



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1CPY / pdb_00001cpy
Title : SITE-DIRECTED MUTAGENESIS ON (SERINE) CARBOXYPEPTIDASE
Y FROM YEAST. THE SIGNIFICANCE OF THR 60 AND MET 398 IN
HYDROLYSIS AND AMINOLYSIS REACTIONS
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dam, K.
Deposited on : 1995-03-24
Resolution : 2.60 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

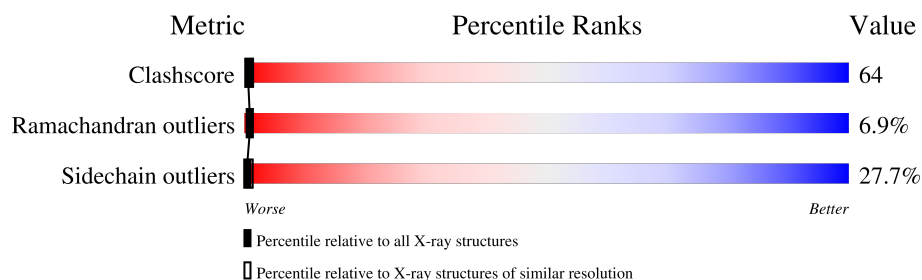
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	421	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3325 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 SERINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3245	2076	526	627	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ALA	GLU	conflict	UNP P00729
A	145	ALA	GLU	conflict	UNP P00729

- 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
2	A	1	14	8	1	5	0	0

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

- Molecule 3 is water.

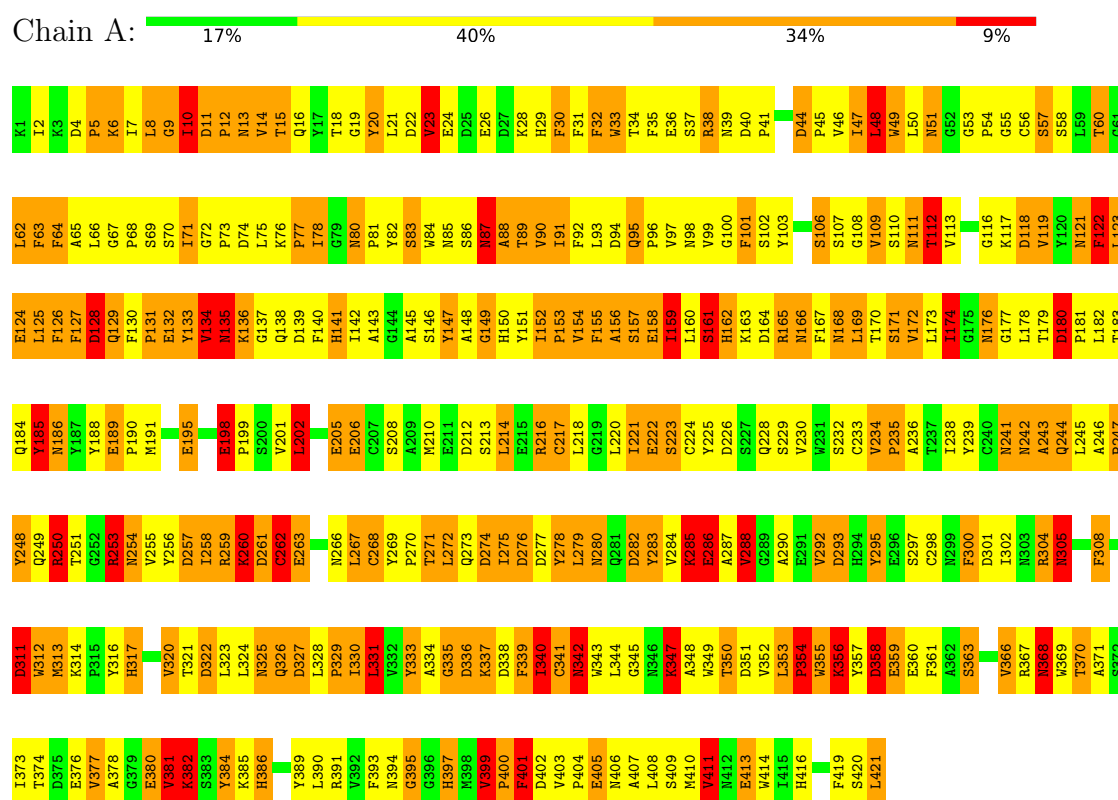
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		

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: SERINE CARBOXYPEPTIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	112.00Å 112.00Å 112.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3325	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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	2.31	70/3343 (2.1%)	2.34	201/4572 (4.4%)

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 (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	LEU	C-OXT	75.17	2.73	1.23
1	A	234	VAL	CA-CB	-8.81	1.49	1.54
1	A	414	TRP	CA-C	-8.19	1.44	1.53
1	A	223	SER	C-N	-7.88	1.23	1.33
1	A	154	VAL	CA-CB	-7.79	1.44	1.54
1	A	242	ASN	CA-C	-7.60	1.45	1.53
1	A	401	PHE	CA-C	-7.52	1.43	1.52
1	A	355	TRP	CA-C	7.51	1.61	1.52
1	A	147	TYR	CA-C	-7.33	1.42	1.52
1	A	49	TRP	CA-C	-7.08	1.44	1.52
1	A	395	GLY	CA-C	7.05	1.57	1.52
1	A	366	VAL	N-CA	-7.05	1.37	1.46
1	A	230	VAL	C-O	-6.98	1.16	1.24
1	A	168	ASN	CA-C	6.89	1.61	1.52
1	A	400	PRO	CA-C	-6.87	1.42	1.52
1	A	411	VAL	N-CA	-6.63	1.38	1.46
1	A	411	VAL	CA-C	-6.62	1.44	1.52
1	A	202	LEU	CA-C	-6.48	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	TRP	C-N	-6.48	1.25	1.33
1	A	222	GLU	CD-OE1	6.48	1.37	1.25
1	A	367	ARG	NE-CZ	6.48	1.40	1.33
1	A	180	ASP	N-CA	-6.40	1.39	1.46
1	A	339	PHE	CA-C	6.30	1.61	1.53
1	A	158	GLU	N-CA	-6.29	1.38	1.46
1	A	340	ILE	CA-CB	-6.27	1.47	1.54
1	A	278	TYR	CA-C	6.22	1.61	1.52
1	A	150	HIS	CE1-NE2	6.19	1.38	1.32
1	A	205	GLU	CD-OE1	6.17	1.37	1.25
1	A	122	PHE	N-CA	-6.15	1.38	1.46
1	A	305	ASN	CA-C	-6.13	1.44	1.52
1	A	189	GLU	N-CA	-6.10	1.41	1.46
1	A	162	HIS	N-CA	-6.07	1.38	1.46
1	A	334	ALA	C-N	6.04	1.38	1.33
1	A	152	ILE	N-CA	-6.00	1.39	1.46
1	A	242	ASN	CA-CB	-6.00	1.46	1.53
1	A	250	ARG	NE-CZ	5.99	1.39	1.33
1	A	301	ASP	CA-C	-5.92	1.45	1.52
1	A	176	ASN	CA-C	5.91	1.60	1.52
1	A	247	PRO	CA-C	-5.81	1.43	1.52
1	A	113	VAL	C-N	-5.79	1.24	1.33
1	A	180	ASP	C-O	5.79	1.30	1.24
1	A	223	SER	CA-C	-5.78	1.45	1.52
1	A	320	VAL	CA-C	5.78	1.60	1.52
1	A	259	ARG	N-CA	5.75	1.53	1.46
1	A	257	ASP	C-N	-5.64	1.27	1.34
1	A	397	HIS	CE1-NE2	5.63	1.38	1.32
1	A	242	ASN	N-CA	-5.55	1.40	1.46
1	A	206	GLU	N-CA	-5.54	1.39	1.46
1	A	7	ILE	C-N	5.50	1.40	1.33
1	A	47	ILE	C-N	5.46	1.41	1.33
1	A	353	LEU	CA-C	-5.43	1.46	1.53
1	A	282	ASP	CG-OD2	5.43	1.35	1.25
1	A	263	GLU	CD-OE2	5.40	1.35	1.25
1	A	30	PHE	C-O	-5.39	1.17	1.23
1	A	405	GLU	CD-OE2	5.39	1.35	1.25
1	A	399	VAL	CA-CB	-5.38	1.50	1.53
1	A	370	THR	CA-C	-5.36	1.46	1.52
1	A	251	THR	CA-C	-5.33	1.45	1.52
1	A	330	ILE	C-O	-5.27	1.18	1.24
1	A	399	VAL	N-CA	-5.26	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	PRO	C-O	5.25	1.30	1.23
1	A	60	THR	N-CA	-5.20	1.40	1.46
1	A	119	VAL	N-CA	-5.16	1.40	1.46
1	A	238	ILE	N-CA	-5.16	1.40	1.46
1	A	235	PRO	N-CA	-5.15	1.40	1.47
1	A	416	HIS	CA-C	5.11	1.58	1.52
1	A	397	HIS	CG-ND1	5.09	1.43	1.38
1	A	63	PHE	CA-C	-5.08	1.45	1.52
1	A	91	ILE	CA-CB	-5.06	1.48	1.54
1	A	400	PRO	CA-CB	-5.00	1.46	1.53

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASN	N-CA-CB	-11.35	98.18	111.79
1	A	257	ASP	CA-CB-CG	11.08	123.68	112.60
1	A	414	TRP	N-CA-C	-9.96	97.92	111.96
1	A	30	PHE	CA-CB-CG	-9.96	103.84	113.80
1	A	80	ASN	CB-CA-C	9.95	121.19	109.85
