



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 09:50 AM UTC

PDB ID : 1FQ7 / pdb_00001fq7
Title : X-RAY STRUCTURE OF INHIBITOR CP-72,647 BOUND TO SACCHAROPEPSIN
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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

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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

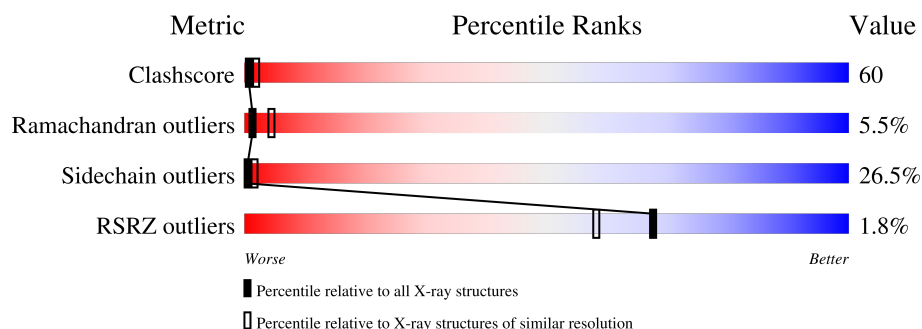
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	2% 19% 33% 38% 10%
2	B	5	60% 40%

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
1	A	329	Total	C	N	O	S	0	0	0
			2528	1618	396	508	6			

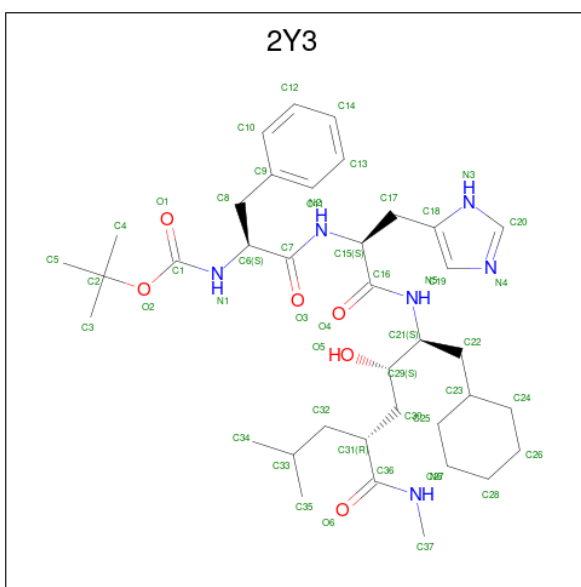
There is a discrepancy between the modelled and reference sequences:

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-glucopyranoside-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- 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 (CCD ID: 2Y3) (formula: C₃₇H₅₈N₆O₆).



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

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



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

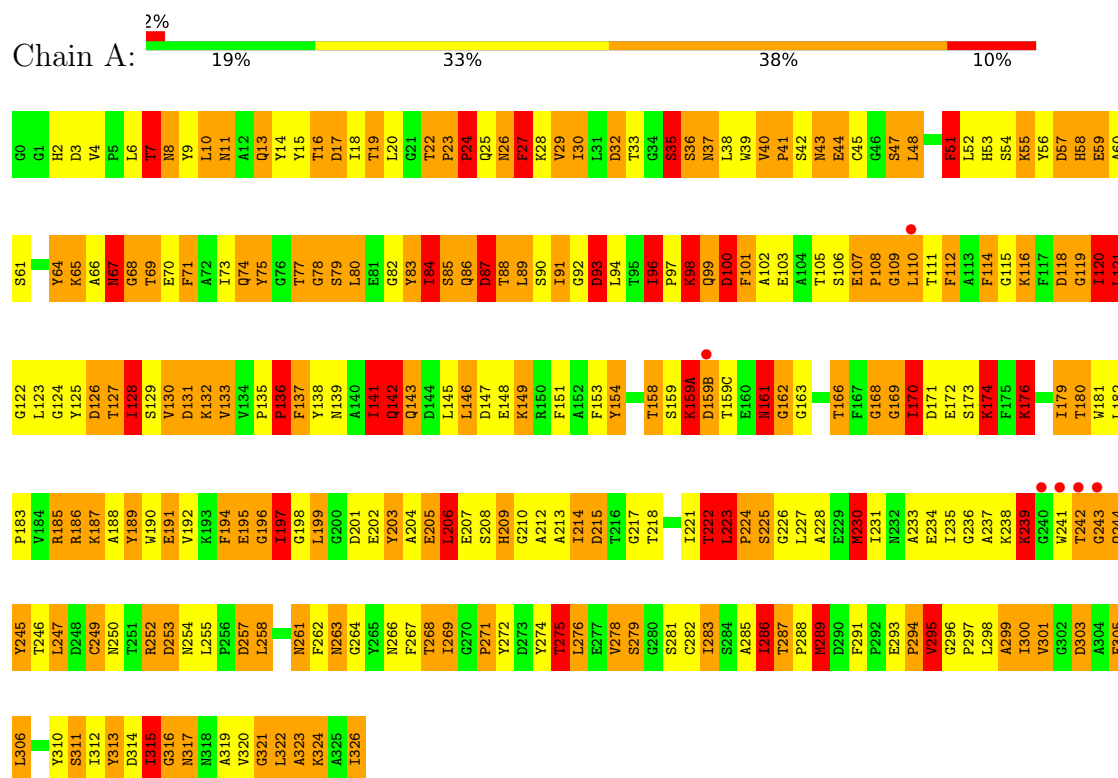
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total 65	O 65	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 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, α , β , γ	86.43Å 86.43Å 109.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.30 – 2.80 28.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.30-2.80) 94.3 (28.30-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.80Å)	Xtriage
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 ²)	53.4	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 114.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2717	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, KBG, 2Y3, 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	1.39	17/2592 (0.7%)	3.02	353/3526 (10.0%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	MET	SD-CE	10.66	2.06	1.79
1	A	245	TYR	N-CA	7.46	1.55	1.46
1	A	269	ILE	N-CA	-6.45	1.38	1.46
1	A	311	SER	N-CA	6.22	1.53	1.45
1	A	202	GLU	CA-CB	-6.06	1.44	1.53
1	A	215	ASP	N-CA	-6.06	1.38	1.46
1	A	222	THR	N-CA	5.81	1.53	1.46
1	A	315	ILE	CA-CB	-5.77	1.46	1.54
1	A	131	ASP	CA-CB	-5.70	1.45	1.53
1	A	161	ASN	N-CA	-5.64	1.39	1.46
1	A	190	TRP	CA-CB	-5.45	1.46	1.52
1	A	121	LEU	N-CA	5.38	1.52	1.46
1	A	179	ILE	CA-CB	5.37	1.60	1.54
1	A	103	GLU	N-CA	5.34	1.52	1.46
1	A	96	ILE	CA-C	5.14	1.57	1.53
1	A	323	ALA	N-CA	-5.04	1.39	1.46
1	A	283	ILE	N-CA	5.04	1.51	1.46

