
2:B:216:GLU:CD	2:B:216:GLU:H	2.21	0.48
1:A:152:LEU:O	1:A:153:ILE:C	2.56	0.48
1:A:165:ASN:O	1:A:166:PRO:C	2.53	0.48
1:A:37:ILE:CB	1:A:237:MET:HE2	2.41	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:145:ASN:N	2:B:145:ASN:ND2	2.54	0.47
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.50	0.47
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
2:B:51:ASP:C	2:B:51:ASP:OD1	2.57	0.46
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:67:THR:O	2:B:68:ALA:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:CG2	1:A:237:MET:HE2	2.46	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:149:MET:HE1	2:B:187:LEU:HD21	1.98	0.45
2:B:48:ILE:HD13	2:B:48:ILE:N	2.31	0.45
2:B:241:TYR:O	2:B:242:PRO:C	2.59	0.45
1:A:181:PHE:HE2	1:A:187:MET:HE1	1.81	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
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
1:A:217:ASP:O	1:A:219:GLY:N	2.51	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
2:B:26:HIS:O	2:B:27:ASP:C	2.58	0.44
2:B:224:ASN:C	2:B:224:ASN:ND2	2.71	0.44
1:A:47:GLY:O	1:A:48:GLU:C	2.59	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: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
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
1:A:115:GLU:CD	1:A:152:LEU:HD21	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:123:THR:O	2:B:124:LEU:C	2.63	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:221:ASN:O	2:B:222:LEU:C	2.62	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
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:81:VAL:O	2:B:82:GLY:C	2.63	0.41
2:B:121:ASP:OD1	2:B:123:THR:OG1	2.25	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: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:186:CYS:O	2:B:187:LEU:C	2.64	0.41
2:B:79:THR:O	2:B:80:ALA:O	2.39	0.41
2:B:235:GLY:O	2:B:236:GLY:C	2.64	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
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%)	196 (82%)	29 (12%)	14 (6%)	1	2
2	B	253/255 (99%)	217 (86%)	24 (10%)	12 (5%)	2	3
All	All	492/496 (99%)	413 (84%)	53 (11%)	26 (5%)	1	3

All (26) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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	193/193 (100%)	135 (70%)	58 (30%)	0	1
2	B	203/203 (100%)	161 (79%)	42 (21%)	1	3
All	All	396/396 (100%)	296 (75%)	100 (25%)	0	2

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	LEU
1	A	8	VAL
1	A	9	THR
1	A	12	THR
1	A	24	LEU
1	A	25	ARG
1	A	30	SER
1	A	34	SER
1	A	42	GLN
1	A	48	GLU
1	A	54	LEU
1	A	58	THR

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Mol	Chain	Res	Type
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	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
1	A	159	SER
1	A	160	GLU
1	A	168	LEU
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	208	VAL
1	A	215	LEU
1	A	222	VAL
1	A	226	ASN

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Mol	Chain	Res	Type
1	A	228	ARG
1	A	229	ASP
1	A	238	LEU
2	B	2	SER
2	B	4	SER
2	B	8	VAL
2	B	17	ASN
2	B	20	VAL
2	B	30	GLN
2	B	36	SER
2	B	38	SER
2	B	41	ASP
2	B	45	LEU
2	B	48	ILE
2	B	88	GLN
2	B	95	ILE
2	B	96	ILE
2	B	97	ASN
2	B	107	SER
2	B	108	SER
2	B	115	LEU
2	B	116	THR
2	B	119	THR
2	B	123	THR
2	B	126	GLN
2	B	129	LEU
2	B	134	THR
2	B	137	ARG
2	B	145	ASN
2	B	149	MET
2	B	155	SER
2	B	160	THR
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

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Mol	Chain	Res	Type
2	B	216	GLU
2	B	224	ASN
2	B	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	59	ASN
1	A	84	GLN
1	A	108	ASN
1	A	120	GLN
1	A	123	GLN
1	A	173	GLN
1	A	176	ASN
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	126	GLN
2	B	145	ASN
2	B	183	GLN
2	B	185	GLN
2	B	198	ASN
2	B	221	ASN
2	B	224	ASN
2	B	248	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 [i](#)

There are no oligosaccharides 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	1.29	2 (14%)	17,19,21	2.87	9 (52%)
3	NAG	A	303	-	14,14,15	1.13	1 (7%)	17,19,21	2.75	6 (35%)
3	NAG	B	301	2	14,14,15	1.49	2 (14%)	17,19,21	3.38	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	-	-	5/6/23/26	0/1/1/1
3	NAG	B	301	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	O7-C7	-4.16	1.13	1.23
3	A	303	NAG	O7-C7	-3.30	1.15	1.23
3	B	302	NAG	O7-C7	-3.05	1.16	1.23
3	B	301	NAG	O5-C5	-2.19	1.39	1.43
3	B	302	NAG	C1-C2	-2.03	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAG	C1-O5-C5	12.73	129.25	112.19
3	A	303	NAG	C4-C3-C2	-7.73	99.69	111.02
3	B	302	NAG	C3-C4-C5	-5.37	100.50	110.23
3	B	302	NAG	O3-C3-C4	5.14	122.49	110.38
3	B	302	NAG	O4-C4-C3	4.92	121.96	110.38
3	A	303	NAG	C1-O5-C5	-4.15	106.63	112.19
3	A	303	NAG	O3-C3-C2	4.14	117.99	109.40
3	B	302	NAG	O7-C7-C8	3.64	128.53	122.05
3	A	303	NAG	C8-C7-N2	3.35	121.68	116.12
3	B	301	NAG	C4-C3-C2	-3.34	106.12	111.02
3	B	302	NAG	O5-C1-C2	-3.34	106.12	111.29
3	A	303	NAG	O7-C7-N2	-3.22	116.28	121.98
3	B	301	NAG	O5-C1-C2	-3.00	106.65	111.29
3	B	302	NAG	O7-C7-N2	-2.90	116.86	121.98
3	B	302	NAG	O4-C4-C5	-2.56	103.02	109.32
3	B	302	NAG	C1-O5-C5	2.43	115.45	112.19
3	B	301	NAG	C6-C5-C4	-2.21	107.59	113.02
3	A	303	NAG	O5-C5-C6	-2.19	103.41	107.66
3	B	302	NAG	O3-C3-C2	-2.13	104.98	109.40

There are no chirality outliers.

All (9) 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	B	302	NAG	O5-C5-C6-O6
3	B	301	NAG	C4-C5-C6-O6
3	A	303	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.