



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:26 PM UTC

PDB ID : 2REN / pdb_00002ren
Title : STRUCTURE OF RECOMBINANT HUMAN RENIN, A TARGET FOR CARDIOVASCULAR-ACTIVE DRUGS, AT 2.5 ANGSTROMS RESOLUTION
Authors : Sielecki, A.R.; James, M.N.G.
Deposited on : 1992-02-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

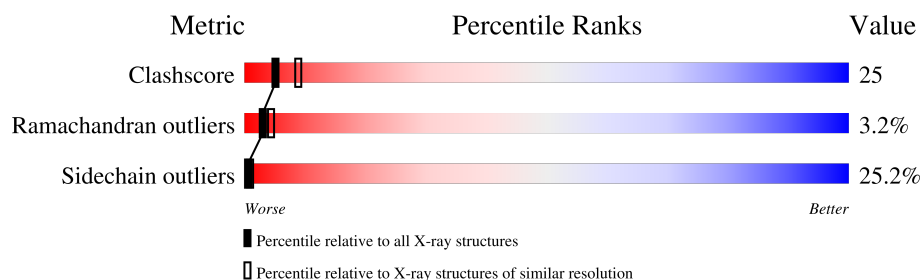
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	340	21% 40% 28% 5% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	341	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2469 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2455	1569	396	476	14	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



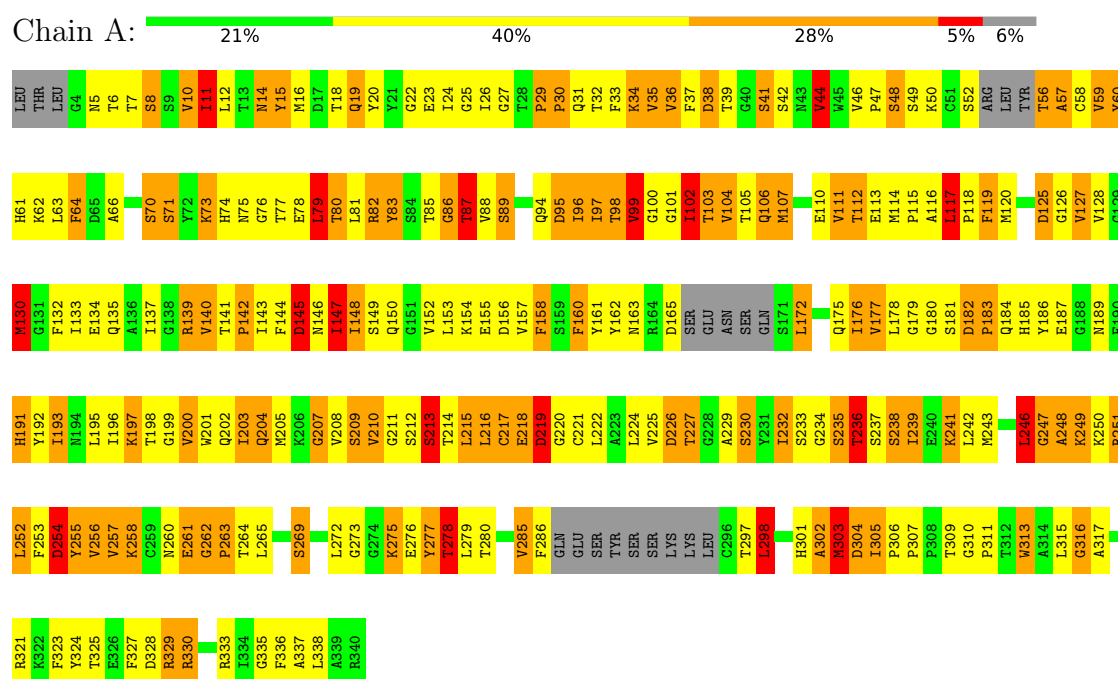
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

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: RENIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	134.08Å 134.08Å 41.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS, PROLSQ, X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2469	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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	1.24	2/2510 (0.1%)	2.88	288/3402 (8.5%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	THR	CA-CB	5.26	1.59	1.52
1	A	180	GLY	N-CA	5.07	1.50	1.45

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	PHE	CA-C-O	16.66	144.33	120.51
1	A	253	PHE	CA-CB-CG	-16.29	97.51	113.80
1	A	307	PRO	N-CA-C	-15.38	95.70	110.47
1	A	253	PHE	CA-C-N	15.30	150.76	121.54
1	A	253	PHE	C-N-CA	15.30	150.76	121.54
1	A	6	THR	N-CA-C	11.83	128.03	110.52
1	A	329	ARG	NE-CZ-NH2	-11.64	108.73	119.20
1	A	11	ILE	CB-CA-C	11.55	127.26	110.98
1	A	107	MET	CA-C-O	-11.48	107.71	120.92
1	A	254	ASP	CA-CB-CG	-11.00	101.60	112.60
1	A	203	ILE	CB-CA-C	10.70	126.25	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ILE	CA-C-O	-10.70	108.93	120.59
1	A	58	CYS	N-CA-C	-10.68	100.39	113.41
1	A	212	SER	N-CA-CB	10.42	131.80	111.07
1	A	336	PHE	CA-CB-CG	10.31	124.11	113.80
1	A	211	GLY	CA-C-N	10.21	135.89	120.17
1	A	211	GLY	C-N-CA	10.21	135.89	120.17
1	A	328	ASP	CA-CB-CG	10.07	122.67	112.60
1	A	30	PRO	N-CA-C	9.97	126.39	111.03
1	A	252	LEU	CA-C-O	9.91	134.43	122.14
1	A	307	PRO	CB-CA-C	9.56	120.38	111.39
1	A	99	VAL	CB-CA-C	9.43	122.95	110.12
1	A	102	ILE	N-CA-C	-9.37	94.63	108.12
1	A	221	CYS	CA-C-O	-9.34	111.24	121.33
1	A	212	SER	N-CA-C	-9.32	98.12	113.50
1	A	252	LEU	CA-C-N	9.24	139.19	121.54
1	A	252	LEU	C-N-CA	9.24	139.19	121.54
1	A	107	MET	N-CA-C	-9.22	94.47	109.96
1	A	207	GLY	N-CA-C	9.09	124.14	112.68