All (353) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ILE	O-C-N	14.80	133.01	121.46
1	A	283	ILE	CA-C-O	-12.91	108.11	121.67
1	A	102	ALA	CA-C-N	-12.53	105.51	123.05
1	A	102	ALA	C-N-CA	-12.53	105.51	123.05
1	A	133	VAL	CA-CB-CG2	12.22	131.18	110.40
1	A	143	GLN	CB-CG-CD	11.87	132.78	112.60
1	A	203	TYR	CA-C-O	-11.71	108.11	120.40
1	A	176	LYS	CA-CB-CG	11.46	137.03	114.10
1	A	286	ILE	CB-CG1-CD1	10.99	136.89	113.80
1	A	244	GLN	CA-C-N	-10.99	107.84	123.00
1	A	244	GLN	C-N-CA	-10.99	107.84	123.00
1	A	214	ILE	CA-C-N	10.97	138.09	122.85
1	A	214	ILE	C-N-CA	10.97	138.09	122.85
1	A	23	PRO	CA-C-N	10.59	133.08	119.84
1	A	23	PRO	C-N-CA	10.59	133.08	119.84
1	A	27	PHE	CA-C-O	-10.58	107.95	120.43
1	A	269	ILE	N-CA-C	10.39	123.25	107.78
1	A	103	GLU	CA-CB-CG	10.35	134.80	114.10
1	A	185	ARG	NE-CZ-NH1	-10.25	111.25	121.50
1	A	320	VAL	CA-C-N	-10.22	114.70	121.65
1	A	320	VAL	C-N-CA	-10.22	114.70	121.65
1	A	215	ASP	CA-CB-CG	-10.14	102.46	112.60
1	A	7	THR	CA-C-N	-10.13	107.74	122.94
1	A	7	THR	C-N-CA	-10.13	107.74	122.94
1	A	170	ILE	CA-C-O	-10.00	109.68	121.28
1	A	27	PHE	O-C-N	9.91	134.78	123.48
1	A	312	ILE	O-C-N	-9.87	113.14	122.71
1	A	244	GLN	CB-CG-CD	9.81	129.28	112.60
1	A	258	LEU	CA-C-O	-9.79	109.76	120.43
1	A	243	GLY	N-CA-C	9.75	129.91	114.90
1	A	142	GLN	CB-CG-CD	-9.54	96.38	112.60
1	A	225	SER	CA-C-N	-9.53	109.22	119.99
1	A	225	SER	C-N-CA	-9.53	109.22	119.99
1	A	244	GLN	CA-C-O	-9.53	110.03	121.56
1	A	283	ILE	O-C-N	9.47	133.56	123.04
1	A	295	VAL	CG1-CB-CG2	9.23	131.10	110.80
1	A	268	THR	CA-C-N	9.21	136.79	122.70
1	A	268	THR	C-N-CA	9.21	136.79	122.70
1	A	11	ASN	OD1-CG-ND2	-9.20	113.40	122.60
1	A	303	ASP	CA-CB-CG	9.16	121.76	112.60
1	A	11	ASN	CA-CB-CG	9.15	121.75	112.60
1	A	223	LEU	CA-C-N	-9.04	110.25	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	LEU	C-N-CA	-9.04	110.25	119.92
1	A	207	GLU	CB-CG-CD	-9.01	97.28	112.60
1	A	261	ASN	OD1-CG-ND2	8.89	131.49	122.60
1	A	183	PRO	O-C-N	8.84	134.26	123.13
1	A	100	ASP	CA-CB-CG	8.62	121.22	112.60
1	A	128	ILE	CB-CG1-CD1	-8.60	95.73	113.80
1	A	112	PHE	CA-CB-CG	-8.60	105.20	113.80
1	A	141	ILE	CA-C-O	8.60	131.53	120.78
1	A	110	LEU	CD1-CG-CD2	8.59	129.70	110.80
1	A	185	ARG	NE-CZ-NH2	8.53	126.87	119.20
1	A	209	HIS	O-C-N	-8.48	113.44	123.03
1	A	33	THR	CA-C-N	-8.43	109.49	122.30
1	A	33	THR	C-N-CA	-8.43	109.49	122.30
1	A	285	ALA	CA-C-N	-8.43	111.50	122.37
1	A	285	ALA	C-N-CA	-8.43	111.50	122.37
1	A	4	VAL	CA-CB-CG2	8.41	124.70	110.40
1	A	78	GLY	CA-C-N	8.41	139.13	123.32
1	A	78	GLY	C-N-CA	8.41	139.13	123.32
1	A	261	ASN	CA-CB-CG	-8.41	104.19	112.60
1	A	154	TYR	CA-C-N	-8.39	111.14	122.72
1	A	154	TYR	C-N-CA	-8.39	111.14	122.72
1	A	206	LEU	CA-C-O	8.33	130.58	121.16
1	A	187	LYS	CB-CG-CD	8.31	130.41	111.30
1	A	114	PHE	CA-CB-CG	-8.26	105.54	113.80
1	A	195	GLU	CA-C-N	-8.10	115.26	122.47
1	A	195	GLU	C-N-CA	-8.10	115.26	122.47
1	A	189	TYR	CA-C-N	-8.06	109.11	122.17
1	A	189	TYR	C-N-CA	-8.06	109.11	122.17
1	A	161	ASN	N-CA-C	8.05	124.22	111.81
1	A	169	GLY	CA-C-N	-8.03	109.92	122.69
1	A	169	GLY	C-N-CA	-8.03	109.92	122.69
1	A	85	SER	CA-C-N	-7.97	109.70	122.53
1	A	85	SER	C-N-CA	-7.97	109.70	122.53
1	A	119	GLY	CA-C-N	7.97	132.65	122.37
1	A	119	GLY	C-N-CA	7.97	132.65	122.37
1	A	271	PRO	N-CD-CG	-7.96	91.25	103.20
1	A	131	ASP	N-CA-CB	7.96	124.14	112.28
1	A	230	MET	CA-C-N	7.94	131.72	120.53
1	A	230	MET	C-N-CA	7.94	131.72	120.53
1	A	89	LEU	CD1-CG-CD2	7.89	128.16	110.80
1	A	267	PHE	O-C-N	7.89	133.38	123.28
1	A	79	SER	O-C-N	7.80	133.89	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	GLY	CA-C-N	7.79	137.53	121.94
1	A	316	GLY	C-N-CA	7.79	137.53	121.94
1	A	250	ASN	CA-CB-CG	7.77	120.37	112.60
1	A	179	ILE	CA-C-N	-7.71	111.38	122.94
1	A	179	ILE	C-N-CA	-7.71	111.38	122.94
1	A	301	VAL	O-C-N	-7.70	113.55	122.94
1	A	215	ASP	N-CA-C	7.68	122.03	107.75
1	A	128	ILE	CA-CB-CG1	7.65	123.41	110.40
1	A	210	GLY	N-CA-C	-7.63	99.96	111.10
1	A	322	LEU	CA-C-N	7.59	134.33	122.94
1	A	322	LEU	C-N-CA	7.59	134.33	122.94
1	A	208	SER	CA-C-O	-7.57	111.42	120.81
1	A	109	GLY	N-CA-C	7.57	125.85	112.53
1	A	130	VAL	CG1-CB-CG2	7.55	127.41	110.80
1	A	281	SER	CA-C-N	-7.53	106.94	122.07
1	A	281	SER	C-N-CA	-7.53	106.94	122.07
1	A	298	LEU	CD1-CG-CD2	-7.52	94.26	110.80
1	A	88	THR	CB-CA-C	7.50	122.82	110.74
1	A	269	ILE	CA-C-O	7.47	127.65	120.25
1	A	166	THR	CA-C-N	-7.40	111.76	122.19
1	A	166	THR	C-N-CA	-7.40	111.76	122.19
1	A	27	PHE	CA-CB-CG	7.38	121.18	113.80
1	A	88	THR	CA-C-N	-7.38	112.23	122.93
1	A	88	THR	C-N-CA	-7.38	112.23	122.93
1	A	108	PRO	CA-C-N	7.34	132.80	121.42
1	A	108	PRO	C-N-CA	7.34	132.80	121.42
1	A	126	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	108	PRO	O-C-N	7.33	132.10	123.01
1	A	315	ILE	CA-CB-CG1	7.28	122.78	110.40
1	A	315	ILE	CA-C-O	7.27	128.86	119.85
1	A	172	GLU	CA-C-O	7.25	127.83	119.35
1	A	190	TRP	CA-C-O	7.24	128.80	120.98
1	A	51	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	70	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	120	ILE	CB-CA-C	-7.18	102.00	110.91
