



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:37 AM BST

PDB ID : 1FQ7  
Title : X-RAY STRUCTURE OF INHIBITOR CP-72,647 BOUND TO SACCHAROPEPSIN  
Authors : Cronin, N.B.; Badasso, M.O.; Tickle, I.J.; Dreyer, T.; Hoover, D.J.; Rosati, R.L.; Humblet, C.C.; Lunney, E.A.; Cooper, J.B.  
Deposited on : 2000-09-04  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

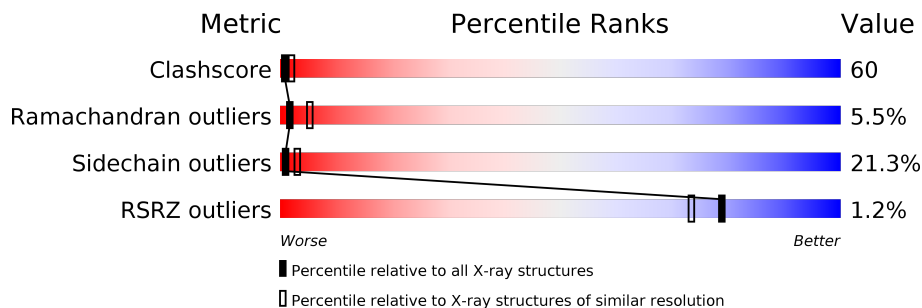
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	 26% 36% 33% 5%
2	B	5	 40% 60%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2717 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 SACCHAROPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2528	1618	396	508	6	0	0	0

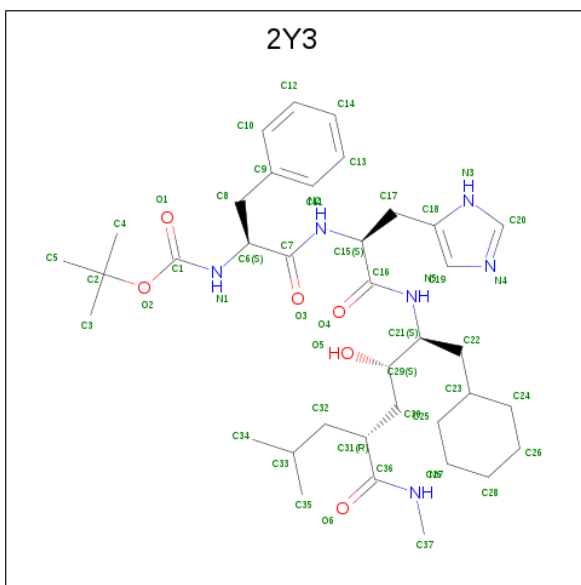
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	conflict	UNP P07267

- Molecule 2 is an oligosaccharide called beta-D-arabino-hexopyranos-2-ulose-(1-2)-beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

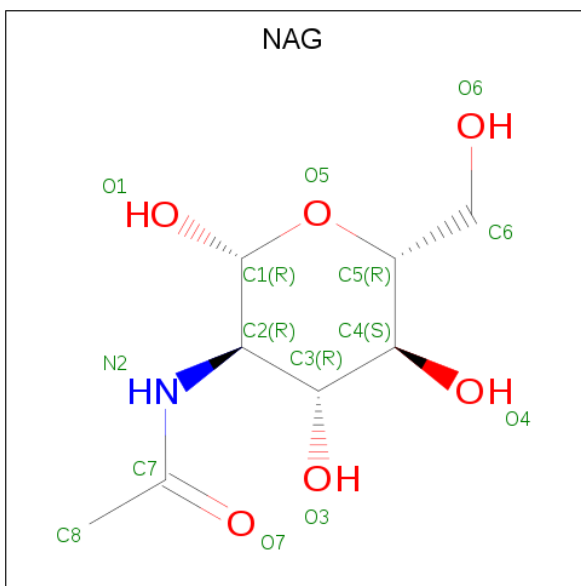
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

- Molecule 3 is N-(tert-butoxycarbonyl)-L-phenylalanyl-N-[(2S,3S,5R)-1-cyclohexyl-3-hydroxy-7-methyl-5-(methylcarbamoyl)octan-2-yl]-L-histidinamide (three-letter code: 2Y3) (formula: C<sub>37</sub>H<sub>58</sub>N<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	49	37	6	6	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

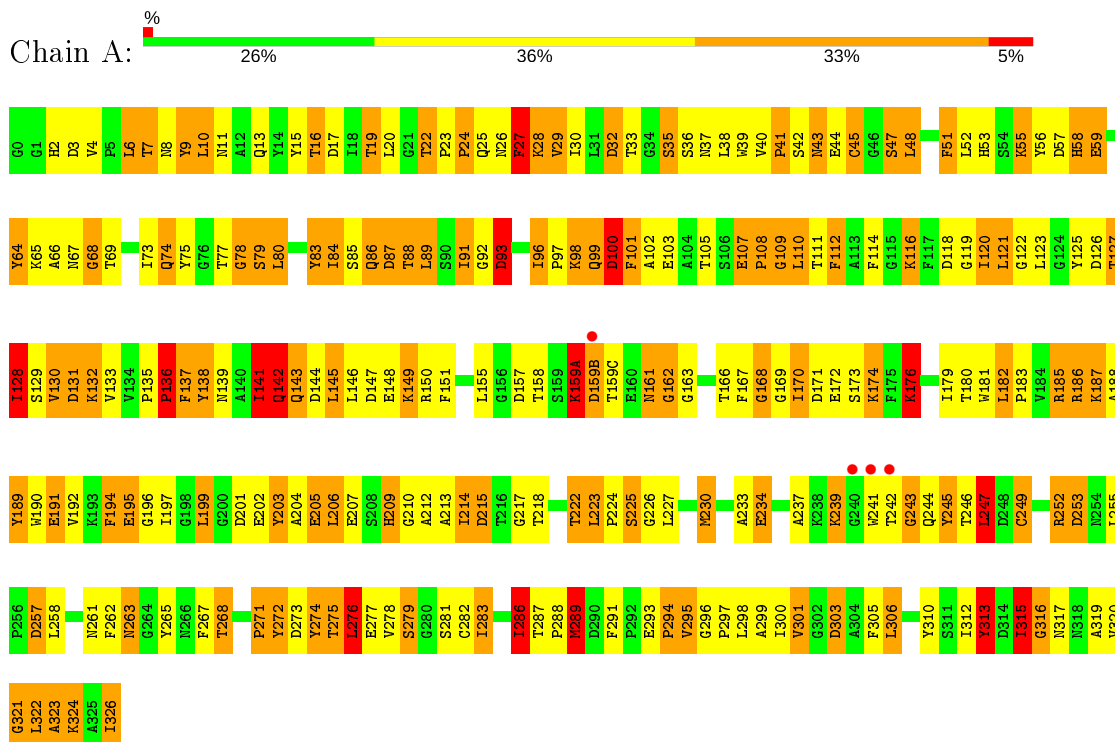
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	65	Total	O	0	0
			65	65		

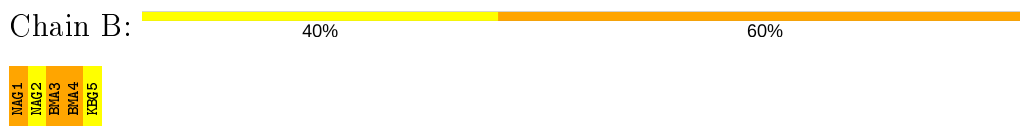
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SACCHAROPEPSIN



- Molecule 2: beta-D-arabino-hexopyranos-2-ulose-(1-2)-beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.43Å 86.43Å 109.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.30 – 2.80 27.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.30-2.80) 94.5 (27.40-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.80Å)	Xtrriage
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.190 , 0.270 0.187 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	0.286	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 100.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 2Y3, BMA, KBG, 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	1.06	1/2592 (0.0%)	2.44	178/3526 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	MET	SD-CE	5.07	2.06	1.77