1	A	302	ILE	N-CA-CB	9.71	121.28	110.51
1	A	347	LYS	CB-CA-C	-9.55	95.81	110.90
1	A	381	VAL	N-CA-C	9.50	122.66	109.55
1	A	163	LYS	N-CA-C	-8.92	102.53	113.50
1	A	368	ASN	CA-CB-CG	8.57	121.17	112.60
1	A	212	ASP	CA-CB-CG	-8.50	104.10	112.60
1	A	368	ASN	N-CA-CB	8.50	122.69	109.69
1	A	353	LEU	C-N-CD	-8.31	90.91	125.00
1	A	386	HIS	CA-CB-CG	-8.27	105.53	113.80
1	A	358	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	2	ILE	N-CA-C	8.08	121.15	108.87
1	A	112	THR	N-CA-C	8.04	119.83	111.14
1	A	214	LEU	N-CA-C	8.02	119.94	111.03
1	A	168	ASN	CA-CB-CG	8.02	120.62	112.60
1	A	286	GLU	N-CA-C	7.98	119.76	111.14
1	A	267	LEU	N-CA-C	7.97	121.79	110.23
1	A	162	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	381	VAL	CA-C-N	7.92	133.91	121.72
1	A	381	VAL	C-N-CA	7.92	133.91	121.72
1	A	335	GLY	O-C-N	-7.88	115.84	122.77
1	A	301	ASP	O-C-N	7.76	130.11	122.03
1	A	253	ARG	N-CA-C	-7.72	96.81	109.40
1	A	48	LEU	CA-C-N	-7.67	112.41	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	C-N-CA	-7.67	112.41	123.00
1	A	325	ASN	CA-C-N	-7.62	111.82	123.17
1	A	325	ASN	C-N-CA	-7.62	111.82	123.17
1	A	343	TRP	N-CA-C	-7.54	103.55	112.89
1	A	247	PRO	N-CA-CB	7.45	111.52	103.33
1	A	419	PHE	CA-CB-CG	-7.36	106.44	113.80
1	A	317	HIS	CA-CB-CG	-7.24	106.56	113.80
1	A	232	SER	N-CA-C	-7.17	105.15	114.04
1	A	121	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	44	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	355	TRP	O-C-N	-7.05	116.63	123.26
1	A	172	VAL	N-CA-C	7.04	118.88	108.45
1	A	180	ASP	CB-CA-C	7.02	121.97	110.87
1	A	308	PHE	CA-CB-CG	-6.99	106.81	113.80
1	A	201	VAL	N-CA-CB	6.99	121.27	112.26
1	A	198	GLU	N-CA-CB	6.96	120.12	110.03
1	A	202	LEU	CA-C-O	-6.95	111.83	120.23
1	A	11	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	121	ASN	CA-C-N	-6.87	108.83	120.58
1	A	121	ASN	C-N-CA	-6.87	108.83	120.58
1	A	384	TYR	N-CA-CB	6.79	120.28	110.37
1	A	285	LYS	CA-C-N	6.78	129.66	120.44
1	A	285	LYS	C-N-CA	6.78	129.66	120.44
1	A	400	PRO	N-CA-CB	6.77	110.36	103.25
1	A	382	LYS	CB-CA-C	-6.76	102.56	111.42
1	A	282	ASP	N-CA-C	6.72	118.60	111.28
1	A	233	CYS	CA-C-N	-6.72	114.96	120.33
1	A	233	CYS	C-N-CA	-6.72	114.96	120.33
1	A	327	ASP	N-CA-C	6.63	120.56	111.54
1	A	118	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	185	TYR	N-CA-C	6.61	124.88	110.80
1	A	322	ASP	N-CA-CB	6.60	119.82	110.12
1	A	250	ARG	N-CA-CB	6.59	119.81	110.12
1	A	267	LEU	N-CA-CB	6.57	119.75	109.83
1	A	221	ILE	N-CA-CB	6.53	118.19	110.55
1	A	250	ARG	CD-NE-CZ	-6.51	115.28	124.40
1	A	111	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	245	LEU	CA-C-O	6.48	127.44	120.24
1	A	330	ILE	N-CA-C	6.44	117.57	108.17
1	A	377	VAL	N-CA-CB	6.42	120.47	110.14
1	A	20	TYR	N-CA-C	6.41	119.95	109.06
1	A	342	ASN	CB-CA-C	-6.39	97.71	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	356	LYS	N-CA-C	6.39	119.06	111.33
1	A	153	PRO	N-CA-CB	6.36	110.03	103.23
1	A	241	ASN	N-CA-C	-6.33	104.65	112.38
1	A	118	ASP	CA-C-N	-6.33	111.69	120.74
1	A	118	ASP	C-N-CA	-6.33	111.69	120.74
1	A	87	ASN	N-CA-C	6.28	117.82	110.41
1	A	381	VAL	CA-CB-CG2	6.26	121.03	110.40
1	A	259	ARG	CD-NE-CZ	6.24	133.14	124.40
1	A	238	ILE	N-CA-C	6.23	116.90	110.36
1	A	411	VAL	CA-CB-CG2	-6.22	99.82	110.40
1	A	90	VAL	N-CA-C	6.22	117.44	108.48
1	A	174	ILE	CA-C-N	-6.22	116.56	122.66
1	A	174	ILE	C-N-CA	-6.22	116.56	122.66
1	A	80	ASN	N-CA-CB	6.22	119.09	110.01
1	A	272	LEU	N-CA-CB	6.20	119.23	110.12
1	A	302	ILE	CB-CA-C	-6.17	103.99	111.88
1	A	256	TYR	CB-CA-C	-6.14	99.83	110.09
1	A	312	TRP	CB-CA-C	-6.14	98.21	110.42
1	A	214	LEU	CB-CA-C	6.12	120.44	110.95
1	A	268	CYS	N-CA-C	-6.12	105.82	113.28
1	A	154	VAL	CA-C-O	-6.09	114.62	120.95
1	A	110	SER	N-CA-C	-6.07	105.19	112.59
1	A	401	PHE	N-CA-C	-6.03	105.83	113.43
1	A	331	LEU	O-C-N	6.01	130.24	123.27
1	A	287	ALA	O-C-N	6.01	128.49	122.12
1	A	400	PRO	CB-CA-C	-5.97	101.71	111.56
1	A	127	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	165	ARG	N-CA-C	5.93	119.08	110.42
1	A	124	GLU	CB-CA-C	5.92	120.62	110.79
1	A	156	ALA	CB-CA-C	-5.92	101.59	110.88
1	A	117	LYS	CA-C-N	-5.91	110.05	121.58
1	A	117	LYS	C-N-CA	-5.91	110.05	121.58
1	A	368	ASN	CA-C-N	5.88	131.12	123.00
1	A	368	ASN	C-N-CA	5.88	131.12	123.00
1	A	305	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	71	ILE	CB-CA-C	5.87	118.35	110.42