1	A	225	SER	O-C-N	-7.17	113.97	122.15
1	A	266	ASN	CA-C-N	7.16	132.99	122.39
1	A	266	ASN	C-N-CA	7.16	132.99	122.39
1	A	281	SER	O-C-N	-7.15	114.68	123.33
1	A	124	GLY	CA-C-O	-7.13	114.77	122.47
1	A	100	ASP	N-CA-CB	7.12	120.58	109.69
1	A	96	ILE	CA-C-O	-7.10	114.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	PRO	N-CD-CG	-7.08	95.30	103.80
1	A	194	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	158	THR	CA-C-O	7.04	128.35	119.12
1	A	106	SER	CA-C-N	-7.03	114.27	123.34
1	A	106	SER	C-N-CA	-7.03	114.27	123.34
1	A	221	ILE	CA-C-N	-7.03	111.98	122.39
1	A	221	ILE	C-N-CA	-7.03	111.98	122.39
1	A	195	GLU	CB-CG-CD	-7.02	100.67	112.60
1	A	90	SER	CA-C-N	6.96	131.18	122.48
1	A	90	SER	C-N-CA	6.96	131.18	122.48
1	A	88	THR	N-CA-CB	6.94	121.62	110.65
1	A	102	ALA	O-C-N	-6.88	115.11	123.30
1	A	180	THR	CA-C-O	-6.84	113.31	120.70
1	A	37	ASN	CA-C-N	6.84	132.74	121.39
1	A	37	ASN	C-N-CA	6.84	132.74	121.39
1	A	142	GLN	CA-CB-CG	-6.83	100.44	114.10
1	A	173	SER	CA-CB-OG	6.82	124.74	111.10
1	A	209	HIS	CA-C-N	-6.76	114.32	121.48
1	A	209	HIS	C-N-CA	-6.76	114.32	121.48
1	A	185	ARG	CD-NE-CZ	-6.75	114.94	124.40
1	A	190	TRP	CB-CA-C	6.72	122.41	111.05
1	A	206	LEU	O-C-N	-6.71	114.70	123.16
1	A	137	PHE	CG-CD2-CE2	-6.69	109.32	120.70
1	A	299	ALA	O-C-N	6.68	130.58	123.03
1	A	3	ASP	N-CA-CB	6.67	119.78	110.17
1	A	159	SER	CA-CB-OG	-6.67	97.76	111.10
1	A	267	PHE	CA-C-O	-6.66	112.08	120.20
1	A	149	LYS	CG-CD-CE	6.65	126.60	111.30
1	A	137	PHE	CZ-CE2-CD2	6.62	131.92	120.00
1	A	323	ALA	N-CA-CB	6.62	122.34	110.83
1	A	36	SER	CA-C-N	6.61	132.31	123.00
1	A	36	SER	C-N-CA	6.61	132.31	123.00
1	A	108	PRO	CA-N-CD	-6.61	102.75	112.00
1	A	315	ILE	O-C-N	-6.60	113.41	122.05
1	A	255	LEU	CA-C-O	-6.59	114.05	120.97
1	A	297	PRO	CA-C-N	-6.59	111.03	122.37
1	A	297	PRO	C-N-CA	-6.59	111.03	122.37
1	A	244	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	A	238	LYS	CA-C-O	-6.54	113.46	121.11
1	A	136	PRO	N-CD-CG	-6.52	93.42	103.20
1	A	183	PRO	CA-C-O	-6.50	113.92	121.86
1	A	137	PHE	O-C-N	-6.50	113.88	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	VAL	CA-CB-CG1	-6.48	99.39	110.40
1	A	321	GLY	N-CA-C	-6.48	100.13	111.46
1	A	319	ALA	O-C-N	6.46	130.85	123.48
1	A	99	GLN	CA-CB-CG	6.46	127.01	114.10
1	A	98	LYS	CA-C-O	6.41	129.67	120.51
1	A	71	PHE	CA-CB-CG	-6.40	107.40	113.80
1	A	93	ASP	CA-CB-CG	-6.37	106.23	112.60
1	A	202	GLU	N-CA-CB	6.36	120.57	110.65
1	A	32	ASP	O-C-N	-6.36	115.12	123.13
1	A	206	LEU	CA-C-N	-6.34	111.69	122.33
1	A	206	LEU	C-N-CA	-6.34	111.69	122.33
1	A	159(A)	LYS	C-N-CA	6.33	137.53	121.70
1	A	303	ASP	CA-C-N	6.29	130.25	120.82
1	A	303	ASP	C-N-CA	6.29	130.25	120.82
1	A	300	ILE	CA-C-N	-6.25	114.55	122.37
1	A	300	ILE	C-N-CA	-6.25	114.55	122.37
1	A	37	ASN	CA-C-O	-6.24	113.62	120.30
1	A	289	MET	CG-SD-CE	-6.24	87.17	100.90
1	A	13	GLN	CB-CG-CD	-6.23	102.01	112.60
1	A	103	GLU	CA-C-O	-6.22	113.47	120.32
1	A	239	LYS	CA-CB-CG	6.22	126.54	114.10
1	A	98	LYS	CA-C-N	-6.21	113.48	123.23
1	A	98	LYS	C-N-CA	-6.21	113.48	123.23
1	A	289	MET	CA-C-N	-6.20	114.24	122.99
1	A	289	MET	C-N-CA	-6.20	114.24	122.99
1	A	43	ASN	CB-CA-C	-6.20	100.37	110.79
1	A	43	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	A	30	ILE	CA-C-N	-6.18	112.78	121.99
1	A	30	ILE	C-N-CA	-6.18	112.78	121.99
1	A	51	PHE	CA-C-N	6.17	131.03	120.72
1	A	51	PHE	C-N-CA	6.17	131.03	120.72
1	A	301	VAL	CA-CB-CG2	6.15	120.85	110.40
1	A	128	ILE	N-CA-CB	-6.14	105.02	112.33
1	A	131	ASP	O-C-N	6.14	133.71	122.11
1	A	108	PRO	CA-C-O	-6.12	114.46	121.56
1	A	128	ILE	N-CA-C	-6.12	107.29	113.47
1	A	82	GLY	CA-C-N	-6.11	112.32	122.21
1	A	82	GLY	C-N-CA	-6.11	112.32	122.21
1	A	228	ALA	O-C-N	6.10	129.77	122.27
1	A	190	TRP	CA-C-N	-6.09	114.21	122.86
1	A	190	TRP	C-N-CA	-6.09	114.21	122.86
1	A	236	GLY	N-CA-C	6.07	123.83	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASN	CA-C-N	-6.06	114.25	122.86
1	A	8	ASN	C-N-CA	-6.06	114.25	122.86
1	A	190	TRP	O-C-N	-6.03	114.49	122.57
1	A	189	TYR	CA-CB-CG	6.01	124.72	113.90
1	A	168	GLY	CA-C-N	-6.00	109.37	120.84
1	A	168	GLY	C-N-CA	-6.00	109.37	120.84
1	A	312	ILE	N-CA-CB	-6.00	105.21	112.35
1	A	172	GLU	CB-CG-CD	5.99	122.78	112.60
1	A	287	THR	O-C-N	5.96	126.42	121.35
1	A	17	ASP	CA-C-N	-5.96	115.75	122.48
1	A	17	ASP	C-N-CA	-5.96	115.75	122.48
1	A	96	ILE	CA-C-N	-5.95	112.40	119.84
1	A	96	ILE	C-N-CA	-5.95	112.40	119.84
1	A	40	VAL	N-CA-C	5.95	114.07	109.19
1	A	192	VAL	CG1-CB-CG2	-5.95	97.72	110.80
1	A	208	SER	CA-CB-OG	-5.95	99.21	111.10
1	A	29	VAL	CA-CB-CG1	-5.89	100.38	110.40
1	A	257	ASP	CA-C-N	-5.89	114.60	122.72
1	A	257	ASP	C-N-CA	-5.89	114.60	122.72
1	A	301	VAL	CA-C-N	-5.88	109.89	121.41
1	A	301	VAL	C-N-CA	-5.88	109.89	121.41
1	A	65	LYS	O-C-N	-5.88	115.42	122.65
1	A	303	ASP	N-CA-CB	5.87	120.42	110.49
1	A	253	ASP	N-CA-CB	5.87	120.27	110.41
1	A	310	TYR	CG-CD1-CE1	5.86	130.00	121.20
1	A	61	SER	CA-C-N	5.86	131.98	121.66
1	A	61	SER	C-N-CA	5.86	131.98	121.66
1	A	93	ASP	CB-CA-C	-5.82	101.93	110.95