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	-18.10	111.25	120.30
1	A	101	PHE	CB-CG-CD1	-13.58	111.29	120.80
1	A	133	VAL	CA-CB-CG2	13.52	131.18	110.90
1	A	185	ARG	NE-CZ-NH2	13.15	126.87	120.30
1	A	201	ASP	CB-CG-OD2	-13.01	106.60	118.30
1	A	203	TYR	CB-CG-CD1	-12.85	113.29	121.00
1	A	295	VAL	CG1-CB-CG2	12.63	131.10	110.90
1	A	252	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	A	203	TYR	CB-CG-CD2	11.55	127.93	121.00
1	A	310	TYR	CG-CD1-CE1	10.87	130.00	121.30
1	A	176	LYS	CA-CB-CG	10.74	137.03	113.40
1	A	137	PHE	CG-CD2-CE2	-10.43	109.32	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	CG1-CB-CG2	10.32	127.41	110.90
1	A	150	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	A	137	PHE	CZ-CE2-CD2	9.85	131.92	120.10
1	A	103	GLU	CA-CB-CG	9.73	134.80	113.40
1	A	157	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	A	157	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	4	VAL	CA-CB-CG2	9.20	124.70	110.90
1	A	255	LEU	CB-CG-CD2	-8.80	96.05	111.00
1	A	323	ALA	N-CA-CB	8.74	122.34	110.10
1	A	137	PHE	CD1-CE1-CZ	-8.68	109.69	120.10
1	A	171	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	121	LEU	CB-CG-CD1	8.34	125.18	111.00
1	A	303	ASP	CB-CG-OD2	8.32	125.79	118.30
1	A	192	VAL	CG1-CB-CG2	-8.24	97.72	110.90
1	A	286	ILE	CB-CG1-CD1	8.21	136.89	113.90
1	A	143	GLN	CB-CG-CD	8.15	132.78	111.60
1	A	289	MET	CG-SD-CE	-8.14	87.17	100.20
1	A	150	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	83	TYR	CB-CG-CD2	-8.04	116.17	121.00
1	A	271	PRO	N-CD-CG	-7.96	91.25	103.20
1	A	320	VAL	CA-CB-CG1	-7.67	99.39	110.90
1	A	247	LEU	CA-CB-CG	7.64	132.88	115.30
1	A	147	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	149	LYS	CD-CE-NZ	7.58	129.13	111.70
1	A	27	PHE	O-C-N	7.55	134.78	122.70
1	A	206	LEU	CB-CG-CD1	7.55	123.83	111.00
1	A	131	ASP	N-CA-CB	7.52	124.14	110.60
1	A	182	LEU	CB-CG-CD1	7.52	123.78	111.00
1	A	171	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	137	PHE	CG-CD1-CE1	7.43	128.97	120.80
1	A	9	TYR	CB-CG-CD1	-7.34	116.59	121.00
1	A	112	PHE	CB-CG-CD1	-7.28	115.70	120.80
1	A	244	GLN	CA-C-N	7.23	133.12	117.20
1	A	187	LYS	CB-CG-CD	7.23	130.41	111.60
1	A	183	PRO	O-C-N	7.23	134.26	122.70
1	A	310	TYR	CB-CG-CD2	7.22	125.33	121.00
1	A	110	LEU	CB-CG-CD2	7.10	123.07	111.00
1	A	313	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	A	29	VAL	CA-CB-CG1	-7.01	100.38	110.90
1	A	245	TYR	CD1-CE1-CZ	7.00	126.10	119.80
1	A	79	SER	O-C-N	7.00	133.89	122.70
1	A	78	GLY	C-N-CA	6.97	139.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	LYS	CD-CE-NZ	6.97	127.74	111.70
1	A	227	LEU	CB-CG-CD2	-6.96	99.17	111.00
1	A	273	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	131	ASP	O-C-N	6.88	133.71	122.70
1	A	310	TYR	CG-CD2-CE2	-6.83	115.84	121.30
1	A	93	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	244	GLN	CB-CG-CD	6.80	129.28	111.60
1	A	283	ILE	O-C-N	6.79	133.56	122.70
1	A	234	GLU	OE1-CD-OE2	6.75	131.40	123.30
1	A	243	GLY	N-CA-C	6.72	129.91	113.10
1	A	320	VAL	CG1-CB-CG2	-6.72	100.14	110.90
1	A	267	PHE	O-C-N	6.67	133.38	122.70
1	A	144	ASP	CB-CG-OD1	-6.65	112.31	118.30
1	A	301	VAL	CA-CB-CG2	6.63	120.85	110.90
1	A	214	ILE	C-N-CA	6.56	138.09	121.70
1	A	128	ILE	CA-CB-CG1	6.53	123.41	111.00
1	A	136	PRO	N-CD-CG	-6.52	93.42	103.20
1	A	201	ASP	OD1-CG-OD2	6.52	135.68	123.30
1	A	128	ILE	CB-CG1-CD1	-6.49	95.73	113.90
1	A	138	TYR	CG-CD2-CE2	6.48	126.48	121.30
1	A	102	ALA	C-N-CA	-6.47	105.51	121.70
1	A	273	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	110	LEU	CD1-CG-CD2	6.40	129.70	110.50
1	A	138	TYR	CG-CD1-CE1	-6.33	116.23	121.30
1	A	159(A)	LYS	C-N-CA	6.33	137.53	121.70
1	A	316	GLY	C-N-CA	6.33	137.53	121.70
1	A	141	ILE	CA-C-N	-6.33	103.28	117.20
1	A	192	VAL	CA-CB-CG2	-6.32	101.42	110.90
1	A	215	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	145	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	A	298	LEU	CB-CG-CD1	6.27	121.66	111.00
1	A	207	GLU	CB-CG-CD	-6.27	97.28	114.20
1	A	96	ILE	O-C-N	6.27	133.01	121.10
1	A	107	GLU	C-N-CD	-6.25	106.85	120.60
1	A	108	PRO	CA-N-CD	-6.25	102.75	111.50
1	A	225	SER	C-N-CA	-6.23	109.22	122.30
1	A	315	ILE	CA-CB-CG1	6.20	122.78	111.00
1	A	99	GLN	CA-CB-CG	6.19	127.01	113.40
1	A	185	ARG	CD-NE-CZ	-6.18	114.94	123.60
1	A	168	GLY	C-N-CA	-6.16	109.37	122.30
1	A	33	THR	C-N-CA	-6.10	109.49	122.30
1	A	274	TYR	CB-CG-CD1	6.08	124.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LEU	CB-CG-CD1	-6.07	100.67	111.00
1	A	29	VAL	CA-CB-CG2	6.04	119.96	110.90
1	A	268	THR	C-N-CA	6.04	136.79	121.70
1	A	190	TRP	CB-CA-C	6.00	122.41	110.40
1	A	312	ILE	O-C-N	-5.98	113.14	122.70
1	A	239	LYS	CA-CB-CG	5.97	126.54	113.40
1	A	247	LEU	CB-CG-CD2	5.96	121.13	111.00
1	A	88	THR	N-CA-CB	5.96	121.62	110.30
1	A	189	TYR	CA-CB-CG	5.96	124.72	113.40
1	A	301	VAL	C-N-CA	-5.91	109.89	122.30
1	A	281	SER	C-N-CA	-5.91	106.94	121.70
1	A	142	GLN	CA-CB-CG	-5.89	100.44	113.40
1	A	89	LEU	CD1-CG-CD2	5.89	128.16	110.50
1	A	247	LEU	CB-CG-CD1	5.88	120.99	111.00
1	A	205	GLU	OE1-CD-OE2	-5.86	116.26	123.30
1	A	142	GLN	CB-CG-CD	-5.85	96.38	111.60
1	A	167	PHE	CZ-CE2-CD2	5.81	127.07	120.10
1	A	182	LEU	CB-CG-CD2	5.80	120.86	111.00
1	A	27	PHE	CA-C-O	-5.79	107.95	120.10
1	A	101	PHE	CB-CG-CD2	5.76	124.83	120.80
1	A	315	ILE	O-C-N	-5.76	113.41	123.20
1	A	297	PRO	O-C-N	-5.75	113.50	122.70
1	A	209	HIS	O-C-N	-5.74	113.44	123.20
1	A	277	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	A	203	TYR	CA-C-O	-5.71	108.11	120.10
1	A	283	ILE	CA-C-O	-5.71	108.11	120.10
1	A	310	TYR	CD1-CE1-CZ	-5.70	114.67	119.80
1	A	138	TYR	CB-CG-CD1	5.69	124.41	121.00
1	A	301	VAL	O-C-N	-5.68	113.55	123.20
1	A	297	PRO	CA-C-N	5.62	129.55	117.20
1	A	145	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	A	203	TYR	CD1-CE1-CZ	5.59	124.83	119.80
1	A	7	THR	C-N-CA	-5.58	107.74	121.70
1	A	100	ASP	N-CA-CB	5.54	120.58	110.60
1	A	244	GLN	C-N-CA	-5.54	107.84	121.70
1	A	202	GLU	N-CA-CB	5.54	120.57	110.60
1	A	167	PHE	CG-CD2-CE2	-5.53	114.72	120.80
1	A	137	PHE	O-C-N	-5.51	113.88	122.70
1	A	32	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	130	VAL	CA-CB-CG1	-5.48	102.68	110.90
1	A	303	ASP	N-CA-CB	5.45	120.42	110.60
1	A	272	TYR	CD1-CE1-CZ	-5.45	114.90	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ILE	CA-C-O	5.44	131.53	120.10
1	A	194	PHE	CB-CG-CD1	5.43	124.60	120.80
1	A	225	SER	O-C-N	-5.43	113.97	123.20
1	A	298	LEU	CD1-CG-CD2	-5.42	94.26	110.50
1	A	244	GLN	CA-CB-CG	5.41	125.29	113.40
1	A	83	TYR	CG-CD1-CE1	-5.38	116.99	121.30
1	A	310	TYR	CZ-CE2-CD2	5.38	124.65	119.80
1	A	265	TYR	CG-CD1-CE1	5.38	125.60	121.30
1	A	253	ASP	N-CA-CB	5.37	120.27	110.60
1	A	10	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	176	LYS	CD-CE-NZ	5.33	123.96	111.70
1	A	19	THR	N-CA-CB	5.31	120.40	110.30
1	A	257	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	294	PRO	N-CD-CG	-5.27	95.30	103.20
1	A	210	GLY	N-CA-C	-5.26	99.96	113.10
1	A	28	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	A	108	PRO	O-C-N	5.24	132.10	123.20
1	A	155	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	194	PHE	CD1-CE1-CZ	5.20	126.34	120.10
1	A	172	GLU	CA-CB-CG	5.20	124.83	113.40
1	A	321	GLY	N-CA-C	-5.19	100.13	113.10
1	A	207	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	10	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	190	TRP	O-C-N	-5.13	114.49	122.70
1	A	136	PRO	CA-CB-CG	-5.13	94.25	104.00
1	A	6	LEU	CB-CG-CD1	5.12	119.70	111.00
1	A	109	GLY	N-CA-C	5.10	125.85	113.10
1	A	3	ASP	N-CA-CB	5.10	119.78	110.60
1	A	319	ALA	O-C-N	5.09	130.85	122.70
1	A	144	ASP	OD1-CG-OD2	5.09	132.97	123.30
1	A	315	ILE	C-N-CA	-5.08	111.63	122.30
1	A	83	TYR	CA-CB-CG	-5.07	103.76	113.40
1	A	322	LEU	C-N-CA	5.05	134.33	121.70
1	A	189	TYR	C-N-CA	-5.04	109.11	121.70
1	A	303	ASP	CB-CA-C	5.02	120.44	110.40
1	A	43	ASN	CB-CA-C	-5.01	100.37	110.40
1	A	173	SER	CA-CB-OG	5.01	124.74	111.20
1	A	281	SER	O-C-N	-5.01	114.68	122.70
1	A	195	GLU	CB-CG-CD	-5.01	100.67	114.20
1	A	108	PRO	C-N-CA	5.00	132.80	122.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	88	THR	CA
1	A	161	ASN	CA
1	A	315	ILE	CB