1	A	126	GLY	CA-C-O	-9.01	112.86	121.41
1	A	184	GLN	OE1-CD-NE2	8.99	131.59	122.60
1	A	82	ARG	N-CA-C	8.66	123.01	109.07
1	A	135	GLN	OE1-CD-NE2	8.65	131.25	122.60
1	A	6	THR	CA-C-N	8.64	135.02	121.72
1	A	6	THR	C-N-CA	8.64	135.02	121.72
1	A	191	HIS	CA-C-O	-8.54	110.84	120.32
1	A	37	PHE	CB-CA-C	8.43	123.85	110.19
1	A	263	PRO	CA-C-N	8.42	132.41	120.28
1	A	263	PRO	C-N-CA	8.42	132.41	120.28
1	A	329	ARG	CA-C-O	-8.34	111.58	120.42
1	A	325	THR	CA-CB-OG1	-8.29	97.16	109.60
1	A	191	HIS	N-CA-C	-8.28	94.77	108.76
1	A	198	THR	CA-CB-CG2	8.22	124.47	110.50
1	A	64	PHE	CA-CB-CG	-8.21	105.59	113.80
1	A	20	TYR	CA-C-O	-8.19	111.52	120.36
1	A	218	GLU	CB-CG-CD	8.13	126.42	112.60
1	A	58	CYS	CB-CA-C	8.12	123.44	109.24
1	A	313	TRP	N-CA-C	-8.10	98.53	110.52
1	A	38	ASP	N-CA-C	8.06	124.55	107.70
1	A	60	TYR	N-CA-C	8.05	123.10	113.28
1	A	253	PHE	O-C-N	-8.04	111.89	122.59
1	A	278	THR	CA-C-N	8.04	134.58	122.93
1	A	278	THR	C-N-CA	8.04	134.58	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ILE	CB-CA-C	-8.03	101.25	110.96
1	A	103	THR	N-CA-C	-8.01	95.22	108.76
1	A	86	GLY	CA-C-O	7.89	132.41	122.23
1	A	112	THR	N-CA-CB	-7.85	99.11	110.65
1	A	232	ILE	N-CA-CB	7.84	120.38	111.21
1	A	5	ASN	CA-CB-CG	-7.83	104.78	112.60
1	A	31	GLN	N-CA-C	-7.76	96.08	108.73
1	A	127	VAL	CA-C-N	7.75	133.51	123.13
1	A	127	VAL	C-N-CA	7.75	133.51	123.13
1	A	301	HIS	CA-CB-CG	7.65	121.45	113.80
1	A	77	THR	CA-C-O	-7.58	112.28	120.92
1	A	6	THR	CA-CB-OG1	-7.54	98.30	109.60
1	A	233	SER	CA-C-O	7.48	130.22	121.46
1	A	323	PHE	O-C-N	7.37	131.89	123.27
1	A	31	GLN	O-C-N	7.32	131.56	123.22
1	A	83	TYR	N-CA-C	7.28	121.35	109.85
1	A	285	VAL	N-CA-C	-7.24	98.03	108.17
1	A	172	LEU	CA-CB-CG	7.22	141.59	116.30
1	A	329	ARG	NH1-CZ-NH2	7.22	128.68	119.30
1	A	76	GLY	CA-C-N	7.17	130.94	120.82
1	A	76	GLY	C-N-CA	7.17	130.94	120.82
1	A	249	LYS	CA-C-N	7.17	130.93	120.82
1	A	249	LYS	C-N-CA	7.17	130.93	120.82
1	A	146	ASN	CA-C-O	-7.14	113.35	120.70
1	A	301	HIS	CA-C-O	-7.11	113.55	121.51
1	A	119	PHE	N-CA-C	7.11	121.21	112.54
1	A	163	ASN	CA-CB-CG	7.08	119.67	112.60
1	A	191	HIS	N-CA-CB	7.06	123.02	110.80
1	A	76	GLY	N-CA-C	7.01	124.65	115.40
1	A	302	ALA	CA-C-O	-7.00	113.12	121.66
1	A	158	PHE	CA-C-N	6.98	135.20	122.92
1	A	158	PHE	C-N-CA	6.98	135.20	122.92
1	A	227	THR	O-C-N	6.96	130.36	122.22
1	A	261	GLU	CB-CG-CD	6.92	124.36	112.60
1	A	44	VAL	N-CA-C	-6.90	98.41	108.89
1	A	199	GLY	N-CA-C	-6.87	105.75	113.79
1	A	79	LEU	CB-CA-C	6.84	120.74	109.72
1	A	316	GLY	CA-C-O	-6.82	114.95	121.90
1	A	329	ARG	CD-NE-CZ	6.81	133.94	124.40
1	A	218	GLU	N-CA-C	-6.81	96.67	108.52
1	A	145	ASP	CA-C-N	6.79	129.68	120.44