1	A	394	ASN	N-CA-CB	5.87	121.22	112.30
1	A	300	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	333	TYR	N-CA-CB	-5.83	100.77	111.37
1	A	83	SER	N-CA-C	5.82	117.81	110.24
1	A	11	ASP	CA-C-N	5.82	127.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASP	C-N-CA	5.82	127.11	119.84
1	A	293	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	157	SER	O-C-N	5.76	128.08	122.09
1	A	258	ILE	CA-C-N	5.74	128.25	120.44
1	A	258	ILE	C-N-CA	5.74	128.25	120.44
1	A	414	TRP	N-CA-CB	5.72	120.51	110.27
1	A	301	ASP	CA-C-O	-5.72	115.00	121.00
1	A	312	TRP	N-CA-CB	-5.70	100.86	110.49
1	A	238	ILE	CB-CA-C	-5.67	104.63	111.88
1	A	101	PHE	CA-C-N	-5.66	112.16	122.12
1	A	101	PHE	C-N-CA	-5.66	112.16	122.12
1	A	336	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	150	HIS	N-CA-C	-5.64	105.43	112.93
1	A	202	LEU	CA-C-N	5.63	125.95	119.92
1	A	202	LEU	C-N-CA	5.63	125.95	119.92
1	A	331	LEU	CA-C-N	5.63	130.77	123.11
1	A	331	LEU	C-N-CA	5.63	130.77	123.11
1	A	133	TYR	CA-C-O	5.63	125.33	119.14
1	A	67	GLY	CA-C-N	5.61	124.81	118.97
1	A	67	GLY	C-N-CA	5.61	124.81	118.97
1	A	280	ASN	CB-CA-C	-5.60	98.18	109.55
1	A	48	LEU	CA-C-O	5.59	126.56	120.58
1	A	221	ILE	O-C-N	5.59	127.39	121.91
1	A	57	SER	CA-C-O	-5.57	114.92	121.16
1	A	325	ASN	N-CA-CB	5.54	119.58	110.39
1	A	117	LYS	N-CA-CB	5.53	118.36	110.06
1	A	63	PHE	CB-CA-C	-5.52	104.28	111.40
1	A	155	PHE	CA-C-N	5.49	127.58	120.44
1	A	155	PHE	C-N-CA	5.49	127.58	120.44
1	A	286	GLU	CB-CA-C	-5.48	102.24	110.90
1	A	149	GLY	CA-C-N	5.47	132.09	122.79
1	A	149	GLY	C-N-CA	5.47	132.09	122.79
1	A	297	SER	N-CA-C	5.46	117.04	111.14
1	A	161	SER	CA-CB-OG	-5.45	100.21	111.10
1	A	176	ASN	CB-CA-C	5.45	121.26	110.42
1	A	381	VAL	N-CA-CB	5.42	119.98	110.49
1	A	260	LYS	CB-CA-C	-5.42	100.24	109.51
1	A	312	TRP	CE2-CD2-CE3	5.41	124.21	118.80
1	A	165	ARG	CB-CA-C	5.39	117.21	109.71
1	A	47	ILE	CA-C-N	5.39	129.59	122.42
1	A	47	ILE	C-N-CA	5.39	129.59	122.42
1	A	60	THR	CA-C-N	-5.39	113.55	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	C-N-CA	-5.39	113.55	120.34
1	A	20	TYR	CB-CA-C	-5.37	98.47	109.38
1	A	340	ILE	N-CA-C	5.31	116.68	110.62
1	A	23	VAL	CB-CA-C	5.31	120.00	111.29
1	A	262	CYS	N-CA-C	-5.31	99.49	110.80
1	A	195	GLU	CB-CA-C	-5.29	102.46	111.02
1	A	111	ASN	N-CA-C	5.28	116.23	107.73
1	A	128	ASP	CB-CA-C	-5.28	102.56	110.90
1	A	354	PRO	N-CA-CB	5.27	108.78	103.25
1	A	355	TRP	N-CA-CB	-5.27	100.65	111.87
1	A	179	THR	CA-C-N	-5.25	116.57	123.34
1	A	179	THR	C-N-CA	-5.25	116.57	123.34
1	A	359	GLU	N-CA-CB	5.22	117.90	110.06
1	A	275	ILE	CA-CB-CG1	5.21	119.26	110.40
1	A	128	ASP	O-C-N	5.20	127.71	122.09
1	A	229	SER	N-CA-C	5.19	118.53	110.17
1	A	171	SER	O-C-N	5.19	128.44	123.04
1	A	288	VAL	O-C-N	5.19	127.66	121.80
1	A	169	LEU	CA-C-N	-5.18	112.95	121.92
1	A	169	LEU	C-N-CA	-5.18	112.95	121.92
1	A	163	LYS	CA-C-N	5.17	128.96	120.63
1	A	163	LYS	C-N-CA	5.17	128.96	120.63
1	A	325	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	5	PRO	O-C-N	5.16	129.15	122.24
1	A	312	TRP	CG-CD2-CE3	-5.14	128.76	133.90
1	A	159	ILE	N-CA-CB	5.12	117.50	110.54
1	A	32	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	13	ASN	CA-C-N	5.09	131.14	121.97
1	A	13	ASN	C-N-CA	5.09	131.14	121.97
1	A	251	THR	N-CA-CB	5.08	118.17	110.14
1	A	311	ASP	N-CA-C	5.08	121.62	110.80
1	A	145	ALA	N-CA-C	5.07	116.89	109.24
1	A	243	ALA	CB-CA-C	-5.06	99.65	110.32
1	A	341	CYS	N-CA-C	5.05	116.50	110.44
1	A	312	TRP	CB-CG-CD2	-5.05	119.73	126.80
1	A	51	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	241	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	226	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	133	TYR	CA-CB-CG	-5.02	104.87	113.90
1	A	248	TYR	N-CA-C	-5.01	105.70	111.07
1	A	30	PHE	O-C-N	-5.01	116.94	122.86
1	A	133	TYR	CA-C-N	-5.01	112.95	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	TYR	C-N-CA	-5.01	112.95	121.97
1	A	80	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	254	ASN	CA-C-N	5.01	128.95	120.64
1	A	254	ASN	C-N-CA	5.01	128.95	120.64
1	A	295	TYR	N-CA-C	5.00	116.91	108.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3245	0	2919	398	0
2	A	42	0	39	10	0
3	A	38	0	0	12	0
All	All	3325	0	2958	399	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 64.