There are no planarity outliers.

## 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	2528	0	2401	301	0
2	B	61	0	42	3	0
3	A	49	0	58	17	0
4	A	14	0	13	0	0
5	A	65	0	0	10	0
All	All	2717	0	2514	309	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 60.

All (309) 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:289:MET:SD	1:A:289:MET:CE	2.06	1.42
1:A:242:THR:HG22	1:A:242:THR:O	1.41	1.15
1:A:287:THR:HG23	1:A:288:PRO:HD2	1.24	1.14
1:A:84:ILE:HG22	1:A:85:SER:H	1.09	1.12
1:A:84:ILE:CG2	1:A:85:SER:H	1.62	1.10
1:A:242:THR:O	1:A:242:THR:CG2	1.99	1.09
1:A:108:PRO:O	1:A:108:PRO:HD2	1.52	1.06
3:A:400:2Y3:O6	3:A:400:2Y3:H35A	1.57	1.05
1:A:86:GLN:O	1:A:87:ASP:HB2	1.54	1.02
1:A:89:LEU:HD23	1:A:96:ILE:HD13	1.42	1.02
1:A:74:GLN:HG3	1:A:79:SER:HB3	1.44	0.99
1:A:84:ILE:HG22	1:A:85:SER:N	1.67	0.99
1:A:252:ARG:HD3	1:A:275:THR:HG21	1.44	0.97
1:A:287:THR:HG23	1:A:288:PRO:CD	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:O	1:A:77:THR:HG22	1.67	0.94
1:A:108:PRO:O	1:A:108:PRO:CD	2.16	0.93
1:A:287:THR:CG2	1:A:288:PRO:HD2	1.99	0.92
1:A:176:LYS:HZ1	1:A:326:ILE:HG13	1.35	0.91
1:A:191:GLU:O	1:A:191:GLU:HG2	1.70	0.90
1:A:6:LEU:HB2	1:A:163:GLY:HA3	1.53	0.90
1:A:121:LEU:HD23	1:A:122:GLY:N	1.85	0.90
1:A:6:LEU:HB2	1:A:163:GLY:CA	2.03	0.89
1:A:135:PRO:HG2	1:A:138:TYR:CD1	2.08	0.88
1:A:97:PRO:O	1:A:98:LYS:HB2	1.70	0.88
1:A:203:TYR:C	1:A:203:TYR:CD1	2.45	0.88
1:A:176:LYS:NZ	1:A:326:ILE:HG13	1.89	0.88
1:A:237:ALA:HB1	1:A:245:TYR:HB3	1.56	0.87
1:A:218:THR:HG23	3:A:400:2Y3:H15	1.57	0.87
1:A:27:PHE:CZ	1:A:56:TYR:HB2	2.10	0.87
1:A:261:ASN:C	1:A:261:ASN:OD1	2.14	0.86
1:A:252:ARG:CD	1:A:275:THR:HG21	2.05	0.86
1:A:35:SER:HB2	1:A:75:TYR:HE1	1.41	0.85
1:A:191:GLU:CG	1:A:191:GLU:O	2.25	0.84
1:A:121:LEU:C	1:A:121:LEU:CD2	2.46	0.83
1:A:159(A):LYS:CG	1:A:159(B):ASP:H	1.89	0.83
1:A:143:GLN:HB2	1:A:145:LEU:HD11	1.60	0.82
1:A:27:PHE:HZ	1:A:56:TYR:HB2	1.41	0.82
3:A:400:2Y3:C36	3:A:400:2Y3:H35A	2.09	0.82
1:A:252:ARG:HH11	1:A:275:THR:CG2	1.92	0.82
1:A:58:HIS:CD2	1:A:58:HIS:H	1.98	0.81
1:A:282:CYS:HB2	5:A:616:HOH:O	1.81	0.80
1:A:179:ILE:HG21	1:A:181:TRP:CZ2	2.17	0.80
1:A:214:ILE:HD12	1:A:214:ILE:N	1.95	0.80
1:A:121:LEU:C	1:A:121:LEU:HD23	2.02	0.80
1:A:196:GLY:HA3	1:A:203:TYR:OH	1.82	0.80
1:A:159(A):LYS:HG3	1:A:159(B):ASP:H	1.46	0.79
1:A:189:TYR:CZ	3:A:400:2Y3:H34	2.18	0.79
1:A:48:LEU:O	1:A:48:LEU:HD23	1.82	0.79
1:A:223:LEU:HD22	1:A:286:ILE:HG23	1.64	0.78
1:A:313:TYR:N	1:A:313:TYR:CD1	2.50	0.78
1:A:29:VAL:HA	1:A:119:GLY:O	1.84	0.78
1:A:239:LYS:CG	1:A:243:GLY:HA2	2.14	0.78
1:A:143:GLN:HB2	1:A:145:LEU:CD1	2.13	0.78
1:A:278:VAL:HG12	1:A:278:VAL:O	1.82	0.78
1:A:287:THR:CG2	1:A:288:PRO:CD	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:HB2	5:A:581:HOH:O	1.84	0.77
1:A:194:PHE:HZ	1:A:197:ILE:HD12	1.47	0.77
1:A:10:LEU:HD23	1:A:10:LEU:N	2.00	0.77
1:A:77:THR:CG2	1:A:111:THR:HG21	2.15	0.76
1:A:16:THR:O	1:A:28:LYS:HA	1.85	0.76
1:A:11:ASN:OD1	1:A:158:THR:HG23	1.86	0.76
1:A:203:TYR:HD1	1:A:203:TYR:O	1.69	0.76
1:A:51:PHE:C	1:A:51:PHE:HD1	1.90	0.75
1:A:16:THR:HG23	1:A:17:ASP:N	1.99	0.74
1:A:203:TYR:HD1	1:A:203:TYR:C	1.88	0.74
1:A:23:PRO:HB2	1:A:24:PRO:HD2	1.67	0.74
1:A:57:ASP:OD1	1:A:59:GLU:HG2	1.86	0.74
1:A:7:THR:HG21	1:A:15:TYR:CE2	2.22	0.74
1:A:125:TYR:O	1:A:128:ILE:HG22	1.88	0.74
1:A:38:LEU:HD12	1:A:39:TRP:H	1.52	0.74
1:A:41:PRO:HG3	1:A:107:GLU:OE2	1.88	0.74
1:A:249:CYS:SG	1:A:282:CYS:N	2.61	0.73
1:A:99:GLN:NE2	1:A:136:PRO:HA	2.03	0.73
1:A:25:GLN:NE2	1:A:56:TYR:HA	2.04	0.73
1:A:10:LEU:O	1:A:11:ASN:HB2	1.89	0.73
1:A:239:LYS:HG3	1:A:243:GLY:HA2	1.72	0.72
1:A:263:ASN:HB2	5:A:612:HOH:O	1.89	0.72
1:A:38:LEU:HA	1:A:121:LEU:HA	1.71	0.72
1:A:145:LEU:HD12	1:A:145:LEU:H	1.55	0.71
1:A:58:HIS:H	1:A:58:HIS:HD2	1.39	0.71
1:A:247:LEU:HG	5:A:616:HOH:O	1.89	0.70
1:A:289:MET:CG	1:A:289:MET:CE	2.69	0.70
1:A:23:PRO:CB	1:A:24:PRO:HD2	2.22	0.70
1:A:10:LEU:H	1:A:10:LEU:HD23	1.54	0.70
3:A:400:2Y3:O1	3:A:400:2Y3:H5A	1.91	0.69
1:A:51:PHE:C	1:A:51:PHE:CD1	2.64	0.69
1:A:271:PRO:O	1:A:275:THR:HB	1.91	0.69
1:A:45:CYS:SG	1:A:47:SER:HB2	2.33	0.69
1:A:223:LEU:HD22	1:A:286:ILE:CG2	2.23	0.69
1:A:79:SER:C	1:A:80:LEU:HD23	2.12	0.69
1:A:84:ILE:HG23	1:A:101:PHE:O	1.93	0.68
1:A:137:PHE:HE2	1:A:315:ILE:CG1	2.06	0.68
1:A:222:THR:HB	1:A:300:ILE:HB	1.74	0.68
1:A:77:THR:HG22	1:A:111:THR:HG21	1.75	0.68
1:A:74:GLN:CG	1:A:79:SER:HB3	2.22	0.68
1:A:25:GLN:HE22	1:A:57:ASP:N	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HD22	1:A:317:ASN:N	1.92	0.67
1:A:252:ARG:HH11	1:A:275:THR:HG22	1.58	0.67
1:A:39:TRP:HZ3	1:A:41:PRO:HD3	1.58	0.67