1	A	145	ASP	C-N-CA	6.79	129.68	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	HIS	N-CA-C	6.78	121.62	112.88
1	A	130	MET	CA-C-N	6.77	131.47	121.05
1	A	130	MET	C-N-CA	6.77	131.47	121.05
1	A	226	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	251	ARG	CD-NE-CZ	6.76	133.87	124.40
1	A	94	GLN	OE1-CD-NE2	6.74	129.34	122.60
1	A	306	PRO	N-CA-C	6.72	118.89	110.70
1	A	181	SER	N-CA-CB	6.71	124.00	111.52
1	A	38	ASP	N-CA-CB	-6.69	99.96	110.87
1	A	181	SER	CA-C-O	-6.68	113.50	120.99
1	A	103	THR	CB-CA-C	6.68	121.78	109.70
1	A	111	VAL	CA-C-O	6.63	128.56	120.74
1	A	144	PHE	CA-C-O	-6.62	113.41	120.42
1	A	304	ASP	CB-CA-C	6.57	119.19	110.06
1	A	216	LEU	N-CA-C	-6.56	99.98	110.14
1	A	101	GLY	CA-C-N	6.54	132.08	122.99
1	A	101	GLY	C-N-CA	6.54	132.08	122.99
1	A	175	GLN	CA-C-N	6.53	131.28	123.19
1	A	175	GLN	C-N-CA	6.53	131.28	123.19
1	A	146	ASN	N-CA-CB	-6.50	100.64	110.07
1	A	323	PHE	CA-C-O	-6.50	113.35	120.24
1	A	184	GLN	O-C-N	6.49	131.41	122.46
1	A	307	PRO	O-C-N	6.47	124.29	121.31
1	A	95	ASP	CA-C-O	-6.44	114.23	121.25
1	A	50	LYS	N-CA-CB	6.42	120.27	110.44
1	A	237	SER	O-C-N	6.41	128.76	122.09
1	A	277	TYR	CA-CB-CG	-6.41	102.37	113.90
1	A	156	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	59	VAL	CB-CA-C	-6.38	103.69	112.04
1	A	117	LEU	O-C-N	6.37	128.65	121.32
1	A	191	HIS	O-C-N	6.35	130.74	123.31
1	A	25	GLY	CA-C-O	-6.33	114.56	120.57
1	A	86	GLY	CA-C-N	6.33	135.47	121.81
1	A	86	GLY	C-N-CA	6.33	135.47	121.81
1	A	31	GLN	CB-CA-C	6.32	120.43	110.19
1	A	200	VAL	CA-C-O	-6.30	114.60	121.28
1	A	307	PRO	CA-C-O	-6.29	116.37	120.90
1	A	5	ASN	O-C-N	6.27	130.97	122.82
1	A	73	LYS	N-CA-C	-6.26	95.36	107.44
1	A	87	THR	CA-CB-OG1	-6.23	100.25	109.60
1	A	146	ASN	OD1-CG-ND2	6.23	128.83	122.60
1	A	285	VAL	N-CA-CB	6.22	119.71	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	VAL	O-C-N	6.18	130.01	123.02
1	A	58	CYS	CA-C-O	6.18	126.40	119.41
1	A	130	MET	N-CA-CB	-6.18	101.49	110.70
1	A	79	LEU	CA-C-O	6.17	127.29	120.31
1	A	148	ILE	CA-CB-CG1	6.17	120.90	110.40
1	A	73	LYS	N-CA-CB	6.15	121.58	110.95
1	A	111	VAL	CA-C-N	6.14	132.02	122.26
1	A	111	VAL	C-N-CA	6.14	132.02	122.26
1	A	262	GLY	N-CA-C	-6.14	99.82	112.34
1	A	112	THR	CA-CB-OG1	-6.12	100.43	109.60
1	A	87	THR	N-CA-CB	6.10	120.90	110.77
1	A	142	PRO	CB-CA-C	6.09	119.02	111.23
1	A	177	VAL	O-C-N	6.07	129.75	123.20
1	A	338	LEU	CB-CA-C	6.05	119.58	109.89
1	A	46	VAL	CA-CB-CG1	6.01	120.62	110.40
1	A	52	SER	N-CA-CB	6.01	120.72	110.50
1	A	95	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	213	SER	N-CA-CB	-6.00	100.34	110.49
1	A	29	PRO	CA-C-N	5.98	126.29	119.83