All (399) 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:259:ARG:HD3	1:A:337:LYS:HD2	1.34	1.09
1:A:329:PRO:HA	1:A:386:HIS:HB2	1.39	0.99
1:A:77:PRO:HD3	1:A:278:TYR:CE2	2.01	0.96
1:A:168:ASN:HD21	2:A:1681:NAG:HN2	1.15	0.93
1:A:262:CYS:HB2	1:A:268:CYS:HA	1.52	0.92
1:A:173:LEU:HD23	1:A:331:LEU:CD2	1.99	0.92
1:A:77:PRO:HD3	1:A:278:TYR:HE2	1.34	0.91
1:A:95:GLN:HG2	1:A:96:PRO:CD	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD23	1:A:331:LEU:HD23	1.54	0.89
1:A:10:ILE:HD12	1:A:10:ILE:H	1.38	0.88
1:A:262:CYS:CB	1:A:268:CYS:HA	2.02	0.88
1:A:10:ILE:HG22	1:A:11:ASP:H	1.36	0.88
1:A:329:PRO:CA	1:A:386:HIS:HB2	2.03	0.88
1:A:355:TRP:CH2	1:A:357:TYR:HB2	2.10	0.87
1:A:279:LEU:HD23	1:A:295:TYR:CE1	2.10	0.86
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.57	0.85
1:A:21:LEU:HD23	1:A:125:LEU:HB2	1.56	0.85
1:A:191:MET:HG2	1:A:342:ASN:ND2	1.91	0.85
1:A:355:TRP:CZ2	1:A:357:TYR:HB2	2.11	0.85
1:A:71:ILE:HD13	1:A:278:TYR:CG	2.13	0.83
1:A:48:LEU:HD12	1:A:49:TRP:N	1.92	0.83
1:A:34:THR:HG22	1:A:35:PHE:H	1.44	0.82
1:A:180:ASP:HB2	1:A:317:HIS:HB3	1.59	0.82
1:A:26:GLU:CB	1:A:28:LYS:HD2	2.10	0.81
1:A:38:ARG:HG3	1:A:86:SER:HA	1.62	0.81
1:A:20:TYR:HE1	1:A:290:ALA:HA	1.45	0.81
1:A:93:LEU:HD12	1:A:94:ASP:H	1.45	0.80
1:A:50:LEU:HD22	1:A:95:GLN:HE22	1.44	0.80
1:A:320:VAL:HG12	1:A:353:LEU:HD21	1.62	0.80
1:A:189:GLU:HB3	1:A:190:PRO:HD3	1.64	0.79
1:A:65:ALA:O	1:A:400:PRO:HB2	1.83	0.79
1:A:420:SER:O	1:A:421:LEU:HD23	1.82	0.79
1:A:10:ILE:O	1:A:12:PRO:HD3	1.84	0.78
1:A:84:TRP:CZ2	1:A:411:VAL:HG21	2.18	0.78
1:A:373:ILE:HD12	1:A:409:SER:OG	1.84	0.78
1:A:37:SER:HB2	1:A:88:ALA:C	2.09	0.78
1:A:48:LEU:HB3	1:A:142:ILE:HG23	1.66	0.77
1:A:378:ALA:HB1	1:A:406:ASN:HD22	1.50	0.77
1:A:29:HIS:O	1:A:102:SER:HB3	1.83	0.76
1:A:168:ASN:ND2	2:A:1681:NAG:HN2	1.84	0.76
1:A:37:SER:HB2	1:A:88:ALA:CA	2.16	0.76
1:A:56:CYS:HB3	3:A:472:HOH:O	1.87	0.75
1:A:162:HIS:ND1	1:A:162:HIS:N	2.30	0.75
1:A:390:LEU:CD2	1:A:410:MET:HG3	2.17	0.75
1:A:89:THR:HG22	3:A:461:HOH:O	1.86	0.74
1:A:45:PRO:HB3	1:A:139:ASP:HB2	1.70	0.74
1:A:125:LEU:N	1:A:125:LEU:HD23	2.02	0.74
1:A:93:LEU:HD12	1:A:94:ASP:N	2.03	0.73
1:A:95:GLN:HG2	1:A:96:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:N	1:A:99:VAL:HG21	2.02	0.73
1:A:180:ASP:HB2	1:A:317:HIS:CB	2.19	0.72
1:A:133:TYR:O	1:A:138:GLN:HB2	1.89	0.72
1:A:366:VAL:HA	1:A:381:VAL:O	1.89	0.72
1:A:191:MET:HG2	1:A:342:ASN:HD21	1.55	0.72
1:A:257:ASP:HA	1:A:337:LYS:O	1.90	0.72
1:A:369:TRP:CZ3	1:A:378:ALA:HB3	2.24	0.72
1:A:34:THR:HG22	1:A:35:PHE:N	2.05	0.71
1:A:171:SER:HA	1:A:328:LEU:HD21	1.70	0.71
1:A:283:TYR:O	1:A:286:GLU:HB2	1.88	0.71
1:A:329:PRO:HA	1:A:386:HIS:O	1.89	0.71
1:A:368:ASN:ND2	2:A:3681:NAG:HN2	1.87	0.71
1:A:352:VAL:O	1:A:354:PRO:HD3	1.91	0.71
1:A:84:TRP:CH2	1:A:411:VAL:HG21	2.26	0.71
1:A:20:TYR:CE1	1:A:290:ALA:HA	2.26	0.71
1:A:10:ILE:HG22	1:A:11:ASP:N	2.04	0.70
1:A:41:PRO:HA	3:A:461:HOH:O	1.91	0.69
1:A:18:THR:HG21	1:A:33:TRP:CD2	2.28	0.68
1:A:337:LYS:N	1:A:395:GLY:O	2.26	0.68
1:A:253:ARG:HH11	1:A:253:ARG:HB2	1.59	0.68
1:A:347:LYS:O	1:A:350:THR:HG22	1.94	0.68
1:A:282:ASP:O	1:A:286:GLU:HG2	1.93	0.67
1:A:327:ASP:OD1	1:A:356:LYS:NZ	2.28	0.67
2:A:3681:NAG:O3	2:A:3681:NAG:H82	1.95	0.67
1:A:72:GLY:O	1:A:75:LEU:N	2.26	0.67
1:A:202:LEU:CD2	1:A:210:MET:HE3	2.25	0.67
1:A:12:PRO:O	1:A:14:VAL:N	2.28	0.66
1:A:48:LEU:HD12	1:A:49:TRP:H	1.58	0.66
1:A:249:GLN:HA	3:A:483:HOH:O	1.95	0.66
1:A:18:THR:HG22	1:A:33:TRP:HA	1.77	0.65
1:A:180:ASP:HB2	1:A:317:HIS:CG	2.30	0.65
1:A:5:PRO:O	1:A:8:LEU:N	2.27	0.65
1:A:353:LEU:HG	1:A:354:PRO:N	2.11	0.65
1:A:60:THR:O	1:A:64:PHE:HB3	1.97	0.65
1:A:191:MET:HE2	1:A:342:ASN:ND2	2.12	0.65
1:A:95:GLN:HG2	1:A:96:PRO:N	2.08	0.65
1:A:345:GLY:HA3	3:A:471:HOH:O	1.96	0.64
1:A:116:GLY:O	1:A:119:VAL:N	2.28	0.64
1:A:202:LEU:HD23	1:A:206:GLU:HB3	1.80	0.64
1:A:94:ASP:OD2	1:A:101:PHE:N	2.24	0.64
1:A:304:ARG:NH1	1:A:305:ASN:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:O	1:A:409:SER:HB2	1.99	0.63
1:A:50:LEU:HD22	1:A:95:GLN:NE2	2.13	0.63
1:A:354:PRO:O	1:A:355:TRP:HB3	1.98	0.63
1:A:8:LEU:HD13	1:A:10:ILE:CD1	2.29	0.63
1:A:75:LEU:HD21	1:A:277:ASP:HB3	1.80	0.63
1:A:140:PHE:HB3	1:A:168:ASN:O	1.98	0.63
1:A:181:PRO:HD2	1:A:225:TYR:OH	1.99	0.63
1:A:373:ILE:HG22	1:A:374:THR:N	2.14	0.63