1:A:137:PHE:CE2	1:A:315:ILE:HD11	2.30	0.67
1:A:89:LEU:CD2	1:A:96:ILE:HD13	2.23	0.67
1:A:77:THR:CG2	1:A:77:THR:O	2.42	0.66
1:A:143:GLN:CB	1:A:145:LEU:HD11	2.25	0.66
1:A:159(A):LYS:HD2	1:A:159(B):ASP:HB2	1.77	0.66
1:A:313:TYR:H	1:A:313:TYR:HD1	1.43	0.66
1:A:278:VAL:O	1:A:278:VAL:CG1	2.43	0.65
1:A:180:THR:O	1:A:321:GLY:HA2	1.96	0.65
1:A:239:LYS:HG2	1:A:243:GLY:HA2	1.78	0.64
1:A:206:LEU:HD13	1:A:209:HIS:CD2	2.33	0.64
1:A:35:SER:HB2	1:A:75:TYR:CE1	2.30	0.64
1:A:145:LEU:HD12	1:A:145:LEU:N	2.12	0.64
1:A:111:THR:HG22	3:A:400:2Y3:H12	1.79	0.63
1:A:15:TYR:CE1	1:A:116:LYS:HB3	2.33	0.63
1:A:203:TYR:O	1:A:203:TYR:CD1	2.49	0.63
1:A:214:ILE:HG23	1:A:306:LEU:HD11	1.79	0.63
1:A:99:GLN:HE22	1:A:136:PRO:HA	1.63	0.62
1:A:225:SER:O	1:A:226:GLY:C	2.35	0.62
1:A:38:LEU:HD12	1:A:39:TRP:N	2.15	0.62
1:A:246:THR:HA	1:A:283:ILE:HA	1.82	0.61
1:A:25:GLN:HE22	1:A:57:ASP:H	1.48	0.61
1:A:58:HIS:HB2	1:A:64:TYR:CD2	2.35	0.61
1:A:73:ILE:HD12	1:A:130:VAL:HG21	1.82	0.61
1:A:48:LEU:C	1:A:48:LEU:HD23	2.21	0.61
1:A:278:VAL:O	1:A:279:SER:HB2	2.00	0.61
3:A:400:2Y3:H3	5:A:659:HOH:O	2.00	0.61
1:A:159(A):LYS:HD2	1:A:159(B):ASP:CB	2.31	0.60
1:A:111:THR:CG2	3:A:400:2Y3:H12	2.32	0.60
1:A:58:HIS:CD2	1:A:58:HIS:N	2.69	0.60
1:A:194:PHE:CZ	1:A:197:ILE:HD12	2.34	0.60
1:A:13:GLN:HE22	1:A:116:LYS:H	1.48	0.59
1:A:42:SER:OG	1:A:43:ASN:N	2.36	0.59
1:A:45:CYS:HB2	1:A:105:THR:O	2.01	0.59
1:A:179:ILE:HA	1:A:323:ALA:HB2	1.85	0.59
1:A:84:ILE:HG23	1:A:85:SER:H	1.65	0.59
1:A:301:VAL:HG12	1:A:305:PHE:HB3	1.84	0.59
1:A:315:ILE:O	1:A:316:GLY:C	2.38	0.59
1:A:30:ILE:HD13	3:A:400:2Y3:C25	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:HD21	1:A:174:LYS:NZ	2.01	0.58
1:A:39:TRP:CZ3	1:A:41:PRO:HD3	2.39	0.58
1:A:89:LEU:HD22	1:A:99:GLN:HG2	1.85	0.58
1:A:121:LEU:CD2	1:A:122:GLY:N	2.63	0.58
1:A:30:ILE:HD13	3:A:400:2Y3:H25A	1.86	0.58
1:A:301:VAL:CG1	1:A:305:PHE:CB	2.82	0.58
1:A:86:GLN:O	1:A:87:ASP:CB	2.35	0.57
1:A:176:LYS:NZ	1:A:326:ILE:HA	2.20	0.57
1:A:56:TYR:CD2	1:A:56:TYR:O	2.57	0.57
1:A:230:MET:O	1:A:233:ALA:HB3	2.05	0.57
1:A:68:GLY:HA2	1:A:83:TYR:CD1	2.40	0.57
1:A:137:PHE:HE2	1:A:315:ILE:HG13	1.68	0.56
1:A:141:ILE:HD13	1:A:149:LYS:HD3	1.87	0.56
1:A:32:ASP:OD2	1:A:35:SER:HB3	2.05	0.56
1:A:25:GLN:HE22	1:A:56:TYR:HA	1.70	0.56
1:A:136:PRO:HD2	5:A:501:HOH:O	2.06	0.56
1:A:85:SER:O	1:A:100:ASP:HA	2.05	0.56
1:A:109:GLY:O	1:A:110:LEU:HD12	2.06	0.56
1:A:23:PRO:CB	1:A:24:PRO:CD	2.83	0.56
1:A:77:THR:HG21	1:A:111:THR:HG21	1.86	0.55
1:A:138:TYR:O	1:A:142:GLN:HB2	2.07	0.55
1:A:161:ASN:O	1:A:163:GLY:N	2.40	0.54
1:A:84:ILE:CG2	1:A:85:SER:N	2.31	0.54
1:A:142:GLN:CD	2:B:4:BMA:H62	2.27	0.54
1:A:317:ASN:N	1:A:317:ASN:ND2	2.55	0.54
1:A:135:PRO:HB2	5:A:501:HOH:O	2.08	0.54
1:A:6:LEU:CB	1:A:163:GLY:HA3	2.33	0.54
1:A:189:TYR:CE1	3:A:400:2Y3:H34	2.43	0.54
1:A:75:TYR:CD1	3:A:400:2Y3:H37A	2.43	0.54
1:A:215:ASP:C	1:A:215:ASP:OD1	2.45	0.53
1:A:182:LEU:HD13	1:A:262:PHE:HB3	1.89	0.53
1:A:189:TYR:CE1	3:A:400:2Y3:C34	2.92	0.53
1:A:214:ILE:HD12	1:A:214:ILE:H	1.73	0.53
1:A:161:ASN:O	1:A:162:GLY:C	2.45	0.53
1:A:38:LEU:HA	1:A:120:ILE:O	2.09	0.53
1:A:196:GLY:H	1:A:261:ASN:HB3	1.73	0.53
1:A:137:PHE:HE2	1:A:315:ILE:CD1	2.22	0.53
1:A:38:LEU:HD13	1:A:121:LEU:HB2	1.90	0.53
1:A:214:ILE:N	1:A:214:ILE:CD1	2.70	0.52
1:A:242:THR:HG23	1:A:242:THR:O	2.04	0.52
1:A:32:ASP:OD1	1:A:217:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:CG2	1:A:288:PRO:N	2.71	0.52
1:A:274:TYR:HB2	1:A:286:ILE:CD1	2.39	0.52
1:A:137:PHE:CD2	1:A:315:ILE:HD11	2.44	0.52
1:A:65:LYS:HG3	1:A:66:ALA:N	2.25	0.52
3:A:400:2Y3:O1	3:A:400:2Y3:C5	2.59	0.51
1:A:159(A):LYS:CD	1:A:159(B):ASP:HB2	2.40	0.51
1:A:287:THR:HG22	1:A:288:PRO:N	2.24	0.51
1:A:291:PHE:O	1:A:296:GLY:HA3	2.10	0.51
1:A:205:GLU:C	1:A:206:LEU:HD23	2.31	0.51
1:A:257:ASP:HB3	1:A:268:THR:CG2	2.40	0.51
1:A:58:HIS:HB2	1:A:64:TYR:CE2	2.45	0.51
1:A:271:PRO:HA	1:A:274:TYR:CE1	2.45	0.50
1:A:252:ARG:HD2	1:A:275:THR:HG21	1.92	0.50
1:A:109:GLY:C	1:A:110:LEU:HD12	2.32	0.50
1:A:39:TRP:CH2	1:A:119:GLY:HA2	2.47	0.50
1:A:186:ARG:NH1	1:A:191:GLU:OE2	2.45	0.50
1:A:222:THR:HG22	1:A:222:THR:O	2.11	0.50
1:A:301:VAL:CG1	1:A:305:PHE:HB3	2.42	0.49
1:A:58:HIS:ND1	1:A:64:TYR:CZ	2.79	0.49
1:A:110:LEU:O	1:A:114:PHE:HD2	1.94	0.49
1:A:179:ILE:HG21	1:A:181:TRP:CH2	2.48	0.49
1:A:42:SER:O	1:A:55:LYS:HG2	2.12	0.49
1:A:159(A):LYS:HE2	1:A:326:ILE:O	2.12	0.49
1:A:25:GLN:NE2	1:A:57:ASP:H	2.10	0.49
1:A:223:LEU:O	1:A:224:PRO:C	2.48	0.49
1:A:161:ASN:ND2	1:A:174:LYS:NZ	2.61	0.49
1:A:13:GLN:HE22	1:A:116:LYS:HB2	1.77	0.48
1:A:191:GLU:HA	1:A:212:ALA:O	2.13	0.48