1	A	29	PRO	C-N-CA	5.98	126.29	119.83
1	A	114	MET	O-C-N	5.97	127.11	121.38
1	A	44	VAL	CA-CB-CG1	5.97	120.55	110.40
1	A	104	VAL	N-CA-CB	-5.97	100.89	111.93
1	A	18	THR	OG1-CB-CG2	5.93	121.17	109.30
1	A	7	THR	N-CA-C	5.93	117.14	107.23
1	A	147	ILE	CA-C-O	-5.93	111.77	119.53
1	A	15	TYR	CA-C-N	5.92	130.81	122.46
1	A	15	TYR	C-N-CA	5.92	130.81	122.46
1	A	221	CYS	N-CA-C	-5.87	100.15	109.07
1	A	106	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	A	94	GLN	CA-CB-CG	-5.85	102.41	114.10
1	A	140	VAL	O-C-N	5.84	130.07	122.94
1	A	226	ASP	N-CA-C	5.84	119.43	107.69
1	A	154	LYS	N-CA-C	5.84	118.42	111.71
1	A	298	LEU	CB-CA-C	5.84	119.29	109.48
1	A	137	ILE	N-CA-CB	-5.83	105.22	111.46
1	A	313	TRP	CA-CB-CG	5.83	124.68	113.60
1	A	229	ALA	CA-C-O	5.82	127.68	121.05
1	A	11	ILE	CA-C-O	5.80	127.57	120.84
1	A	236	THR	O-C-N	5.79	128.11	122.09
1	A	275	LYS	N-CA-CB	-5.79	102.41	110.29
1	A	78	GLU	N-CA-CB	5.79	119.24	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASN	O-C-N	5.77	130.34	123.24
1	A	163	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	337	ALA	CA-C-N	-5.76	112.89	120.95
1	A	337	ALA	C-N-CA	-5.76	112.89	120.95
1	A	86	GLY	O-C-N	-5.73	116.98	123.11
1	A	213	SER	CA-C-O	-5.72	112.33	120.51
1	A	307	PRO	N-CA-CB	5.72	106.39	103.19
1	A	14	ASN	CA-C-O	5.72	127.02	120.84
1	A	161	TYR	CA-C-N	-5.71	115.12	123.00
1	A	161	TYR	C-N-CA	-5.71	115.12	123.00
1	A	315	LEU	CA-C-N	5.71	129.74	122.83
1	A	315	LEU	C-N-CA	5.71	129.74	122.83
1	A	42	SER	N-CA-C	5.70	122.15	113.61
1	A	101	GLY	CA-C-O	5.68	126.79	119.68
1	A	37	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	253	PHE	CB-CA-C	5.68	121.72	110.42
1	A	7	THR	CB-CA-C	-5.66	104.01	111.42
1	A	24	ILE	CB-CA-C	5.64	119.84	110.30
1	A	31	GLN	CA-C-O	-5.64	114.32	120.36
1	A	256	VAL	CB-CA-C	5.64	119.03	110.62
1	A	269	SER	N-CA-C	5.64	118.09	108.90
1	A	101	GLY	N-CA-C	5.64	124.35	114.76
1	A	60	TYR	N-CA-CB	-5.63	101.61	110.46
1	A	186	TYR	N-CA-C	-5.63	100.51	109.07
1	A	74	HIS	CA-C-N	5.63	130.84	122.17
1	A	74	HIS	C-N-CA	5.63	130.84	122.17
1	A	146	ASN	CB-CA-C	5.63	119.79	110.90
1	A	130	MET	CB-CA-C	5.63	120.22	110.94
1	A	213	SER	N-CA-C	5.62	122.77	110.80
1	A	83	TYR	N-CA-CB	-5.62	102.10	111.20
1	A	113	GLU	N-CA-CB	5.60	119.82	110.59
1	A	143	ILE	N-CA-C	5.59	117.00	110.62
1	A	10	VAL	CB-CA-C	5.55	118.43	110.33
1	A	178	LEU	CA-C-O	-5.53	114.84	120.71
1	A	66	ALA	CA-C-O	-5.49	114.05	120.20
1	A	5	ASN	N-CA-CB	5.49	118.72	109.94
1	A	31	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	A	49	SER	N-CA-C	-5.48	106.67	113.19
1	A	329	ARG	CA-CB-CG	-5.48	103.15	114.10
1	A	104	VAL	CA-CB-CG2	5.44	119.65	110.40