1:A:125:LEU:O	1:A:128:ASP:HB2	1.98	0.63
1:A:330:ILE:N	1:A:386:HIS:O	2.31	0.62
1:A:38:ARG:HG2	1:A:85:ASN:O	1.98	0.62
1:A:181:PRO:O	1:A:185:TYR:HB2	1.98	0.62
1:A:335:GLY:CA	1:A:395:GLY:HA3	2.29	0.62
1:A:85:ASN:HB2	1:A:88:ALA:O	2.00	0.62
1:A:305:ASN:OD1	1:A:305:ASN:N	2.30	0.62
1:A:39:ASN:HB3	1:A:44:ASP:OD2	2.00	0.61
1:A:270:PRO:HD2	3:A:484:HOH:O	2.00	0.61
1:A:31:PHE:O	1:A:93:LEU:HD12	2.01	0.61
1:A:160:LEU:HD11	1:A:328:LEU:HD12	1.82	0.61
1:A:166:ASN:OD1	1:A:167:PHE:HD1	1.84	0.61
1:A:360:GLU:O	1:A:363:SER:N	2.26	0.61
1:A:259:ARG:HD3	1:A:337:LYS:CD	2.22	0.60
1:A:123:LEU:HB3	1:A:167:PHE:CZ	2.36	0.60
1:A:57:SER:HB2	1:A:100:GLY:HA3	1.83	0.60
1:A:191:MET:HE3	1:A:338:ASP:O	2.02	0.60
1:A:361:PHE:CE1	1:A:382:LYS:HD2	2.37	0.60
1:A:131:PRO:HD2	1:A:132:GLU:OE2	2.02	0.60
1:A:143:ALA:CB	1:A:173:LEU:HB2	2.32	0.60
1:A:127:PHE:HD2	1:A:167:PHE:CD1	2.20	0.59
1:A:159:ILE:C	1:A:161:SER:H	2.10	0.59
1:A:30:PHE:CZ	1:A:118:ASP:HB3	2.36	0.59
1:A:95:GLN:CB	1:A:96:PRO:HA	2.30	0.59
1:A:71:ILE:HD13	1:A:278:TYR:CD2	2.38	0.58
1:A:336:ASP:OD1	1:A:337:LYS:HE2	2.02	0.58
1:A:53:GLY:HA3	1:A:54:PRO:C	2.27	0.58
1:A:180:ASP:OD2	1:A:183:THR:HB	2.03	0.58
1:A:182:LEU:HB2	1:A:221:ILE:CG2	2.33	0.58
1:A:274:ASP:O	1:A:277:ASP:HB2	2.02	0.58
1:A:304:ARG:HG2	1:A:305:ASN:OD1	2.04	0.58
1:A:121:ASN:O	1:A:125:LEU:HG	2.03	0.57
1:A:5:PRO:HD2	1:A:16:GLN:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.87	0.57
1:A:71:ILE:HG21	1:A:278:TYR:HB2	1.87	0.57
1:A:172:VAL:HG22	1:A:330:ILE:HG12	1.87	0.57
1:A:279:LEU:O	1:A:285:LYS:HG2	2.05	0.57
1:A:21:LEU:HD23	1:A:125:LEU:CB	2.32	0.56
1:A:143:ALA:HB2	1:A:173:LEU:HB2	1.86	0.56
1:A:186:ASN:ND2	1:A:186:ASN:H	2.03	0.56
1:A:44:ASP:HB3	1:A:88:ALA:HA	1.85	0.56
1:A:130:PHE:C	1:A:132:GLU:H	2.13	0.56
1:A:173:LEU:HD23	1:A:331:LEU:HD22	1.83	0.56
1:A:328:LEU:HD23	1:A:329:PRO:CD	2.34	0.56
1:A:335:GLY:HA2	1:A:395:GLY:HA3	1.86	0.56
1:A:12:PRO:C	1:A:14:VAL:H	2.12	0.56
1:A:62:LEU:C	1:A:62:LEU:HD23	2.30	0.56
1:A:127:PHE:HD2	1:A:167:PHE:CG	2.23	0.56
1:A:176:ASN:HB2	3:A:458:HOH:O	2.05	0.56
1:A:378:ALA:CB	1:A:406:ASN:HD22	2.18	0.56
1:A:10:ILE:HD12	1:A:10:ILE:N	2.14	0.56
1:A:63:PHE:HA	1:A:69:SER:O	2.05	0.56
1:A:77:PRO:O	1:A:78:ILE:HG13	2.05	0.56
1:A:146:SER:CA	1:A:177:GLY:HA2	2.36	0.56
1:A:30:PHE:HZ	1:A:118:ASP:HB3	1.70	0.56
1:A:320:VAL:HG12	1:A:353:LEU:CD2	2.35	0.56
1:A:159:ILE:HD11	1:A:169:LEU:HB2	1.86	0.56
1:A:268:CYS:HB2	3:A:482:HOH:O	2.05	0.55
1:A:410:MET:CE	1:A:411:VAL:HG23	2.36	0.55
1:A:127:PHE:CD2	1:A:167:PHE:CG	2.94	0.55
1:A:198:GLU:OE2	1:A:259:ARG:HG2	2.06	0.55
1:A:254:ASN:OD1	1:A:268:CYS:HB3	2.07	0.55
1:A:413:GLU:HG3	1:A:413:GLU:O	2.05	0.55
1:A:158:GLU:O	1:A:161:SER:HB2	2.06	0.55
1:A:28:LYS:HE2	1:A:118:ASP:OD2	2.07	0.55
1:A:253:ARG:HD2	1:A:260:LYS:O	2.07	0.55
1:A:146:SER:HA	1:A:177:GLY:HA2	1.89	0.54
1:A:350:THR:HG21	1:A:389:TYR:HB2	1.89	0.54
1:A:355:TRP:O	1:A:358:ASP:HB2	2.08	0.54
1:A:148:ALA:O	1:A:152:ILE:HG13	2.08	0.54
1:A:32:PHE:CD1	1:A:32:PHE:N	2.76	0.54
1:A:148:ALA:HA	1:A:151:TYR:CD2	2.43	0.53
1:A:159:ILE:HD13	1:A:169:LEU:HD22	1.90	0.53
1:A:68:PRO:O	1:A:80:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:O	1:A:161:SER:N	2.41	0.53
1:A:154:VAL:HG21	1:A:316:TYR:CD1	2.43	0.53
1:A:48:LEU:HD12	1:A:48:LEU:C	2.27	0.53
1:A:317:HIS:H	1:A:317:HIS:CD2	2.27	0.53
1:A:198:GLU:HG3	1:A:199:PRO:HD2	1.91	0.53
1:A:106:SER:O	1:A:106:SER:OG	2.27	0.53
1:A:216:ARG:HG2	1:A:239:TYR:CZ	2.44	0.52
1:A:8:LEU:HD13	1:A:10:ILE:HD13	1.91	0.52
1:A:109:VAL:HG23	1:A:109:VAL:O	2.09	0.52
1:A:180:ASP:CB	1:A:317:HIS:HB3	2.35	0.52
1:A:10:ILE:H	1:A:10:ILE:CD1	2.17	0.52
1:A:220:LEU:HD13	1:A:236:ALA:HA	1.91	0.52
1:A:189:GLU:HB3	1:A:190:PRO:CD	2.36	0.52
1:A:146:SER:HA	1:A:176:ASN:O	2.10	0.52
1:A:126:PHE:HE1	1:A:127:PHE:CE1	2.28	0.52
1:A:15:THR:O	1:A:36:GLU:HG3	2.09	0.52
1:A:62:LEU:HB2	1:A:92:PHE:CE1	2.46	0.51
1:A:83:SER:O	1:A:408:LEU:HD22	2.09	0.51
1:A:122:PHE:CD1	1:A:122:PHE:C	2.89	0.51
1:A:182:LEU:HB2	1:A:221:ILE:HG21	1.93	0.51
1:A:329:PRO:CB	1:A:386:HIS:HB2	2.39	0.51
1:A:378:ALA:HB1	1:A:406:ASN:ND2	2.23	0.51
1:A:380:GLU:N	1:A:391:ARG:O	2.44	0.51
1:A:261:ASP:N	1:A:261:ASP:OD1	2.44	0.51
1:A:317:HIS:CD2	1:A:317:HIS:N	2.78	0.51
1:A:224:CYS:O	1:A:228:GLN:N	2.33	0.51
1:A:155:PHE:CD1	1:A:155:PHE:N	2.78	0.51
1:A:403:VAL:HG23	1:A:403:VAL:O	2.11	0.51