1:A:166:THR:HG22	1:A:169:GLY:O	2.11	0.48
1:A:315:ILE:HD13	1:A:315:ILE:HG21	1.63	0.48
1:A:73:ILE:HD12	1:A:130:VAL:CG2	2.42	0.48
3:A:400:2Y3:C36	3:A:400:2Y3:C35	2.80	0.48
1:A:77:THR:CG2	1:A:111:THR:CG2	2.89	0.48
1:A:246:THR:HG22	1:A:283:ILE:HG22	1.94	0.48
1:A:15:TYR:CE1	1:A:116:LYS:CB	2.96	0.48
1:A:53:HIS:HB3	1:A:118:ASP:OD1	2.13	0.48
1:A:36:SER:HB2	1:A:128:ILE:HG23	1.96	0.48
1:A:276:LEU:O	1:A:282:CYS:HA	2.13	0.48
1:A:35:SER:CB	1:A:75:TYR:HE1	2.19	0.48
1:A:8:ASN:OD1	1:A:9:TYR:N	2.47	0.48
1:A:48:LEU:CD2	1:A:48:LEU:C	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:VAL:HG12	1:A:296:GLY:N	2.29	0.47
1:A:96:ILE:H	1:A:96:ILE:HD12	1.80	0.47
1:A:141:ILE:CD1	1:A:149:LYS:HG2	2.44	0.47
1:A:128:ILE:HG21	1:A:128:ILE:HD12	1.47	0.47
1:A:159(A):LYS:HG3	1:A:159(B):ASP:N	2.24	0.47
1:A:222:THR:HG22	5:A:676:HOH:O	2.13	0.47
1:A:291:PHE:HB3	1:A:295:VAL:HG12	1.97	0.47
1:A:88:THR:OG1	1:A:97:PRO:HA	2.14	0.47
1:A:135:PRO:O	1:A:136:PRO:C	2.52	0.47
1:A:75:TYR:HD1	3:A:400:2Y3:H37A	1.79	0.47
1:A:135:PRO:HG2	1:A:138:TYR:HD1	1.71	0.47
1:A:137:PHE:CE2	1:A:315:ILE:CD1	2.97	0.47
1:A:6:LEU:HB2	1:A:163:GLY:C	2.36	0.46
1:A:97:PRO:O	1:A:98:LYS:CB	2.45	0.46
2:B:3:BMA:O2	2:B:4:BMA:C1	2.60	0.46
1:A:151:PHE:HA	1:A:166:THR:O	2.14	0.46
1:A:278:VAL:O	1:A:279:SER:CB	2.63	0.46
1:A:74:GLN:HA	1:A:79:SER:HB3	1.98	0.46
1:A:39:TRP:HE1	1:A:120:ILE:HG13	1.81	0.46
1:A:222:THR:O	1:A:299:ALA:HA	2.16	0.46
1:A:39:TRP:C	1:A:39:TRP:CE3	2.89	0.46
1:A:39:TRP:NE1	1:A:120:ILE:HG13	2.30	0.46
1:A:135:PRO:HD2	1:A:138:TYR:HB2	1.97	0.46
1:A:37:ASN:HD21	1:A:130:VAL:N	2.14	0.46
1:A:83:TYR:CD1	1:A:83:TYR:C	2.89	0.46
1:A:65:LYS:HG3	1:A:66:ALA:H	1.79	0.45
1:A:7:THR:CG2	1:A:15:TYR:CE2	2.97	0.45
1:A:203:TYR:CE1	1:A:204:ALA:O	2.70	0.45
1:A:215:ASP:OD1	1:A:217:GLY:N	2.49	0.45
1:A:239:LYS:HG3	1:A:243:GLY:CA	2.43	0.45
1:A:43:ASN:C	1:A:45:CYS:H	2.20	0.45
1:A:75:TYR:HB2	1:A:78:GLY:O	2.15	0.45
1:A:139:ASN:O	1:A:143:GLN:HG3	2.16	0.45
1:A:83:TYR:HD1	1:A:84:ILE:O	2.00	0.45
1:A:83:TYR:N	1:A:83:TYR:CD2	2.84	0.45
1:A:68:GLY:HA2	1:A:83:TYR:HD1	1.82	0.45
1:A:301:VAL:CG1	1:A:305:PHE:CG	2.99	0.45
1:A:48:LEU:CD2	1:A:52:LEU:CD1	2.94	0.45
1:A:25:GLN:HE22	1:A:56:TYR:CA	2.30	0.44
1:A:159(B):ASP:OD1	1:A:161:ASN:HA	2.18	0.44
1:A:289:MET:HG2	1:A:289:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:HG21	1:A:111:THR:CG2	2.48	0.44
1:A:247:LEU:HD21	1:A:275:THR:OG1	2.18	0.44
1:A:326:ILE:OXT	1:A:326:ILE:HG22	2.18	0.44
1:A:121:LEU:C	1:A:121:LEU:HD22	2.33	0.44
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.83	0.44
1:A:20:LEU:O	1:A:25:GLN:HB2	2.18	0.44
1:A:197:ILE:HG21	1:A:197:ILE:HD13	1.67	0.43
1:A:242:THR:HG22	5:A:598:HOH:O	2.18	0.43
3:A:400:2Y3:H24	3:A:400:2Y3:H21	1.64	0.43
1:A:39:TRP:O	1:A:40:VAL:HG13	2.17	0.43
1:A:85:SER:O	1:A:100:ASP:HB3	2.18	0.43
1:A:130:VAL:HG12	1:A:131:ASP:N	2.32	0.43
1:A:146:LEU:HD22	1:A:168:GLY:HA3	2.01	0.43
1:A:13:GLN:NE2	1:A:116:LYS:H	2.14	0.43
1:A:213:ALA:HB3	1:A:300:ILE:HD13	1.99	0.43
1:A:22:THR:HA	1:A:23:PRO:HA	1.68	0.43
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.76	0.43
1:A:294:PRO:HD2	1:A:295:VAL:N	2.34	0.43
1:A:222:THR:HA	1:A:287:THR:O	2.19	0.43
1:A:48:LEU:HD21	1:A:52:LEU:HD11	2.01	0.43
1:A:289:MET:HE3	1:A:289:MET:HG2	2.02	0.42
1:A:8:ASN:C	1:A:8:ASN:OD1	2.57	0.42
1:A:96:ILE:HD12	1:A:96:ILE:N	2.34	0.42
1:A:253:ASP:OD1	1:A:272:TYR:HE2	2.03	0.42
1:A:161:ASN:HD21	1:A:174:LYS:HZ3	1.67	0.42
1:A:91:ILE:O	1:A:92:GLY:C	2.56	0.42
1:A:83:TYR:CD1	1:A:83:TYR:O	2.73	0.42
1:A:182:LEU:HD13	1:A:262:PHE:CB	2.50	0.42
1:A:130:VAL:C	1:A:132:LYS:H	2.23	0.42
1:A:56:TYR:CG	1:A:56:TYR:O	2.73	0.42
1:A:199:LEU:HB2	1:A:258:LEU:HA	2.02	0.41
1:A:65:LYS:HZ1	2:B:1:NAG:H81	1.85	0.41
1:A:53:HIS:HE1	1:A:112:PHE:O	2.03	0.41
1:A:195:GLU:HB2	1:A:261:ASN:OD1	2.20	0.41
1:A:170:ILE:HG12	1:A:170:ILE:O	2.20	0.41
1:A:176:LYS:HZ2	1:A:326:ILE:HG13	1.82	0.41
1:A:39:TRP:HE3	1:A:40:VAL:N	2.18	0.41
1:A:75:TYR:C	1:A:77:THR:N	2.73	0.41
1:A:13:GLN:NE2	1:A:116:LYS:HB2	2.36	0.41
1:A:73:ILE:O	1:A:79:SER:HA	2.20	0.41
1:A:126:ASP:C	1:A:128:ILE:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159(C):THR:O	1:A:159(C):THR:HG22	2.21	0.40
1:A:222:THR:HG23	1:A:289:MET:HB2	2.03	0.40
1:A:48:LEU:HD21	1:A:52:LEU:CD1	2.51	0.40
1:A:2:HIS:HB3	5:A:581:HOH:O	2.21	0.40
1:A:301:VAL:HG11	1:A:305:PHE:CG	2.56	0.40
1:A:80:LEU:HD23	1:A:80:LEU:N	2.37	0.40
1:A:107:GLU:HA	1:A:108:PRO:HD3	1.87	0.40
1:A:127:THR:HG22	1:A:127:THR:O	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	327/329 (99%)	278 (85%)	31 (10%)	18 (6%)	<b>2</b> <b>5</b>