1	A	119	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	321	ARG	CA-C-N	5.44	129.93	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	C-N-CA	5.44	129.93	120.68
1	A	246	LEU	N-CA-CB	-5.43	101.31	110.49
1	A	256	VAL	N-CA-CB	-5.43	101.94	111.39
1	A	315	LEU	CB-CA-C	5.43	120.53	111.30
1	A	330	ARG	CB-CG-CD	5.42	123.76	111.30
1	A	19	GLN	O-C-N	5.41	129.60	123.27
1	A	183	PRO	CA-C-O	-5.40	111.34	119.55
1	A	63	LEU	N-CA-CB	-5.40	102.09	110.57
1	A	133	ILE	CA-CB-CG1	-5.40	101.23	110.40
1	A	305	ILE	O-C-N	5.39	126.26	121.41
1	A	172	LEU	N-CA-CB	-5.38	101.39	110.49
1	A	311	PRO	N-CD-CG	-5.38	97.34	103.80
1	A	184	GLN	CA-C-O	-5.38	112.05	119.05
1	A	241	LYS	N-CA-C	-5.38	104.97	112.45
1	A	280	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	71	SER	N-CA-CB	-5.35	102.37	111.20
1	A	335	GLY	N-CA-C	-5.35	101.82	111.19
1	A	277	TYR	CA-C-N	-5.35	114.92	122.94
1	A	277	TYR	C-N-CA	-5.35	114.92	122.94
1	A	105	THR	N-CA-CB	5.33	119.11	110.42
1	A	70	SER	CB-CA-C	-5.30	99.35	110.17
1	A	75	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	333	ARG	CD-NE-CZ	5.27	131.78	124.40
1	A	154	LYS	CA-C-N	5.27	131.44	121.69
1	A	154	LYS	C-N-CA	5.27	131.44	121.69
1	A	177	VAL	N-CA-C	-5.26	100.54	108.12
1	A	162	TYR	N-CA-C	-5.26	100.60	109.07
1	A	158	PHE	CB-CA-C	5.25	120.08	109.68
1	A	262	GLY	O-C-N	5.25	127.02	121.77
1	A	260	ASN	N-CA-C	-5.23	105.66	111.36
1	A	279	LEU	N-CA-CB	5.23	119.11	110.69
1	A	125	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	58	CYS	CA-C-N	5.22	127.89	120.53
1	A	58	CYS	C-N-CA	5.22	127.89	120.53
1	A	260	ASN	CB-CA-C	5.22	119.72	110.85
1	A	182	ASP	CB-CA-C	5.22	115.96	110.17
1	A	324	TYR	N-CA-C	-5.19	102.22	109.96
1	A	235	SER	CA-C-O	-5.19	115.90	121.56
1	A	304	ASP	N-CA-C	-5.18	102.53	110.30
1	A	219	ASP	CA-C-N	5.17	129.53	122.54
1	A	219	ASP	C-N-CA	5.17	129.53	122.54
1	A	19	GLN	CA-C-N	-5.16	115.71	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLN	C-N-CA	-5.16	115.71	122.99
1	A	36	VAL	CA-C-O	-5.16	114.47	121.02
1	A	324	TYR	O-C-N	5.16	129.87	123.01
1	A	116	ALA	N-CA-C	5.16	120.48	113.37
1	A	12	LEU	CA-CB-CG	5.15	134.33	116.30
1	A	241	LYS	CA-C-O	5.15	126.28	120.00
1	A	225	VAL	CB-CA-C	5.13	117.24	111.80
1	A	98	THR	N-CA-CB	5.09	118.76	110.77
1	A	160	PHE	CB-CA-C	-5.09	99.05	109.38
1	A	140	VAL	N-CA-C	-5.08	100.46	108.23
1	A	232	ILE	N-CA-C	-5.07	100.59	107.99
1	A	202	GLN	CA-C-N	-5.07	116.75	122.48
1	A	202	GLN	C-N-CA	-5.07	116.75	122.48
1	A	37	PHE	O-C-N	-5.06	117.45	123.22
1	A	162	TYR	CB-CA-C	5.06	118.47	109.72
1	A	239	ILE	CA-C-O	-5.06	115.16	120.57
1	A	337	ALA	O-C-N	5.05	129.01	123.25