1:A:335:GLY:HA3	1:A:395:GLY:C	2.36	0.50
1:A:141:HIS:N	1:A:141:HIS:CD2	2.79	0.50
1:A:206:GLU:OE2	1:A:247:PRO:HB3	2.10	0.50
1:A:95:GLN:HG2	1:A:96:PRO:CG	2.42	0.50
1:A:147:TYR:C	1:A:149:GLY:H	2.18	0.50
1:A:153:PRO:O	1:A:156:ALA:HB3	2.11	0.50
1:A:202:LEU:CD2	1:A:206:GLU:HB3	2.42	0.50
1:A:328:LEU:HD23	1:A:328:LEU:C	2.36	0.50
1:A:168:ASN:ND2	2:A:1681:NAG:C1	2.75	0.50
1:A:210:MET:HE2	1:A:247:PRO:HG2	1.93	0.50
1:A:217:CYS:HB2	1:A:239:TYR:HD2	1.76	0.50
1:A:50:LEU:N	1:A:143:ALA:O	2.41	0.50
1:A:217:CYS:HB2	1:A:239:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:C	1:A:21:LEU:HD12	2.37	0.50
1:A:174:ILE:HG22	1:A:174:ILE:O	2.11	0.50
1:A:18:THR:CG2	1:A:33:TRP:HA	2.42	0.49
1:A:130:PHE:N	1:A:131:PRO:HD3	2.27	0.49
1:A:191:MET:CE	1:A:342:ASN:ND2	2.75	0.49
1:A:171:SER:HA	1:A:328:LEU:CD2	2.40	0.49
1:A:247:PRO:HA	1:A:250:ARG:HG3	1.94	0.49
1:A:34:THR:CG2	1:A:35:PHE:H	2.22	0.49
1:A:55:GLY:O	1:A:298:CYS:HA	2.12	0.49
1:A:72:GLY:O	1:A:74:ASP:N	2.46	0.49
1:A:182:LEU:HB3	1:A:225:TYR:CE2	2.48	0.49
1:A:323:LEU:O	1:A:326:GLN:N	2.42	0.49
1:A:378:ALA:CB	1:A:406:ASN:ND2	2.76	0.49
1:A:20:TYR:CE2	1:A:31:PHE:HB2	2.48	0.49
1:A:21:LEU:CD2	1:A:126:PHE:H	2.25	0.49
1:A:368:ASN:OD1	2:A:3681:NAG:O5	2.29	0.49
1:A:390:LEU:HD22	1:A:410:MET:HG3	1.92	0.49
1:A:34:THR:HG23	1:A:90:VAL:O	2.12	0.48
1:A:234:VAL:HB	1:A:235:PRO:CD	2.43	0.48
1:A:279:LEU:CD1	1:A:279:LEU:N	2.76	0.48
1:A:23:VAL:HG11	1:A:30:PHE:HE2	1.78	0.48
1:A:100:GLY:CA	1:A:295:TYR:CE2	2.96	0.48
1:A:126:PHE:CD1	1:A:126:PHE:C	2.90	0.48
1:A:191:MET:HE2	1:A:342:ASN:HD22	1.78	0.48
1:A:141:HIS:HB3	1:A:171:SER:O	2.13	0.48
1:A:214:LEU:O	1:A:217:CYS:N	2.47	0.48
1:A:279:LEU:HD23	1:A:295:TYR:CZ	2.48	0.48
1:A:9:GLY:O	1:A:10:ILE:O	2.31	0.48
1:A:292:VAL:HG13	1:A:293:ASP:N	2.29	0.48
1:A:95:GLN:HG2	1:A:96:PRO:CA	2.43	0.48
1:A:134:VAL:O	1:A:136:LYS:N	2.46	0.48
1:A:46:VAL:HG22	1:A:89:THR:HG23	1.96	0.48
1:A:202:LEU:HD21	1:A:210:MET:HE3	1.96	0.48
1:A:284:VAL:O	1:A:288:VAL:HG23	2.13	0.47
1:A:368:ASN:ND2	2:A:3681:NAG:C1	2.77	0.47
1:A:399:VAL:N	1:A:400:PRO:CD	2.77	0.47
1:A:102:SER:O	1:A:103:TYR:HB3	2.12	0.47
1:A:410:MET:HB3	1:A:410:MET:HE2	1.59	0.47
1:A:182:LEU:HB2	1:A:221:ILE:HG22	1.95	0.47
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.15	0.47
1:A:80:ASN:HA	1:A:81:PRO:HD3	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TRP:CE3	1:A:378:ALA:HB3	2.50	0.47
1:A:65:ALA:O	1:A:400:PRO:O	2.32	0.47
1:A:80:ASN:OD1	1:A:81:PRO:HD2	2.15	0.47
1:A:87:ASN:ND2	2:A:871:NAG:C1	2.77	0.47
1:A:87:ASN:HD21	2:A:871:NAG:C1	2.27	0.47
1:A:100:GLY:HA2	1:A:295:TYR:CE2	2.50	0.47
1:A:389:TYR:HD2	3:A:469:HOH:O	1.97	0.47
1:A:22:ASP:OD2	1:A:29:HIS:ND1	2.44	0.47
1:A:253:ARG:HH11	1:A:253:ARG:CB	2.27	0.47
1:A:4:ASP:C	1:A:6:LYS:N	2.72	0.47
1:A:407:ALA:HB3	3:A:462:HOH:O	2.15	0.47
1:A:185:TYR:OH	1:A:241:ASN:ND2	2.47	0.46
1:A:21:LEU:HD23	1:A:126:PHE:H	1.80	0.46
1:A:135:ASN:C	1:A:137:GLY:H	2.23	0.46
1:A:247:PRO:O	1:A:250:ARG:HG3	2.16	0.46
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.55	0.46
1:A:50:LEU:CD2	1:A:95:GLN:HE22	2.21	0.46
1:A:368:ASN:ND2	2:A:3681:NAG:N2	2.60	0.46
1:A:10:ILE:CD1	1:A:10:ILE:N	2.78	0.46
1:A:188:TYR:CB	1:A:244:GLN:HG2	2.45	0.46
1:A:213:SER:CB	1:A:243:ALA:HB1	2.46	0.46
1:A:129:GLN:C	1:A:131:PRO:HD3	2.41	0.46
1:A:304:ARG:HG3	1:A:308:PHE:CD2	2.51	0.46
1:A:18:THR:HG21	1:A:33:TRP:CG	2.50	0.46
1:A:86:SER:CB	1:A:408:LEU:HD21	2.46	0.46
1:A:295:TYR:CD1	1:A:295:TYR:C	2.94	0.46
1:A:84:TRP:CE2	1:A:411:VAL:HG21	2.50	0.46
1:A:95:GLN:CG	1:A:96:PRO:HA	2.46	0.46
1:A:188:TYR:HB2	1:A:244:GLN:HG2	1.97	0.46
1:A:23:VAL:HG13	1:A:28:LYS:HB2	1.97	0.46
1:A:50:LEU:CD2	1:A:95:GLN:NE2	2.79	0.46
1:A:183:THR:O	1:A:186:ASN:ND2	2.49	0.46
1:A:304:ARG:HG3	1:A:308:PHE:HD2	1.81	0.46
1:A:80:ASN:C	1:A:82:TYR:H	2.23	0.46
1:A:335:GLY:HA3	1:A:395:GLY:HA3	1.96	0.46
1:A:253:ARG:NE	1:A:258:ILE:O	2.49	0.46
1:A:340:ILE:CG2	1:A:341:CYS:N	2.79	0.46
1:A:147:TYR:C	1:A:149:GLY:N	2.72	0.45
1:A:8:LEU:HD13	1:A:10:ILE:HD11	1.98	0.45
1:A:340:ILE:HG23	1:A:341:CYS:N	2.31	0.45
1:A:136:LYS:HB2	1:A:138:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:O	1:A:393:PHE:HB2	2.17	0.45
1:A:18:THR:CG2	1:A:33:TRP:CD2	2.98	0.45
1:A:186:ASN:HB3	1:A:214:LEU:HD21	1.97	0.45
1:A:5:PRO:O	1:A:8:LEU:HB2	2.16	0.45
1:A:31:PHE:CD1	1:A:31:PHE:C	2.95	0.45