1	A	170	ILE	O-C-N	5.81	129.22	123.00
1	A	197	ILE	CB-CG1-CD1	-5.79	101.63	113.80
1	A	99	GLN	CB-CG-CD	5.76	122.40	112.60
1	A	24	PRO	CA-C-N	5.76	130.59	121.72
1	A	24	PRO	C-N-CA	5.76	130.59	121.72
1	A	112	PHE	O-C-N	5.75	128.75	122.20
1	A	137	PHE	CD1-CE1-CZ	-5.73	109.69	120.00
1	A	198	GLY	CA-C-N	-5.73	112.81	121.86
1	A	198	GLY	C-N-CA	-5.73	112.81	121.86
1	A	179	ILE	CB-CA-C	-5.73	103.38	111.28
1	A	171	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	207	GLU	CA-C-N	-5.71	114.12	122.40
1	A	207	GLU	C-N-CA	-5.71	114.12	122.40
1	A	324	LYS	CA-C-N	-5.71	112.44	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	LYS	C-N-CA	-5.71	112.44	121.86
1	A	14	TYR	CA-C-O	-5.69	112.61	120.52
1	A	196	GLY	CA-C-N	5.69	132.21	121.97
1	A	196	GLY	C-N-CA	5.69	132.21	121.97
1	A	94	LEU	O-C-N	5.66	129.85	123.06
1	A	166	THR	CA-C-O	5.65	126.59	119.98
1	A	222	THR	O-C-N	5.65	130.51	123.28
1	A	215	ASP	O-C-N	-5.65	115.92	122.87
1	A	224	PRO	O-C-N	-5.64	116.08	122.91
1	A	235	ILE	CA-C-N	-5.64	113.00	122.25
1	A	235	ILE	C-N-CA	-5.64	113.00	122.25
1	A	83	TYR	CA-CB-CG	-5.63	103.76	113.90
1	A	267	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	69	THR	N-CA-CB	5.62	119.00	110.45
1	A	29	VAL	CA-CB-CG2	5.62	119.96	110.40
1	A	255	LEU	O-C-N	5.61	128.00	121.21
1	A	37	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	244	GLN	CA-CB-CG	5.60	125.29	114.10
1	A	147	ASP	CA-C-O	-5.59	114.63	120.55
1	A	3	ASP	CA-C-N	5.58	132.46	122.13
1	A	3	ASP	C-N-CA	5.58	132.46	122.13
1	A	43	ASN	O-C-N	5.57	128.91	122.17
1	A	198	GLY	CA-C-O	5.55	126.24	121.19
1	A	264	GLY	CA-C-O	5.54	125.28	119.07
1	A	101	PHE	CB-CG-CD1	-5.54	111.29	120.70
1	A	120	ILE	CB-CG1-CD1	-5.53	102.19	113.80
1	A	79	SER	CA-C-N	5.52	131.27	122.10
1	A	79	SER	C-N-CA	5.52	131.27	122.10
1	A	126	ASP	O-C-N	5.51	128.44	122.15
1	A	131	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	118	ASP	N-CA-C	-5.49	106.26	113.12
1	A	87	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	201	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	19	THR	N-CA-CB	5.45	120.40	111.08
1	A	67	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	275	THR	CA-C-N	-5.43	114.14	122.62
1	A	275	THR	C-N-CA	-5.43	114.14	122.62
1	A	201	ASP	CA-C-O	-5.41	112.98	119.15
1	A	305	PHE	CA-C-O	-5.40	113.56	120.31
1	A	176	LYS	CB-CG-CD	5.40	123.72	111.30
1	A	153	PHE	CA-C-N	-5.40	115.59	122.77
1	A	153	PHE	C-N-CA	-5.40	115.59	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	PRO	CA-CB-CG	-5.39	94.25	104.50
1	A	205	GLU	O-C-N	5.38	129.71	123.30
1	A	149	LYS	CD-CE-NZ	5.38	129.13	111.90
1	A	168	GLY	CA-C-O	5.37	125.68	119.13
1	A	172	GLU	CA-CB-CG	5.37	124.83	114.10
1	A	254	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	A	44	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	147	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	201	ASP	OD1-CG-OD2	5.33	135.68	122.90
1	A	75	TYR	CA-C-O	-5.32	115.69	121.87
1	A	87	ASP	CA-C-O	5.29	128.08	120.51
1	A	36	SER	N-CA-C	5.28	119.48	112.30
1	A	187	LYS	CA-CB-CG	-5.28	103.53	114.10
1	A	192	VAL	CA-CB-CG2	-5.28	101.42	110.40
1	A	115	GLY	N-CA-C	5.28	119.30	112.54
1	A	141	ILE	CB-CG1-CD1	-5.28	102.72	113.80
1	A	314	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	35	SER	CA-C-O	-5.27	114.95	121.11
1	A	61	SER	O-C-N	5.26	128.84	122.94
1	A	315	ILE	CA-CB-CG2	5.24	119.41	110.50
1	A	60	ALA	CA-C-O	5.23	124.80	119.05
1	A	57	ASP	CA-C-N	-5.22	110.51	121.64
1	A	57	ASP	C-N-CA	-5.22	110.51	121.64
1	A	107	GLU	CA-C-O	5.22	127.69	120.80
1	A	43	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	79	SER	CA-C-O	-5.20	115.30	121.60
1	A	323	ALA	N-CA-C	5.20	117.87	109.40
1	A	18	ILE	CB-CA-C	-5.18	104.65	111.70
1	A	3	ASP	N-CA-C	5.18	117.80	110.50
1	A	253	ASP	O-C-N	5.17	129.98	122.43
1	A	101	PHE	CA-C-N	-5.17	115.70	122.99
1	A	101	PHE	C-N-CA	-5.17	115.70	122.99
1	A	208	SER	CA-C-N	5.15	132.12	122.74
1	A	208	SER	C-N-CA	5.15	132.12	122.74
1	A	84	ILE	N-CA-CB	5.14	119.72	111.23
1	A	201	ASP	CB-CG-OD2	-5.13	106.60	118.40
1	A	115	GLY	CA-C-N	5.12	132.22	122.60
1	A	115	GLY	C-N-CA	5.12	132.22	122.60
1	A	146	LEU	CD1-CG-CD2	-5.12	99.55	110.80
1	A	264	GLY	N-CA-C	5.11	121.56	114.92
1	A	317	ASN	CA-C-O	-5.11	112.43	119.12
1	A	54	SER	CA-C-O	-5.09	116.15	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	GLU	CB-CA-C	5.09	118.53	110.19
1	A	305	PHE	O-C-N	5.07	129.15	122.30
1	A	305	PHE	CA-C-N	5.07	127.58	120.28
1	A	305	PHE	C-N-CA	5.07	127.58	120.28
1	A	128	ILE	CA-C-O	5.06	123.54	118.98
1	A	154	TYR	O-C-N	-5.06	117.46	123.22
1	A	252	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	A	322	LEU	CA-C-O	-5.05	114.91	120.36
1	A	303	ASP	CB-CA-C	5.03	120.44	110.42
1	A	174	LYS	N-CA-C	5.03	119.57	113.38
1	A	11	ASN	N-CA-CB	-5.03	105.09	112.78
1	A	286	ILE	CA-C-N	-5.02	113.62	123.56
1	A	286	ILE	C-N-CA	-5.02	113.62	123.56
1	A	88	THR	O-C-N	-5.02	116.50	123.12
1	A	10	LEU	CA-C-N	-5.01	115.58	123.91
1	A	10	LEU	C-N-CA	-5.01	115.58	123.91
1	A	203	TYR	CB-CG-CD1	-5.01	113.29	120.80