1	A	99	VAL	O-C-N	5.04	128.23	123.03
1	A	7	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	12	LEU	CA-C-O	5.02	126.83	121.16
1	A	226	ASP	N-CA-CB	-5.02	102.41	110.69
1	A	323	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	73	LYS	CB-CG-CD	5.01	122.82	111.30
1	A	85	THR	O-C-N	5.00	128.25	122.09
1	A	16	MET	N-CA-C	5.00	118.10	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2382	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	0	0
All	All	2469	0	2395	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:HG2	1:A:255:TYR:CD1	1.88	1.06
1:A:215:LEU:HD12	1:A:218:GLU:HG3	1.39	1.03
1:A:269:SER:OG	1:A:278:THR:HB	1.74	0.87
1:A:305:ILE:O	1:A:310:GLY:HA3	1.75	0.84
1:A:145:ASP:OD1	1:A:329:ARG:NH2	2.10	0.83
1:A:59:VAL:HB	1:A:60:TYR:CD1	2.14	0.82
1:A:80:THR:HG23	1:A:89:SER:HB3	1.62	0.81
1:A:8:SER:HB3	1:A:100:GLY:O	1.81	0.80
1:A:257:VAL:HG22	1:A:258:LYS:HD3	1.66	0.77
1:A:59:VAL:HB	1:A:60:TYR:HD1	1.46	0.77
1:A:196:ILE:HD12	1:A:204:GLN:HB2	1.68	0.76
1:A:303:MET:O	1:A:305:ILE:HG13	1.88	0.74
1:A:210:VAL:CG1	1:A:246:LEU:HD13	2.18	0.74
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.53	0.73
1:A:39:THR:HG21	1:A:327:PHE:CE2	2.24	0.73
1:A:104:VAL:HG21	1:A:147:ILE:HG22	1.71	0.71
1:A:27:GLY:HA2	1:A:95:ASP:OD1	1.90	0.70
1:A:10:VAL:HB	1:A:176:ILE:HG23	1.74	0.69
1:A:192:TYR:C	1:A:193:ILE:HD12	2.16	0.69
1:A:11:ILE:HD13	1:A:172:LEU:HD23	1.73	0.69
1:A:14:ASN:ND2	1:A:165:ASP:HB2	2.07	0.68
1:A:22:GLY:O	1:A:34:LYS:HA	1.94	0.68
1:A:249:LYS:HB2	1:A:256:VAL:O	1.94	0.66
1:A:56:THR:O	1:A:59:VAL:HG23	1.97	0.65
1:A:117:LEU:H	1:A:118:PRO:HD2	1.63	0.63
1:A:210:VAL:HG12	1:A:210:VAL:O	1.99	0.62
1:A:98:THR:HG23	1:A:103:THR:HG22	1.82	0.62
1:A:226:ASP:O	1:A:316:GLY:HA2	1.99	0.62
1:A:44:VAL:HB	1:A:128:VAL:HA	1.80	0.62
1:A:257:VAL:HG22	1:A:258:LYS:CD	2.31	0.60
1:A:152:VAL:HG23	1:A:153:LEU:HD12	1.83	0.59
1:A:88:VAL:HG13	1:A:111:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:OG1	1:A:304:ASP:OD2	2.16	0.58
1:A:139:ARG:HG2	1:A:139:ARG:NH1	2.17	0.58
1:A:191:HIS:NE2	1:A:273:GLY:O	2.32	0.58
1:A:33:PHE:CZ	1:A:64:PHE:HB2	2.39	0.58
1:A:257:VAL:HG22	1:A:258:LYS:H	1.68	0.58
1:A:11:ILE:HD13	1:A:172:LEU:CD2	2.34	0.57
1:A:262:GLY:H	1:A:263:PRO:CD	2.17	0.57
1:A:87:THR:O	1:A:88:VAL:HG23	2.04	0.57
1:A:145:ASP:CG	1:A:329:ARG:HH22	2.13	0.56
1:A:48:SER:HB2	1:A:110:GLU:OE2	2.06	0.56
1:A:97:ILE:HG22	1:A:99:VAL:HG12	1.88	0.56
1:A:305:ILE:C	1:A:310:GLY:HA3	2.31	0.56
1:A:44:VAL:HA	1:A:127:VAL:O	2.05	0.56
1:A:60:TYR:CD1	1:A:60:TYR:N	2.74	0.56
1:A:214:THR:O	1:A:215:LEU:CD2	2.55	0.55
1:A:258:LYS:HD3	1:A:258:LYS:H	1.72	0.54
1:A:262:GLY:H	1:A:263:PRO:HD2	1.71	0.54