1:A:123:LEU:HD11	1:A:140:PHE:CZ	2.52	0.45
1:A:58:SER:HB2	1:A:93:LEU:O	2.17	0.45
1:A:71:ILE:HD13	1:A:278:TYR:CB	2.45	0.45
1:A:198:GLU:CG	1:A:199:PRO:HD2	2.46	0.44
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.63	0.44
1:A:355:TRP:CZ3	1:A:357:TYR:HD2	2.35	0.44
1:A:369:TRP:CZ3	1:A:378:ALA:CB	2.99	0.44
1:A:78:ILE:O	1:A:78:ILE:HG22	2.07	0.44
1:A:159:ILE:CD1	1:A:169:LEU:HB2	2.47	0.44
1:A:348:ALA:HA	1:A:351:ASP:HB2	1.99	0.44
1:A:21:LEU:N	1:A:21:LEU:CD1	2.75	0.44
1:A:401:PHE:CD1	1:A:401:PHE:C	2.96	0.44
1:A:182:LEU:CB	1:A:225:TYR:CE2	3.00	0.44
1:A:320:VAL:CG1	1:A:353:LEU:CD2	2.95	0.44
1:A:74:ASP:O	1:A:76:LYS:HG2	2.17	0.44
1:A:5:PRO:HB3	1:A:33:TRP:CZ2	2.52	0.44
1:A:234:VAL:CB	1:A:235:PRO:CD	2.96	0.44
1:A:321:THR:HG23	1:A:354:PRO:O	2.17	0.44
1:A:134:VAL:O	1:A:137:GLY:N	2.50	0.44
1:A:355:TRP:CH2	1:A:357:TYR:HD2	2.36	0.44
1:A:126:PHE:CE1	1:A:127:PHE:CE1	3.06	0.43
1:A:267:LEU:HB3	1:A:269:TYR:H	1.82	0.43
1:A:62:LEU:HB2	1:A:92:PHE:CD1	2.53	0.43
1:A:324:LEU:HB3	1:A:355:TRP:CE3	2.54	0.43
1:A:130:PHE:N	1:A:130:PHE:CD1	2.87	0.43
1:A:143:ALA:HB1	1:A:173:LEU:HB2	2.00	0.43
1:A:186:ASN:C	1:A:188:TYR:H	2.26	0.43
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.64	0.43
1:A:5:PRO:HG2	1:A:16:GLN:CB	2.49	0.43
1:A:338:ASP:OD1	1:A:339:PHE:N	2.52	0.43
1:A:57:SER:HB2	1:A:100:GLY:CA	2.48	0.43
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.74	0.43
1:A:248:TYR:CE1	1:A:258:ILE:HG13	2.54	0.43
1:A:329:PRO:HB3	1:A:386:HIS:HB2	2.00	0.43
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.36	0.43
1:A:46:VAL:HG21	1:A:133:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:O	1:A:109:VAL:HG22	2.18	0.43
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.74	0.43
1:A:270:PRO:O	1:A:273:GLN:N	2.48	0.43
1:A:271:THR:HA	1:A:274:ASP:OD2	2.19	0.43
1:A:130:PHE:C	1:A:132:GLU:N	2.76	0.42
1:A:39:ASN:HB3	1:A:40:ASP:H	1.62	0.42
1:A:321:THR:OG1	1:A:354:PRO:O	2.30	0.42
1:A:93:LEU:CD1	1:A:94:ASP:N	2.79	0.42
1:A:248:TYR:OH	1:A:258:ILE:HA	2.19	0.42
1:A:91:ILE:HG22	1:A:92:PHE:N	2.34	0.42
1:A:370:THR:CG2	1:A:371:ALA:N	2.78	0.42
1:A:95:GLN:HG3	3:A:476:HOH:O	2.19	0.42
1:A:410:MET:HE3	1:A:411:VAL:HG23	2.01	0.42
1:A:348:ALA:O	1:A:352:VAL:HG22	2.19	0.42
1:A:146:SER:O	1:A:177:GLY:HA2	2.20	0.42
1:A:262:CYS:HB3	1:A:268:CYS:HA	1.96	0.42
1:A:38:ARG:HG3	1:A:86:SER:CA	2.43	0.42
1:A:186:ASN:ND2	1:A:186:ASN:N	2.68	0.42
1:A:221:ILE:CG1	1:A:313:MET:HE3	2.50	0.42
1:A:239:TYR:CD2	1:A:239:TYR:C	2.97	0.42
1:A:275:ILE:C	1:A:277:ASP:N	2.78	0.42
1:A:171:SER:HB3	1:A:329:PRO:HG2	2.01	0.42
1:A:182:LEU:HB3	1:A:225:TYR:HE2	1.84	0.42
1:A:129:GLN:C	1:A:130:PHE:CD1	2.98	0.41
1:A:155:PHE:O	1:A:159:ILE:HG22	2.20	0.41
1:A:320:VAL:CG1	1:A:324:LEU:HD12	2.50	0.41
1:A:69:SER:HA	1:A:78:ILE:O	2.20	0.41
1:A:71:ILE:CD1	1:A:278:TYR:CG	2.94	0.41
1:A:21:LEU:HD21	1:A:126:PHE:N	2.35	0.41
1:A:127:PHE:HB2	1:A:166:ASN:OD1	2.20	0.41
1:A:146:SER:OG	1:A:147:TYR:N	2.53	0.41
1:A:159:ILE:C	1:A:161:SER:N	2.72	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD12	1.83	0.41
1:A:276:ASP:OD1	1:A:295:TYR:CE1	2.73	0.41
1:A:342:ASN:HB2	3:A:471:HOH:O	2.19	0.41
1:A:407:ALA:O	1:A:411:VAL:N	2.35	0.41
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.32	0.41
1:A:390:LEU:HD23	1:A:410:MET:HG3	2.00	0.41
1:A:10:ILE:CG2	1:A:11:ASP:N	2.79	0.41
1:A:135:ASN:C	1:A:137:GLY:N	2.77	0.41
1:A:155:PHE:N	1:A:155:PHE:HD1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:CG1	1:A:293:ASP:N	2.81	0.41
1:A:325:ASN:OD1	1:A:356:LYS:N	2.48	0.41
1:A:19:GLY:C	1:A:32:PHE:CE1	2.99	0.41
1:A:242:ASN:O	1:A:246:ALA:HB3	2.20	0.41
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.72	0.41
1:A:127:PHE:HD1	1:A:127:PHE:HA	1.67	0.41
1:A:142:ILE:HG22	1:A:143:ALA:N	2.36	0.41
1:A:48:LEU:HD13	1:A:48:LEU:HA	1.53	0.41
1:A:54:PRO:HG3	1:A:147:TYR:CE2	2.56	0.41
1:A:112:THR:HG22	1:A:154:VAL:HG11	2.02	0.40
1:A:130:PHE:HA	1:A:132:GLU:CD	2.46	0.40
1:A:130:PHE:HB3	1:A:133:TYR:CE2	2.56	0.40
1:A:214:LEU:HD11	1:A:218:LEU:HD21	2.03	0.40
1:A:322:ASP:O	1:A:326:GLN:N	2.55	0.40
1:A:358:ASP:HB3	1:A:359:GLU:H	1.74	0.40
1:A:82:TYR:HB2	1:A:404:PRO:HB2	2.03	0.40
1:A:247:PRO:HA	1:A:250:ARG:CG	2.51	0.40
1:A:384:TYR:CE1	1:A:385:LYS:CG	3.04	0.40
1:A:210:MET:HE2	1:A:247:PRO:CG	2.52	0.40
1:A:84:TRP:CZ2	1:A:411:VAL:CG2	2.96	0.40