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 ⓘ

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	302	0
2	B	61	0	42	2	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	310	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 (310) 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: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:108:PRO:HD2	1:A:108:PRO:O	1.52	1.06
3:A:400:2Y3:H35A	3:A:400:2Y3:O6	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
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:203:TYR:C	1:A:203:TYR:CD1	2.45	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:261:ASN:OD1	1:A:261:ASN:C	2.14	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: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:121:LEU:C	1:A:121:LEU:CD2	2.46	0.87
1:A:27:PHE:CZ	1:A:56:TYR:HB2	2.10	0.87
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:121:LEU:HD23	1:A:121:LEU:C	2.02	0.84
1:A:191:GLU:O	1:A:191:GLU:CG	2.25	0.84
1:A:159(A):LYS:CG	1:A:159(B):ASP:H	1.89	0.83
1:A:27:PHE:HZ	1:A:56:TYR:HB2	1.41	0.82
1:A:143:GLN:HB2	1:A:145:LEU:HD11	1.60	0.82
3:A:400:2Y3:H35A	3:A:400:2Y3:C36	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HH11	1:A:275:THR:CG2	1.92	0.82
1:A:58:HIS:H	1:A:58:HIS:CD2	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:N	1:A:214:ILE:HD12	1.95	0.80
1:A:51:PHE:C	1:A:51:PHE:HD1	1.90	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:203:TYR:C	1:A:203:TYR:HD1	1.88	0.78
1:A:313:TYR:CD1	1:A:313:TYR:N	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
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:N	1:A:10:LEU:HD23	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:16:THR:HG23	1:A:17:ASP:N	1.99	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: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:125:TYR:O	1:A:128:ILE:HG22	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:79:SER:C	1:A:80:LEU:HD23	2.12	0.73
1:A:10:LEU:O	1:A:11:ASN:HB2	1.89	0.73
1:A:51:PHE:C	1:A:51:PHE:CD1	2.64	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:A:289:MET:CG	2.69	0.70
1:A:23:PRO:CB	1:A:24:PRO:HD2	2.22	0.70
1:A:10:LEU:HD23	1:A:10:LEU:H	1.54	0.70
3:A:400:2Y3:H5A	3:A:400:2Y3:O1	1.91	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: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
1:A:317:ASN:N	1:A:317:ASN:HD22	1.92	0.67
1:A:39:TRP:HZ3	1:A:41:PRO:HD3	1.58	0.67
1:A:252:ARG:HH11	1:A:275:THR:HG22	1.58	0.67
1:A:89:LEU:CD2	1:A:96:ILE:HD13	2.23	0.67
1:A:137:PHE:CE2	1:A:315:ILE:HD11	2.30	0.67
1:A:77:THR:O	1:A:77:THR:CG2	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:HD1	1:A:313:TYR:H	1.43	0.66
1:A:48:LEU:HD23	1:A:48:LEU:C	2.21	0.66
1:A:278:VAL:O	1:A:278:VAL:CG1	2.43	0.65
1:A:225:SER:O	1:A:226:GLY:C	2.35	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:35:SER:HB2	1:A:75:TYR:CE1	2.30	0.64
1:A:206:LEU:HD13	1:A:209:HIS:CD2	2.33	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:315:ILE:O	1:A:316:GLY:C	2.38	0.63
1:A:203:TYR:CD1	1:A:203:TYR:O	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:38:LEU:HD12	1:A:39:TRP:N	2.15	0.62
1:A:25:GLN:HE22	1:A:57:ASP:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HA	1:A:283:ILE:HA	1.82	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: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:58:HIS:CD2	1:A:58:HIS:N	2.69	0.60
1:A:111:THR:CG2	3:A:400:2Y3:H12	2.32	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:84:ILE:HG23	1:A:85:SER:H	1.65	0.59
1:A:142:GLN:CD	2:B:4:BMA:H62	2.27	0.59
1:A:179:ILE:HA	1:A:323:ALA:HB2	1.85	0.59
1:A:301:VAL:HG12	1:A:305:PHE:HB3	1.84	0.59
1:A:30:ILE:HD13	3:A:400:2Y3:C25	2.33	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:161:ASN:HD21	1:A:174:LYS:NZ	2.01	0.58
1:A:30:ILE:HD13	3:A:400:2Y3:H25A	1.86	0.58
1:A:121:LEU:CD2	1:A:122:GLY:N	2.63	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:161:ASN:O	1:A:162:GLY:C	2.45	0.57
1:A:176:LYS:NZ	1:A:326:ILE:HA	2.20	0.57
1:A:215:ASP:C	1:A:215:ASP:OD1	2.45	0.57
1:A:56:TYR:CD2	1:A:56:TYR:O	2.57	0.57
1:A:68:GLY:HA2	1:A:83:TYR:CD1	2.40	0.57
1:A:230:MET:O	1:A:233:ALA:HB3	2.05	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:25:GLN:HE22	1:A:56:TYR:HA	1.70	0.56
1:A:32:ASP:OD2	1:A:35:SER:HB3	2.05	0.56
1:A:85:SER:O	1:A:100:ASP:HA	2.05	0.56
1:A:136:PRO:HD2	5:A:501:HOH:O	2.06	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:109:GLY:C	1:A:110:LEU:HD12	2.32	0.55
1:A:205:GLU:C	1:A:206:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:317:ASN:N	1:A:317:ASN:ND2	2.55	0.54
1:A:6:LEU:CB	1:A:163:GLY:HA3	2.33	0.54
1:A:135:PRO:HB2	5:A:501:HOH:O	2.08	0.54
1:A:75:TYR:CD1	3:A:400:2Y3:H37A	2.43	0.54
1:A:189:TYR:CE1	3:A:400:2Y3:H34	2.43	0.54
1:A:223:LEU:O	1:A:224:PRO:C	2.48	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: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:38:LEU:HD13	1:A:121:LEU:HB2	1.90	0.53
1:A:137:PHE:HE2	1:A:315:ILE:CD1	2.22	0.53
1:A:32:ASP:OD1	1:A:217:GLY:HA3	2.09	0.52
1:A:214:ILE:N	1:A:214:ILE:CD1	2.70	0.52
1:A:287:THR:CG2	1:A:288:PRO:N	2.71	0.52
1:A:48:LEU:C	1:A:48:LEU:CD2	2.83	0.52
1:A:137:PHE:CD2	1:A:315:ILE:HD11	2.44	0.52
1:A:274:TYR:HB2	1:A:286:ILE:CD1	2.39	0.52
1:A:135:PRO:O	1:A:136:PRO:C	2.52	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:6:LEU:HB2	1:A:163:GLY:C	2.36	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:65:LYS:HG3	1:A:66:ALA:N	2.25	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:39:TRP:CE3	1:A:39:TRP:C	2.89	0.51
1:A:271:PRO:HA	1:A:274:TYR:CE1	2.45	0.50
1:A:83:TYR:CD1	1:A:83:TYR:C	2.89	0.50
1:A:252:ARG:HD2	1:A:275:THR:HG21	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:MET:HA	1:A:289:MET:HE2	1.93	0.49
1:A:42:SER:O	1:A:55:LYS:HG2	2.12	0.49
1:A:25:GLN:NE2	1:A:57:ASP:H	2.10	0.49
1:A:159(A):LYS:HE2	1:A:326:ILE:O	2.12	0.49
1:A:43:ASN:C	1:A:45:CYS:H	2.20	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:73:ILE:HD12	1:A:130:VAL:CG2	2.42	0.48
1:A:166:THR:HG22	1:A:169:GLY:O	2.11	0.48
1:A:315:ILE:HG21	1:A:315:ILE:HD13	1.63	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:161:ASN:HD21	1:A:174:LYS:HZ3	1.61	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:121:LEU:C	1:A:121:LEU:HD22	2.33	0.48
1:A:53:HIS:HB3	1:A:118:ASP:OD1	2.13	0.48
1:A:8:ASN:OD1	1:A:9:TYR:N	2.47	0.48
1:A:35:SER:CB	1:A:75:TYR:HE1	2.19	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:295:VAL:HG12	1:A:296:GLY:N	2.29	0.47
1:A:8:ASN:OD1	1:A:8:ASN:C	2.57	0.47
1:A:96:ILE:HD12	1:A:96:ILE:H	1.80	0.47
1:A:141:ILE:CD1	1:A:149:LYS:HG2	2.44	0.47
1:A:88:THR:OG1	1:A:97:PRO:HA	2.14	0.47
1:A:91:ILE:O	1:A:92:GLY:C	2.56	0.47
1:A:128:ILE:HD12	1:A:128:ILE:HG21	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: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:130:VAL:C	1:A:132:LYS:H	2.23	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:74:GLN:HA	1:A:79:SER:HB3	1.98	0.46
1:A:278:VAL:O	1:A:279:SER:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:ASN:HD21	1:A:130:VAL:N	2.14	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:65:LYS:HG3	1:A:66:ALA:H	1.79	0.45
1:A:75:TYR:C	1:A:77:THR:N	2.73	0.45
1:A:7:THR:CG2	1:A:15:TYR:CE2	2.97	0.45
1:A:75:TYR:HB2	1:A:78:GLY:O	2.15	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:83:TYR:HD1	1:A:84:ILE:O	2.00	0.45
1:A:139:ASN:O	1:A:143:GLN:HG3	2.16	0.45
1:A:83:TYR:CD2	1:A:83:TYR:N	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:154:TYR:CD1	1:A:154:TYR:C	2.93	0.45
1:A:25:GLN:HE22	1:A:56:TYR:CA	2.30	0.44
1:A:71:PHE:CD2	1:A:71:PHE:C	2.94	0.44
1:A:130:VAL:C	1:A:132:LYS:N	2.76	0.44
1:A:159(B):ASP:OD1	1:A:161:ASN:HA	2.18	0.44
1:A:289:MET:CE	1:A:289:MET:HG2	2.47	0.44
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:HG22	1:A:326:ILE:OXT	2.18	0.44
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.83	0.44
1:A:20:LEU:O	1:A:25:GLN:HB2	2.18	0.44
1:A:126:ASP:C	1:A:128:ILE:H	2.25	0.44
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: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:H21	3:A:400:2Y3:H24	1.64	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:26:ASN:C	1:A:27:PHE:CD1	2.96	0.43
1:A:13:GLN:NE2	1:A:116:LYS:H	2.14	0.43
1:A:159(B):ASP:CG	1:A:161:ASN:HA	2.44	0.43
1:A:213:ALA:HB3	1:A:300:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:LEU:HD21	1:A:52:LEU:HD11	2.01	0.43
1:A:222:THR:HA	1:A:287:THR:O	2.19	0.43
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:83:TYR:CD1	1:A:83:TYR:O	2.73	0.42
1:A:67:ASN:O	1:A:68:GLY:C	2.61	0.42
1:A:182:LEU:HD13	1:A:262:PHE:CB	2.50	0.42
1:A:56:TYR:O	1:A:56:TYR:CG	2.73	0.42
1:A:199:LEU:HB2	1:A:258:LEU:HA	2.02	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:O	1:A:170:ILE:HG12	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: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:159(C):THR:HG22	1:A:159(C):THR:O	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:80:LEU:HD23	1:A:80:LEU:N	2.37	0.40
1:A:301:VAL:HG11	1:A:305:PHE:CG	2.56	0.40
1:A:107:GLU:HA	1:A:108:PRO:HD3	1.87	0.40
1:A:127:THR:O	1:A:127:THR:HG22	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%)	1 4