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASP
1	A	188	ALA
1	A	24	PRO
1	A	44	GLU
1	A	59	GLU
1	A	64	TYR
1	A	68	GLY
1	A	98	LYS
1	A	159(A)	LYS
1	A	159(B)	ASP
1	A	162	GLY
1	A	241	TRP
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	127	THR
1	A	249	CYS
1	A	263	ASN
1	A	84	ILE
1	A	136	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/268 (100%)	211 (79%)	57 (21%)	<b>1</b> <b>3</b>

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	19	THR
1	A	22	THR
1	A	26	ASN
1	A	27	PHE
1	A	35	SER
1	A	41	PRO
1	A	45	CYS
1	A	47	SER
1	A	48	LEU
1	A	51	PHE
1	A	55	LYS
1	A	58	HIS
1	A	69	THR
1	A	74	GLN
1	A	80	LEU
1	A	86	GLN
1	A	91	ILE
1	A	93	ASP
1	A	100	ASP
1	A	116	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	120	ILE
1	A	123	LEU
1	A	128	ILE
1	A	129	SER
1	A	132	LYS
1	A	141	ILE
1	A	142	GLN
1	A	148	GLU
1	A	159(A)	LYS
1	A	161	ASN
1	A	170	ILE
1	A	174	LYS
1	A	176	LYS
1	A	185	ARG
1	A	186	ARG
1	A	187	LYS
1	A	191	GLU
1	A	199	LEU
1	A	222	THR
1	A	223	LEU
1	A	230	MET
1	A	234	GLU
1	A	247	LEU
1	A	275	THR
1	A	276	LEU
1	A	279	SER
1	A	286	ILE
1	A	289	MET
1	A	293	GLU
1	A	303	ASP
1	A	306	LEU
1	A	313	TYR
1	A	315	ILE
1	A	322	LEU
1	A	324	LYS
1	A	326	ILE

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2	HIS
1	A	13	GLN

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Mol	Chain	Res	Type
1	A	25	GLN
1	A	99	GLN
1	A	142	GLN
1	A	161	ASN
1	A	209	HIS
1	A	232	ASN
1	A	317	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](#)

5 monosaccharides 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	B	1	1,2	14,14,15	1.68	4 (28%)	17,19,21	3.10	6 (35%)
2	NAG	B	2	2	14,14,15	1.34	3 (21%)	17,19,21	2.46	7 (41%)
2	BMA	B	3	2	11,11,12	1.17	1 (9%)	15,15,17	3.73	4 (26%)
2	BMA	B	4	2	11,11,12	2.04	3 (27%)	15,15,17	2.93	8 (53%)
2	KBG	B	5	2	11,11,12	4.20	6 (54%)	12,15,17	2.26	5 (41%)

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	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	KBG	B	5	2	-	1/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	KBG	OAG-C2	11.47	1.41	1.21
2	B	5	KBG	C3-C2	-5.21	1.44	1.52
2	B	5	KBG	C1-C2	-3.64	1.47	1.51
2	B	4	BMA	O5-C5	3.57	1.50	1.43
2	B	4	BMA	C2-C3	3.44	1.57	1.52
2	B	4	BMA	O5-C1	3.07	1.48	1.43
2	B	1	NAG	C1-C2	-3.05	1.47	1.52
2	B	5	KBG	O5-C5	2.96	1.49	1.43
2	B	1	NAG	O3-C3	2.62	1.49	1.43
2	B	1	NAG	C2-N2	2.62	1.50	1.46
2	B	2	NAG	O4-C4	2.50	1.48	1.43
2	B	3	BMA	O4-C4	2.39	1.48	1.43
2	B	2	NAG	O5-C1	2.31	1.47	1.43
2	B	2	NAG	O3-C3	2.20	1.48	1.43
2	B	1	NAG	C7-N2	2.19	1.41	1.34
2	B	5	KBG	O4-C4	2.19	1.48	1.43
2	B	5	KBG	C4-C3	-2.18	1.49	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	13.01	129.82	112.19
2	B	1	NAG	C2-N2-C7	-10.27	108.28	122.90
2	B	4	BMA	O5-C1-C2	-5.86	101.72	110.77
2	B	4	BMA	C1-O5-C5	-5.51	104.72	112.19
2	B	2	NAG	C1-O5-C5	5.26	119.31	112.19
2	B	5	KBG	OAG-C2-C1	-4.51	113.84	121.30
2	B	2	NAG	O5-C5-C6	4.49	114.24	107.20
2	B	4	BMA	O5-C5-C6	-4.31	100.45	107.20
2	B	1	NAG	O5-C1-C2	3.98	117.57	111.29
2	B	3	BMA	O2-C2-C3	3.82	117.79	110.14
2	B	2	NAG	C3-C4-C5	-3.42	104.13	110.24
2	B	2	NAG	C8-C7-N2	-3.42	110.31	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	KBG	O5-C5-C6	-3.38	101.91	107.20
2	B	1	NAG	O3-C3-C4	-3.35	102.61	110.35
2	B	2	NAG	O7-C7-N2	3.14	127.73	121.95
2	B	5	KBG	O5-C5-C4	3.08	118.33	110.83
2	B	4	BMA	O5-C5-C4	3.05	118.24	110.83
2	B	5	KBG	C1-O5-C5	3.04	115.93	111.76
2	B	2	NAG	O3-C3-C4	-3.01	103.39	110.35
2	B	4	BMA	C2-C3-C4	-2.93	105.82	110.89
2	B	1	NAG	C1-O5-C5	2.86	116.07	112.19
2	B	4	BMA	O3-C3-C2	-2.76	104.71	109.99
2	B	3	BMA	C1-C2-C3	2.72	113.01	109.67
2	B	1	NAG	O5-C5-C6	-2.69	102.99	107.20
2	B	5	KBG	O3-C3-C2	2.61	115.08	109.84
2	B	1	NAG	O5-C5-C4	-2.53	104.68	110.83
2	B	2	NAG	O4-C4-C5	-2.43	103.26	109.30
2	B	4	BMA	C3-C4-C5	-2.31	106.11	110.24
2	B	3	BMA	O3-C3-C4	-2.26	105.12	110.35
2	B	4	BMA	O3-C3-C4	-2.22	105.21	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