1:A:130:PHE:N	1:A:131:PRO:CD	2.85	0.40
1:A:202:LEU:CD2	1:A:210:MET:CE	2.98	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	419/421 (100%)	326 (78%)	64 (15%)	29 (7%)	1 1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	12	PRO
1	A	13	ASN
1	A	14	VAL
1	A	15	THR
1	A	24	GLU
1	A	125	LEU
1	A	135	ASN
1	A	266	ASN
1	A	342	ASN
1	A	358	ASP
1	A	98	ASN
1	A	311	ASP
1	A	397	HIS
1	A	73	PRO
1	A	126	PHE
1	A	6	LYS
1	A	64	PHE
1	A	77	PRO
1	A	136	LYS
1	A	185	TYR
1	A	88	ALA
1	A	300	PHE
1	A	411	VAL
1	A	312	TRP
1	A	131	PRO
1	A	9	GLY
1	A	134	VAL
1	A	354	PRO

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	332/363 (92%)	240 (72%)	92 (28%)	0 1

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	ILE
1	A	23	VAL
1	A	33	TRP
1	A	38	ARG
1	A	47	ILE
1	A	48	LEU
1	A	51	ASN
1	A	62	LEU
1	A	66	LEU
1	A	70	SER
1	A	78	ILE
1	A	87	ASN
1	A	89	THR
1	A	95	GLN
1	A	97	VAL
1	A	106	SER
1	A	107	SER
1	A	109	VAL
1	A	111	ASN
1	A	112	THR
1	A	122	PHE
1	A	123	LEU
1	A	124	GLU
1	A	128	ASP
1	A	129	GLN
1	A	132	GLU
1	A	134	VAL
1	A	135	ASN
1	A	141	HIS
1	A	157	SER
1	A	159	ILE
1	A	161	SER
1	A	165	ARG
1	A	166	ASN
1	A	170	THR
1	A	174	ILE
1	A	180	ASP
1	A	184	GLN
1	A	186	ASN
1	A	195	GLU
1	A	198	GLU
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	205	GLU
1	A	208	SER
1	A	216	ARG
1	A	217	CYS
1	A	222	GLU
1	A	223	SER
1	A	244	GLN
1	A	250	ARG
1	A	253	ARG
1	A	255	VAL
1	A	260	LYS
1	A	261	ASP
1	A	262	CYS
1	A	263	GLU
1	A	271	THR
1	A	272	LEU
1	A	274	ASP
1	A	276	ASP
1	A	279	LEU
1	A	280	ASN
1	A	283	TYR
1	A	285	LYS
1	A	286	GLU
1	A	288	VAL
1	A	292	VAL
1	A	304	ARG
1	A	305	ASN
1	A	311	ASP
1	A	313	MET
1	A	314	LYS
1	A	326	GLN
1	A	331	LEU
1	A	337	LYS
1	A	340	ILE
1	A	347	LYS
1	A	350	THR
1	A	356	LYS
1	A	363	SER
1	A	368	ASN
1	A	376	GLU
1	A	377	VAL
1	A	380	GLU

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Mol	Chain	Res	Type
1	A	381	VAL
1	A	382	LYS
1	A	399	VAL
1	A	401	PHE
1	A	402	ASP
1	A	405	GLU
1	A	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	168	ASN
1	A	186	ASN
1	A	241	ASN
1	A	244	GLN
1	A	317	HIS
1	A	342	ASN
1	A	368	ASN
1	A	406	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 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
2	NAG	A	3681	-	14,14,15	0.79	0	17,19,21	4.12	6 (35%)
2	NAG	A	871	-	14,14,15	1.98	4 (28%)	17,19,21	2.75	7 (41%)
2	NAG	A	1681	-	14,14,15	2.12	6 (42%)	17,19,21	2.99	5 (29%)

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	3681	-	-	5/6/23/26	0/1/1/1
2	NAG	A	871	-	-	3/6/23/26	0/1/1/1
2	NAG	A	1681	-	-	5/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	871	NAG	C1-C2	5.07	1.59	1.52
2	A	1681	NAG	C2-N2	5.06	1.54	1.46
2	A	871	NAG	O5-C5	3.05	1.49	1.43
2	A	871	NAG	C3-C2	2.64	1.58	1.52
2	A	1681	NAG	C3-C2	2.63	1.58	1.52
2	A	871	NAG	C2-N2	2.61	1.50	1.46
2	A	1681	NAG	C1-C2	2.60	1.55	1.52
2	A	1681	NAG	O7-C7	2.35	1.28	1.23
2	A	1681	NAG	C7-N2	2.17	1.41	1.34
2	A	1681	NAG	C4-C3	2.02	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3681	NAG	O6-C6-C5	14.97	162.30	111.33
2	A	1681	NAG	O6-C6-C5	8.30	139.59	111.33
2	A	871	NAG	O6-C6-C5	6.99	135.14	111.33
2	A	1681	NAG	C2-N2-C7	6.29	131.33	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	871	NAG	C1-O5-C5	5.53	119.59	112.19
2	A	3681	NAG	O7-C7-C8	-5.24	112.72	122.05
2	A	1681	NAG	O7-C7-C8	-4.80	113.51	122.05
2	A	871	NAG	C1-C2-N2	3.15	115.40	110.43
2	A	3681	NAG	O7-C7-N2	3.06	127.38	121.98
2	A	871	NAG	O7-C7-C8	-2.67	117.31	122.05
2	A	1681	NAG	O7-C7-N2	2.61	126.59	121.98
2	A	871	NAG	C3-C4-C5	2.46	114.69	110.23
2	A	3681	NAG	C1-C2-N2	2.40	114.22	110.43
2	A	3681	NAG	O5-C5-C6	-2.16	103.45	107.66
2	A	3681	NAG	C8-C7-N2	2.16	119.70	116.12
2	A	871	NAG	O7-C7-N2	2.16	125.79	121.98
2	A	871	NAG	O5-C5-C4	2.15	116.06	110.83
2	A	1681	NAG	C1-O5-C5	-2.15	109.30	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	871	NAG	C3-C2-N2-C7
2	A	1681	NAG	C8-C7-N2-C2
2	A	1681	NAG	O7-C7-N2-C2
2	A	3681	NAG	C3-C2-N2-C7
2	A	3681	NAG	C8-C7-N2-C2
2	A	3681	NAG	O7-C7-N2-C2
2	A	871	NAG	C4-C5-C6-O6
2	A	3681	NAG	O5-C5-C6-O6
2	A	871	NAG	O5-C5-C6-O6
2	A	3681	NAG	C4-C5-C6-O6
2	A	1681	NAG	C4-C5-C6-O6
2	A	1681	NAG	O5-C5-C6-O6
2	A	1681	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3681	NAG	5	0
2	A	871	NAG	2	0
2	A	1681	NAG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.