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
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 ⓘ

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%)	197 (74%)	71 (26%)	0 2

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	16	THR
1	A	19	THR

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Mol	Chain	Res	Type
1	A	22	THR
1	A	26	ASN
1	A	27	PHE
1	A	35	SER
1	A	41	PRO
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	77	THR
1	A	80	LEU
1	A	86	GLN
1	A	91	ILE
1	A	93	ASP
1	A	96	ILE
1	A	100	ASP
1	A	116	LYS
1	A	120	ILE
1	A	121	LEU
1	A	123	LEU
1	A	128	ILE
1	A	129	SER
1	A	132	LYS
1	A	133	VAL
1	A	141	ILE
1	A	142	GLN
1	A	148	GLU
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	197	ILE
1	A	199	LEU
1	A	206	LEU
1	A	222	THR

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Mol	Chain	Res	Type
1	A	223	LEU
1	A	227	LEU
1	A	230	MET
1	A	231	ILE
1	A	234	GLU
1	A	239	LYS
1	A	242	THR
1	A	244	GLN
1	A	247	LEU
1	A	269	ILE
1	A	275	THR
1	A	276	LEU
1	A	278	VAL
1	A	279	SER
1	A	286	ILE
1	A	289	MET
1	A	293	GLU
1	A	295	VAL
1	A	303	ASP
1	A	306	LEU
1	A	311	SER
1	A	313	TYR
1	A	315	ILE
1	A	322	LEU
1	A	324	LYS
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	13	GLN
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	254	ASN
1	A	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	1.73	5 (35%)	17,19,21	3.22	6 (35%)
2	NAG	B	2	2	14,14,15	1.31	3 (21%)	17,19,21	2.37	7 (41%)
2	BMA	B	3	2	11,11,12	1.13	1 (9%)	15,15,17	3.73	4 (26%)
2	BMA	B	4	2	11,11,12	2.01	3 (27%)	15,15,17	2.61	8 (53%)
2	KBG	B	5	2	11,11,12	4.41	6 (54%)	11,15,17	2.29	5 (45%)

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	2,1	-	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	KBG	OAG-C2	12.02	1.41	1.21
2	B	5	KBG	C3-C2	-5.75	1.44	1.52
2	B	4	BMA	O5-C5	3.72	1.50	1.43
2	B	5	KBG	C1-C2	-3.64	1.47	1.51
2	B	1	NAG	C1-C2	-3.35	1.47	1.52
2	B	4	BMA	C2-C3	3.33	1.57	1.52
2	B	5	KBG	O5-C5	3.08	1.49	1.43
2	B	4	BMA	O5-C1	2.93	1.48	1.43
2	B	1	NAG	C2-N2	2.72	1.50	1.46
2	B	1	NAG	O3-C3	2.50	1.49	1.43
2	B	2	NAG	O4-C4	2.39	1.48	1.43
2	B	1	NAG	C7-N2	2.34	1.41	1.34
2	B	5	KBG	C4-C3	-2.29	1.49	1.53
2	B	3	BMA	O4-C4	2.28	1.48	1.43
2	B	2	NAG	O5-C1	2.21	1.47	1.43
2	B	2	NAG	O3-C3	2.10	1.48	1.43
2	B	5	KBG	O4-C4	2.09	1.48	1.43
2	B	1	NAG	O5-C5	2.07	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	13.16	129.82	112.19
2	B	1	NAG	C2-N2-C7	-10.91	108.28	122.90
2	B	4	BMA	C1-O5-C5	-5.57	104.72	112.19
2	B	2	NAG	C1-O5-C5	5.32	119.31	112.19
2	B	5	KBG	OAG-C2-C1	-4.51	113.84	121.30
2	B	1	NAG	O5-C1-C2	4.06	117.57	111.29
2	B	4	BMA	O5-C1-C2	-3.80	101.72	110.79
2	B	4	BMA	O5-C5-C6	-3.71	100.45	107.66
2	B	3	BMA	O2-C2-C3	3.69	117.79	110.15
2	B	2	NAG	C8-C7-N2	-3.50	110.31	116.12
2	B	2	NAG	O5-C5-C6	3.38	114.24	107.66
2	B	2	NAG	C3-C4-C5	-3.36	104.13	110.23
2	B	1	NAG	O3-C3-C4	-3.30	102.61	110.38
2	B	2	NAG	O7-C7-N2	3.25	127.73	121.98
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	111.67
2	B	2	NAG	O3-C3-C4	-2.96	103.39	110.38
2	B	5	KBG	O5-C5-C6	-2.95	101.91	107.66
2	B	1	NAG	C1-O5-C5	2.90	116.07	112.19
2	B	4	BMA	C2-C3-C4	-2.87	105.82	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	BMA	O3-C3-C2	-2.62	104.71	110.05
2	B	5	KBG	O3-C3-C2	2.59	115.08	109.84
2	B	1	NAG	O5-C5-C4	-2.53	104.68	110.83
2	B	2	NAG	O4-C4-C5	-2.46	103.26	109.32
2	B	1	NAG	O5-C5-C6	-2.40	102.99	107.66
2	B	3	BMA	C1-C2-C3	2.31	113.01	109.64
2	B	4	BMA	C3-C4-C5	-2.27	106.11	110.23
2	B	3	BMA	O3-C3-C4	-2.23	105.12	110.38
2	B	4	BMA	O3-C3-C4	-2.19	105.21	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