1:A:261:GLU:HG2	1:A:264:THR:HG21	1.90	0.54
1:A:139:ARG:HH11	1:A:139:ARG:CG	2.20	0.54
1:A:57:ALA:HB2	1:A:120:MET:HE2	1.89	0.53
1:A:15:TYR:HB3	1:A:19:GLN:HB2	1.91	0.53
1:A:209:SER:HA	1:A:214:THR:O	2.09	0.53
1:A:88:VAL:HG13	1:A:111:VAL:HG13	1.92	0.51
1:A:257:VAL:CG2	1:A:258:LYS:HD3	2.39	0.51
1:A:269:SER:HG	1:A:278:THR:HB	1.75	0.51
1:A:26:ILE:HD12	1:A:33:PHE:CD1	2.46	0.51
1:A:47:PRO:HD3	1:A:125:ASP:O	2.12	0.50
1:A:234:GLY:O	1:A:302:ALA:HA	2.11	0.50
1:A:210:VAL:HG21	1:A:242:LEU:HG	1.94	0.49
1:A:39:THR:HG21	1:A:327:PHE:CZ	2.47	0.49
1:A:205:MET:CE	1:A:313:TRP:CD1	2.95	0.49
1:A:88:VAL:HG11	1:A:111:VAL:HG21	1.95	0.48
1:A:38:ASP:OD2	1:A:41:SER:HB3	2.13	0.48
1:A:61:HIS:HB3	1:A:125:ASP:OD1	2.13	0.48
1:A:196:ILE:CG2	1:A:197:LYS:HE2	2.43	0.48
1:A:215:LEU:HD12	1:A:218:GLU:CG	2.27	0.48
1:A:115:PRO:HD2	1:A:119:PHE:HD2	1.79	0.48
1:A:117:LEU:N	1:A:118:PRO:HD2	2.29	0.48
1:A:130:MET:HG2	1:A:158:PHE:CE2	2.49	0.47
1:A:215:LEU:CD1	1:A:218:GLU:HG3	2.27	0.47
1:A:235:SER:HB2	1:A:304:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:O	1:A:115:PRO:HD3	2.14	0.47
1:A:285:VAL:HG22	1:A:298:LEU:HD12	1.95	0.47
1:A:71:SER:OG	1:A:95:ASP:OD1	2.32	0.47
1:A:303:MET:O	1:A:304:ASP:C	2.57	0.47
1:A:258:LYS:CD	1:A:258:LYS:H	2.28	0.46
1:A:243:MET:CB	1:A:255:TYR:CE1	2.99	0.46
1:A:193:ILE:HD12	1:A:193:ILE:N	2.31	0.46
1:A:214:THR:O	1:A:215:LEU:HD23	2.15	0.46
1:A:193:ILE:N	1:A:193:ILE:CD1	2.79	0.46
1:A:214:THR:O	1:A:215:LEU:HD22	2.15	0.46
1:A:83:TYR:HB2	1:A:86:GLY:H	1.81	0.45
1:A:207:GLY:HA2	1:A:216:LEU:O	2.16	0.45
1:A:235:SER:OG	1:A:238:SER:HB2	2.17	0.45
1:A:33:PHE:HZ	1:A:64:PHE:HB2	1.82	0.44
1:A:243:MET:CG	1:A:255:TYR:CD1	2.80	0.44
1:A:38:ASP:HA	1:A:227:THR:OG1	2.17	0.44
1:A:254:ASP:O	1:A:255:TYR:O	2.35	0.44
1:A:160:PHE:CZ	1:A:227:THR:HG21	2.53	0.44
1:A:59:VAL:CB	1:A:60:TYR:CD1	2.94	0.43
1:A:196:ILE:HG23	1:A:197:LYS:HE2	2.00	0.43
1:A:132:PHE:HE1	1:A:201:TRP:CG	2.35	0.43
1:A:205:MET:O	1:A:220:GLY:HA2	2.18	0.43
1:A:23:GLU:HA	1:A:33:PHE:O	2.19	0.42
1:A:243:MET:HG2	1:A:255:TYR:HD1	1.66	0.42
1:A:88:VAL:CG1	1:A:111:VAL:CG2	2.97	0.42
1:A:213:SER:O	1:A:214:THR:C	2.63	0.42
1:A:286:PHE:HB2	1:A:297:THR:O	2.20	0.42
1:A:97:ILE:O	1:A:103:THR:HA	2.19	0.42
1:A:132:PHE:HE1	1:A:201:TRP:CD2	2.37	0.42
1:A:182:ASP:HA	1:A:183:PRO:HD2	1.75	0.42
1:A:208:VAL:HB	1:A:216:LEU:HB2	2.02	0.42
1:A:239:ILE:HD11	1:A:313:TRP:CZ3	2.55	0.42
1:A:272:LEU:HD12	1:A:277:TYR:CD1	2.55	0.42
1:A:247:GLY:O	1:A:248:ALA:HB3	2.20	0.41
1:A:148:ILE:HD13	1:A:148:ILE:HG21	1.78	0.41
1:A:243:MET:HE3	1:A:255:TYR:HB3	2.02	0.41
1:A:141:THR:HA	1:A:142:PRO:HD2	1.94	0.41