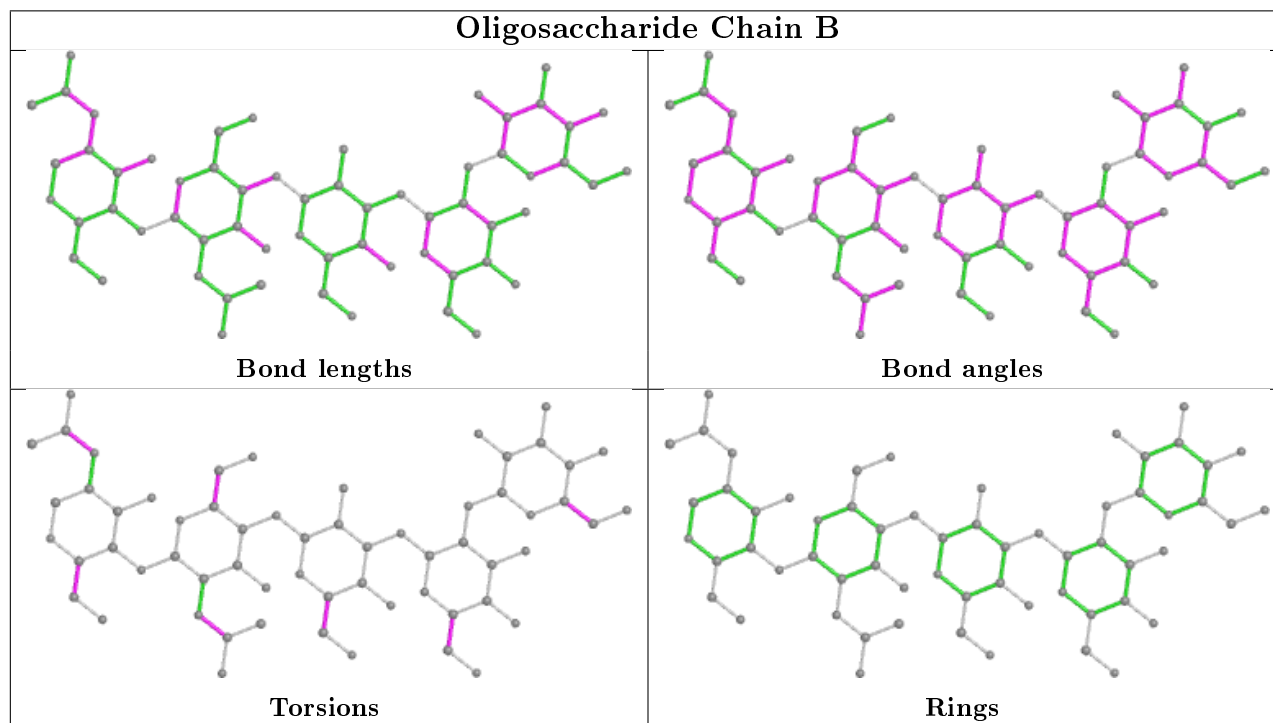
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
2	B	5	KBG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	3	BMA	1	0
2	B	4	BMA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

2 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$
4	NAG	A	337	1	14,14,15	1.35	2 (14%)	17,19,21	2.98	5 (29%)
3	2Y3	A	400	-	47,51,51	1.20	3 (6%)	60,69,69	2.06	17 (28%)

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
4	NAG	A	337	1	-	2/6/23/26	0/1/1/1
3	2Y3	A	400	-	-	13/55/63/63	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	2Y3	O2-C1	5.44	1.45	1.34
4	A	337	NAG	O5-C1	3.29	1.49	1.43
3	A	400	2Y3	C17-C15	-2.71	1.47	1.54
4	A	337	NAG	O4-C4	2.61	1.49	1.43
3	A	400	2Y3	O2-C2	-2.11	1.44	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	337	NAG	O5-C1-C2	-8.09	98.51	111.29
3	A	400	2Y3	O2-C1-N1	7.04	121.86	110.02
4	A	337	NAG	C8-C7-N2	-6.11	105.76	116.10
3	A	400	2Y3	C17-C15-N2	5.24	121.83	110.79
3	A	400	2Y3	O2-C1-O1	-4.86	116.75	125.62
4	A	337	NAG	O7-C7-N2	4.14	129.57	121.95
3	A	400	2Y3	C15-N2-C7	3.79	129.80	121.67
3	A	400	2Y3	C35-C33-C32	-3.70	97.49	111.11
3	A	400	2Y3	O3-C7-C6	-3.69	112.68	120.45
3	A	400	2Y3	C22-C23-C25	3.26	118.83	111.73
3	A	400	2Y3	C28-C27-C25	3.16	117.86	111.42
3	A	400	2Y3	C6-N1-C1	2.51	127.02	120.90
4	A	337	NAG	O6-C6-C5	2.47	119.75	111.29
4	A	337	NAG	C6-C5-C4	2.44	118.72	113.00
3	A	400	2Y3	C21-N5-C16	2.39	127.30	123.07
3	A	400	2Y3	C31-C32-C33	-2.37	110.24	115.68
3	A	400	2Y3	C25-C23-C24	-2.25	103.83	109.33
3	A	400	2Y3	C6-C7-N2	2.19	121.51	116.70
3	A	400	2Y3	C2-O2-C1	-2.14	117.70	120.99
3	A	400	2Y3	O1-C1-N1	-2.12	121.38	124.85
3	A	400	2Y3	C28-C26-C24	-2.06	107.22	111.42
3	A	400	2Y3	C34-C33-C32	2.03	118.58	111.11

There are no chirality outliers.

All (15) torsion outliers are listed below:

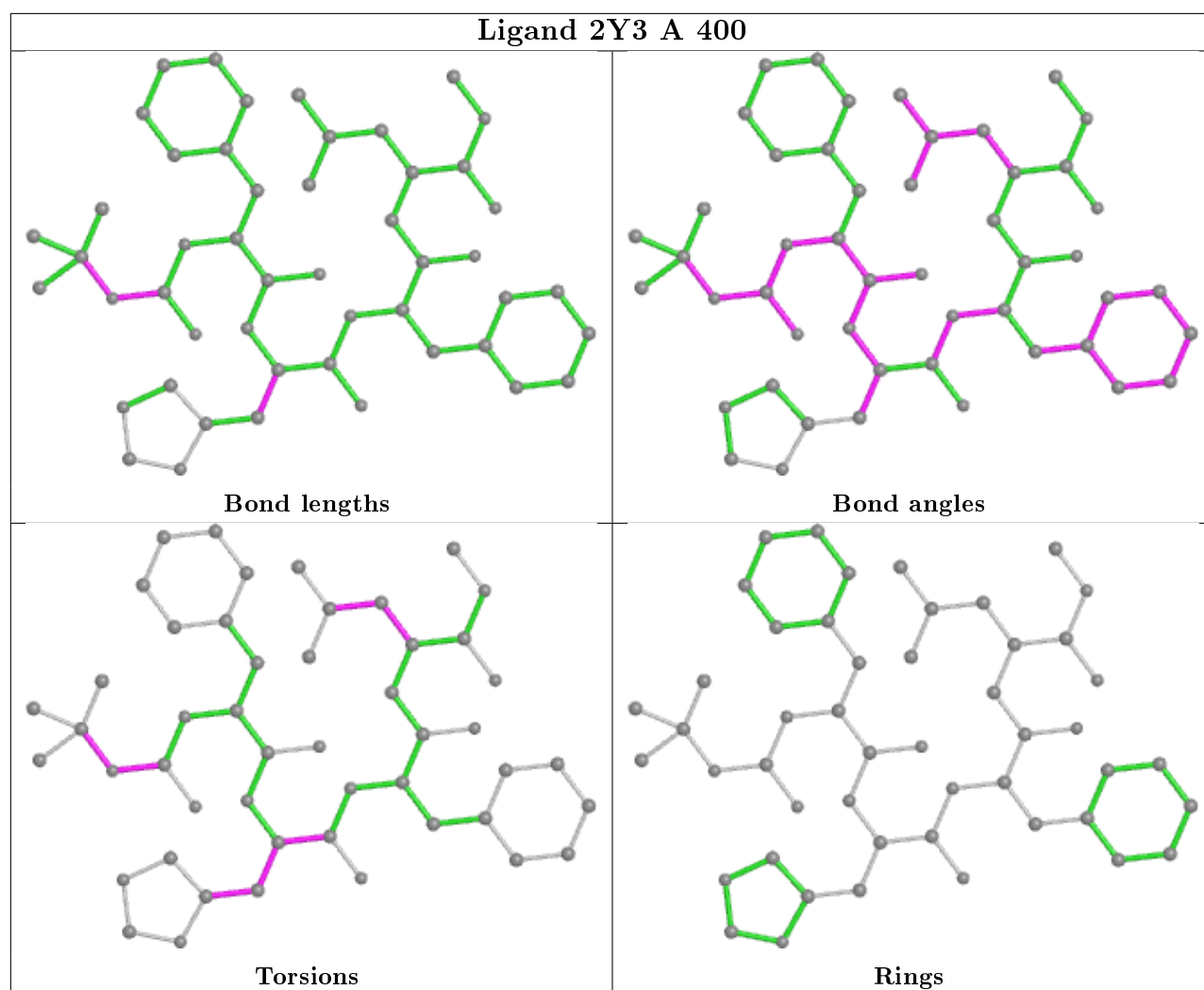
Mol	Chain	Res	Type	Atoms
3	A	400	2Y3	C5-C2-O2-C1
3	A	400	2Y3	C3-C2-O2-C1
3	A	400	2Y3	C4-C2-O2-C1
4	A	337	NAG	C8-C7-N2-C2
3	A	400	2Y3	C31-C32-C33-C34
4	A	337	NAG	O7-C7-N2-C2
3	A	400	2Y3	C31-C32-C33-C35
3	A	400	2Y3	N2-C15-C17-C18
3	A	400	2Y3	C15-C17-C18-N3
3	A	400	2Y3	N1-C1-O2-C2
3	A	400	2Y3	O1-C1-O2-C2
3	A	400	2Y3	N2-C15-C16-O4
3	A	400	2Y3	N2-C15-C16-N5
3	A	400	2Y3	C36-C31-C32-C33
3	A	400	2Y3	C15-C17-C18-C19