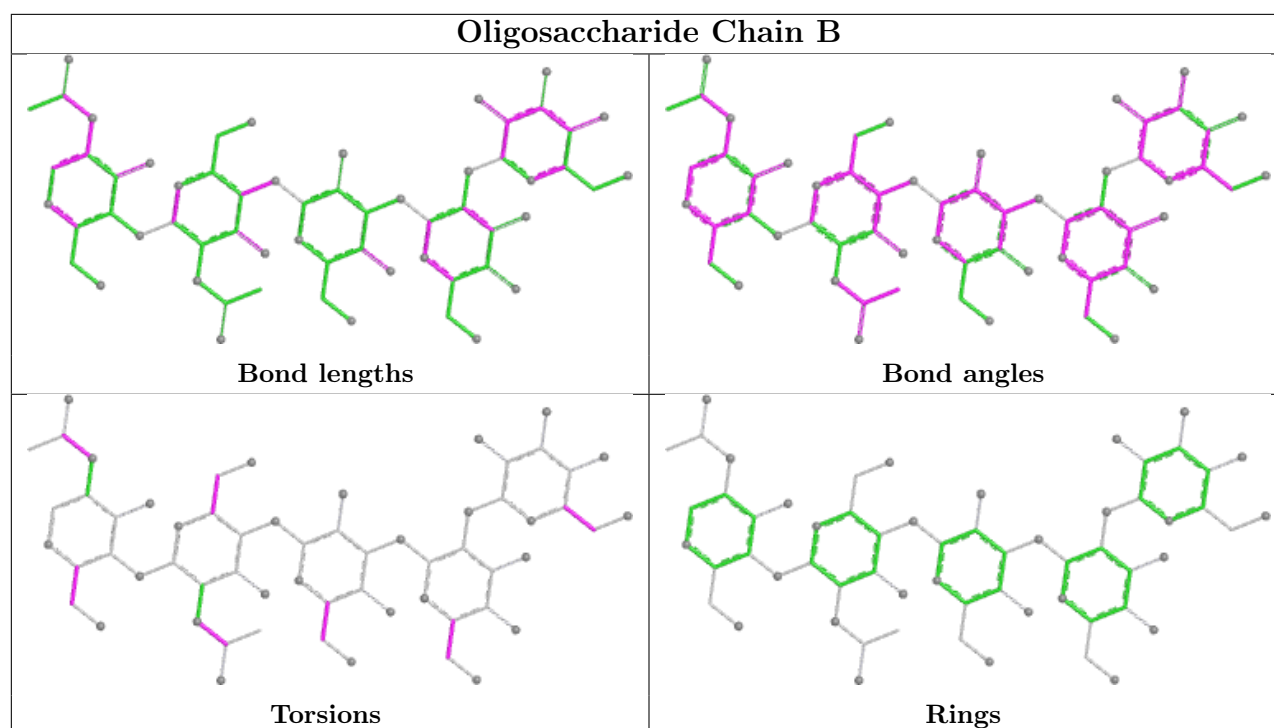
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O7-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	4	BMA	C4-C5-C6-O6
2	B	5	KBG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	1.32	2 (14%)	17,19,21	3.04	5 (29%)
3	2Y3	A	400	-	51,51,51	1.21	3 (5%)	62,69,69	2.20	20 (32%)

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	-	-	14/55/63/63	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	5.69	1.45	1.34
4	A	337	NAG	O5-C1	3.14	1.49	1.43
3	A	400	2Y3	C17-C15	-3.08	1.47	1.53
4	A	337	NAG	O4-C4	2.49	1.49	1.43
3	A	400	2Y3	O2-C2	-2.19	1.44	1.48

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	337	NAG	O5-C1-C2	-8.26	98.51	111.29
3	A	400	2Y3	O2-C1-N1	7.22	121.86	110.03
4	A	337	NAG	C8-C7-N2	-6.24	105.76	116.12
3	A	400	2Y3	C17-C15-N2	5.87	121.83	110.64
3	A	400	2Y3	C15-C17-C18	5.27	122.18	113.27
3	A	400	2Y3	O2-C1-O1	-5.00	116.75	125.64
4	A	337	NAG	O7-C7-N2	4.29	129.57	121.98
3	A	400	2Y3	C15-N2-C7	3.80	129.80	121.65
3	A	400	2Y3	C35-C33-C32	-3.78	97.49	111.08
3	A	400	2Y3	O3-C7-C6	-3.72	112.68	120.48
3	A	400	2Y3	C28-C27-C25	3.13	117.86	111.42
3	A	400	2Y3	C22-C23-C25	3.06	118.83	111.71
3	A	400	2Y3	C31-C32-C33	-2.58	110.24	115.60
4	A	337	NAG	O6-C6-C5	2.47	119.75	111.33
3	A	400	2Y3	C6-N1-C1	2.45	127.02	120.93
3	A	400	2Y3	C21-N5-C16	2.33	127.30	123.25
4	A	337	NAG	C6-C5-C4	2.32	118.72	113.02
3	A	400	2Y3	C6-C7-N2	2.29	121.51	116.63
3	A	400	2Y3	C25-C23-C24	-2.23	103.83	109.29
3	A	400	2Y3	C2-O2-C1	-2.16	117.70	120.97
3	A	400	2Y3	O1-C1-N1	-2.12	121.38	124.86
3	A	400	2Y3	C34-C33-C32	2.08	118.58	111.08
3	A	400	2Y3	O4-C16-N5	-2.07	119.24	122.96
3	A	400	2Y3	C28-C26-C24	-2.04	107.22	111.42
3	A	400	2Y3	O5-C29-C21	2.00	113.83	109.88

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	2Y3	N2-C15-C17-C18
3	A	400	2Y3	C36-C31-C32-C33