1:A:29:PRO:HA	1:A:30:PRO:HD3	1.90	0.41
1:A:155:GLU:O	1:A:179:GLY:HA2	2.21	0.41
1:A:230:SER:O	1:A:317:ALA:HB3	2.20	0.41
1:A:22:GLY:O	1:A:35:VAL:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HA	1:A:102:ILE:O	2.20	0.41
1:A:217:CYS:O	1:A:219:ASP:N	2.53	0.41
1:A:247:GLY:HA3	1:A:257:VAL:HG21	2.02	0.41
1:A:243:MET:HB3	1:A:255:TYR:CE1	2.55	0.40
1:A:88:VAL:HG13	1:A:111:VAL:HG11	2.02	0.40
1:A:79:LEU:O	1:A:89:SER:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	312/340 (92%)	273 (88%)	29 (9%)	10 (3%)	3 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ASP
1	A	57	ALA
1	A	219	ASP
1	A	255	TYR
1	A	246	LEU
1	A	117	LEU
1	A	303	MET
1	A	248	ALA
1	A	247	GLY
1	A	210	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/290 (93%)	202 (75%)	68 (25%)	0 1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	11	ILE
1	A	32	THR
1	A	34	LYS
1	A	36	VAL
1	A	41	SER
1	A	44	VAL
1	A	48	SER
1	A	56	THR
1	A	62	LYS
1	A	70	SER
1	A	73	LYS
1	A	79	LEU
1	A	80	THR
1	A	81	LEU
1	A	82	ARG
1	A	87	THR
1	A	89	SER
1	A	96	ILE
1	A	97	ILE
1	A	99	VAL
1	A	102	ILE
1	A	106	GLN
1	A	107	MET
1	A	112	THR
1	A	130	MET
1	A	134	GLU
1	A	139	ARG
1	A	140	VAL
1	A	145	ASP

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Mol	Chain	Res	Type
1	A	147	ILE
1	A	149	SER
1	A	150	GLN
1	A	157	VAL
1	A	176	ILE
1	A	177	VAL
1	A	187	GLU
1	A	193	ILE
1	A	195	LEU
1	A	197	LYS
1	A	200	VAL
1	A	203	ILE
1	A	204	GLN
1	A	209	SER
1	A	213	SER
1	A	215	LEU
1	A	217	CYS
1	A	219	ASP
1	A	222	LEU
1	A	224	LEU
1	A	230	SER
1	A	232	ILE
1	A	236	THR
1	A	238	SER
1	A	241	LYS
1	A	250	LYS
1	A	251	ARG
1	A	252	LEU
1	A	254	ASP
1	A	257	VAL
1	A	258	LYS
1	A	265	LEU
1	A	275	LYS
1	A	276	GLU
1	A	278	THR
1	A	298	LEU
1	A	303	MET
1	A	309	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	301	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	341	1	14,14,15	1.53	2 (14%)	17,19,21	2.16	6 (35%)

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
2	NAG	A	341	1	1/1/5/7	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	341	NAG	O5-C1	-3.89	1.37	1.43
2	A	341	NAG	C1-C2	-2.94	1.48	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	341	NAG	O5-C1-C2	5.32	119.52	111.29
2	A	341	NAG	C1-O5-C5	3.94	117.46	112.19
2	A	341	NAG	C2-N2-C7	-3.39	118.35	122.90
2	A	341	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	341	NAG	C3-C4-C5	-2.39	105.90	110.23
2	A	341	NAG	C1-C2-N2	2.05	113.66	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	341	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	341	NAG	O5-C5-C6-O6
2	A	341	NAG	C4-C5-C6-O6
2	A	341	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.