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	2Y3	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	329/329 (100%)	-0.63	4 (1%) 79 73	6, 28, 56, 102	4 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	4.8
1	A	240	GLY	4.6
1	A	241	TRP	3.4
1	A	159(B)	ASP	2.8

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

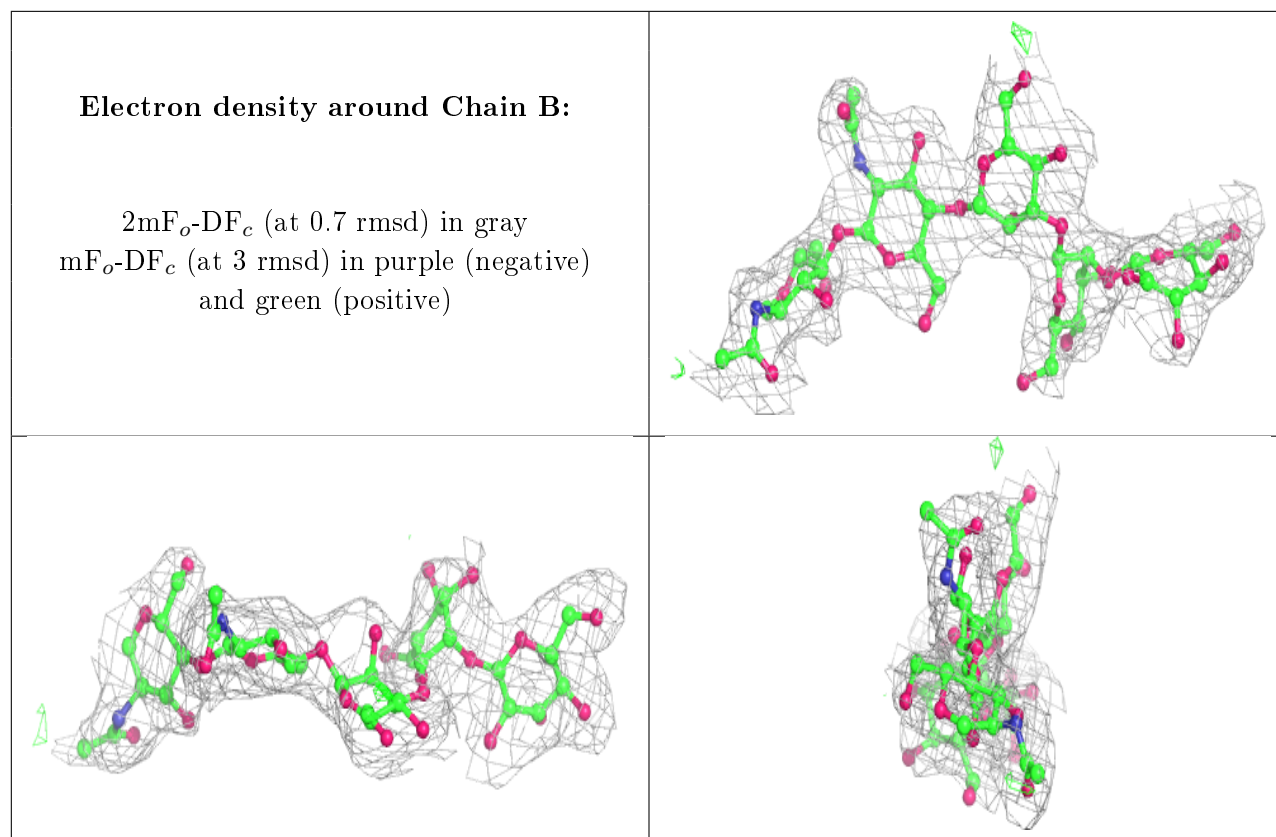
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	KBG	B	5	11/12	0.80	0.16	34,51,156,156	0
2	NAG	B	1	14/15	0.93	0.17	20,43,71,85	0
2	BMA	B	3	11/12	0.93	0.12	15,30,67,83	0
2	NAG	B	2	14/15	0.96	0.12	3,33,62,87	0
2	BMA	B	4	11/12	0.97	0.18	7,25,58,101	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



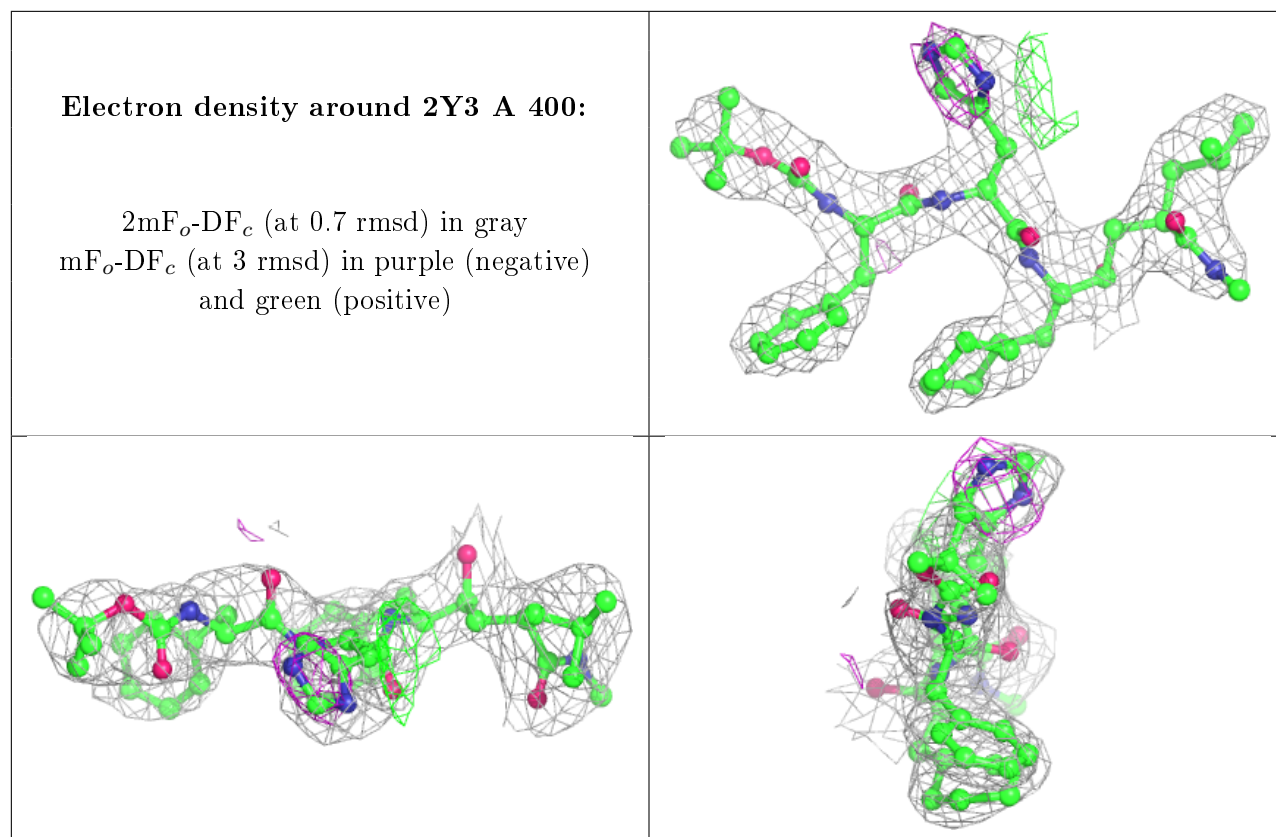
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	337	14/15	0.93	0.08	15,38,146,156	0
3	2Y3	A	400	49/49	0.93	0.16	4,24,49,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.