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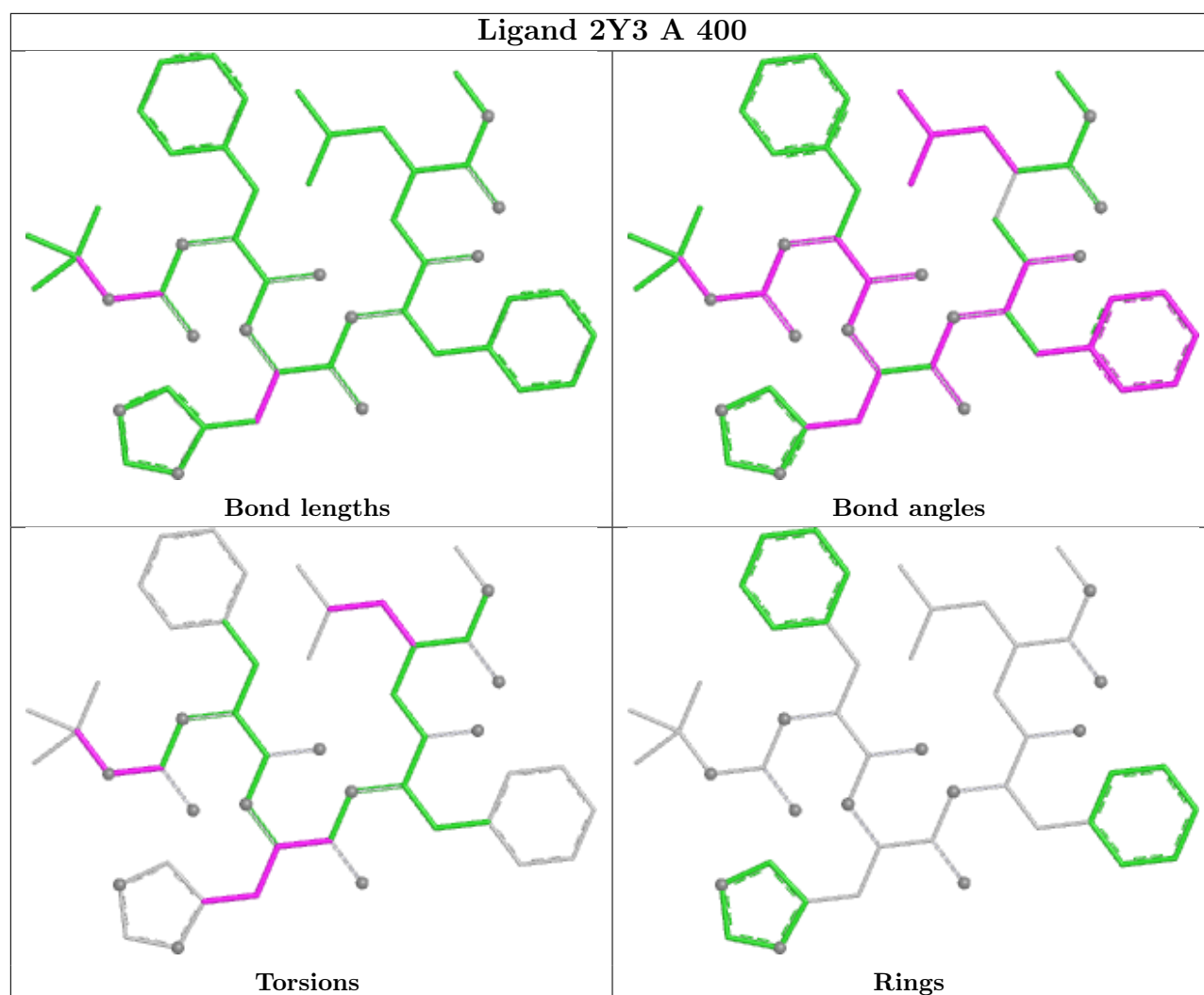
Mol	Chain	Res	Type	Atoms
3	A	400	2Y3	C5-C2-O2-C1
3	A	400	2Y3	C3-C2-O2-C1
3	A	400	2Y3	C4-C2-O2-C1
4	A	337	NAG	C8-C7-N2-C2
4	A	337	NAG	O7-C7-N2-C2
3	A	400	2Y3	C31-C32-C33-C34
3	A	400	2Y3	C31-C32-C33-C35
3	A	400	2Y3	N1-C1-O2-C2
3	A	400	2Y3	N2-C15-C16-O4
3	A	400	2Y3	O1-C1-O2-C2
3	A	400	2Y3	N2-C15-C16-N5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

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, 95th 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 ²)	Q<0.9
1	A	329/329 (100%)	-0.06	6 (1%) 67 58	6, 27, 55, 102	4 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	15.5
1	A	241	TRP	15.1
1	A	240	GLY	14.6
1	A	243	GLY	6.1
1	A	159(B)	ASP	3.6
1	A	110	LEU	2.8

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

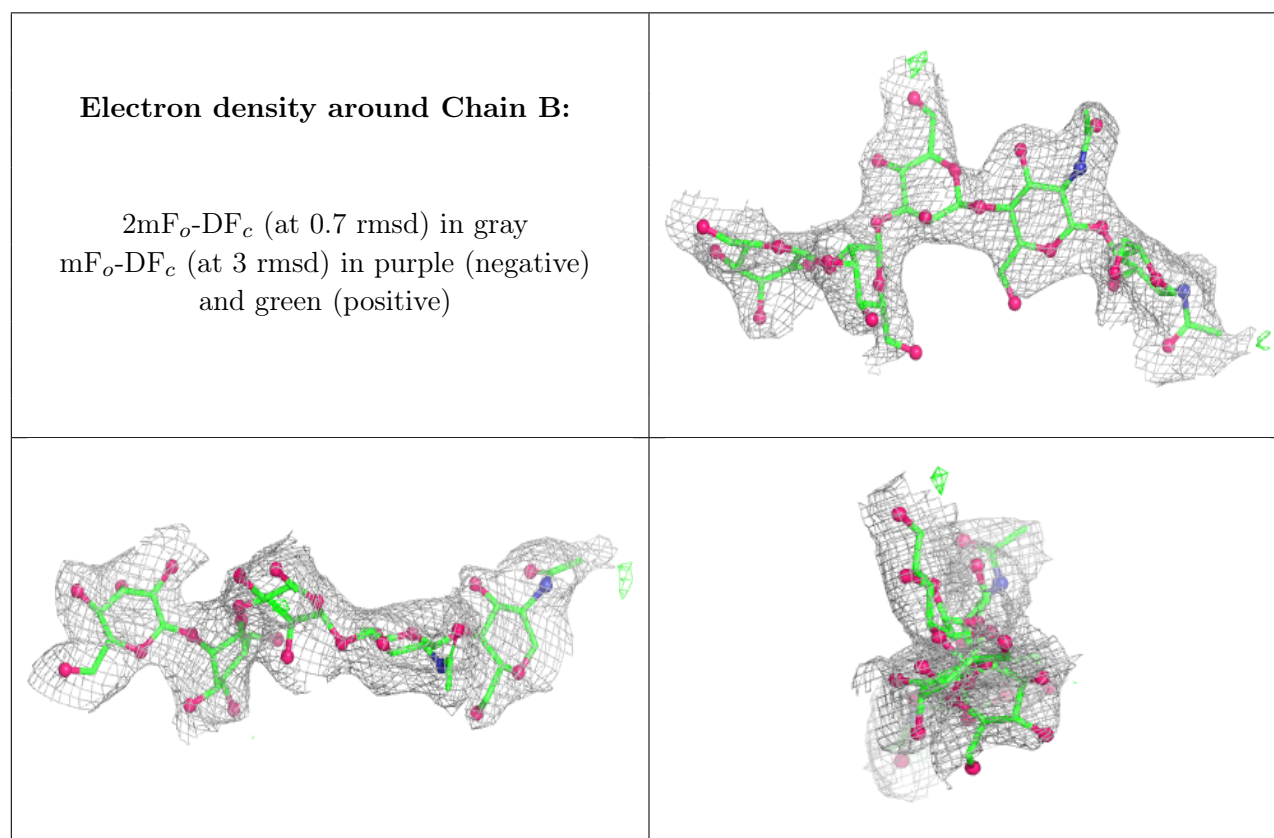
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
2	KBG	B	5	11/12	0.83	0.12	34,51,156,156	0
2	BMA	B	3	11/12	0.84	0.10	15,30,67,83	0
2	NAG	B	1	14/15	0.88	0.09	20,43,71,85	0
2	NAG	B	2	14/15	0.95	0.07	3,33,62,87	0
2	BMA	B	4	11/12	0.96	0.09	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](#)

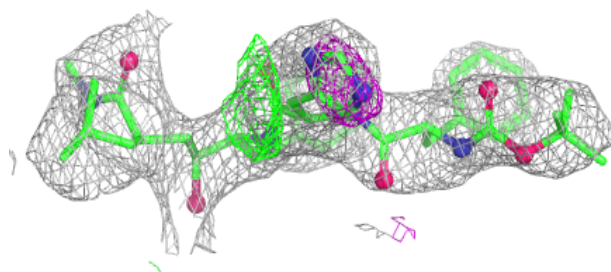
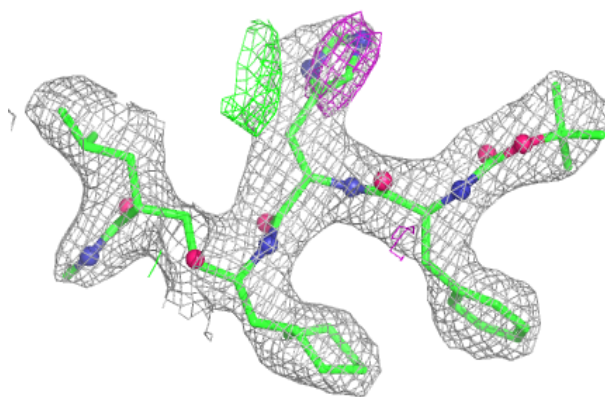
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	2Y3	A	400	49/49	0.90	0.10	4,24,49,77	0
4	NAG	A	337	14/15	0.90	0.10	15,38,146,156	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.

Electron density around 2Y3 A 400:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.