



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:30 AM UTC

PDB ID : 3Q3T / pdb_00003q3t
Title : Alkyl Amine Renin Inhibitors: Filling S1 from S3
Authors : Wu, Z.; McKeever, B.
Deposited on : 2010-12-22
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

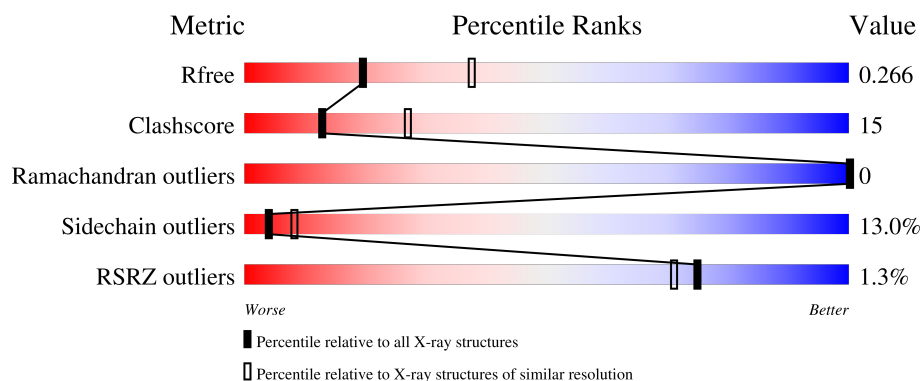
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	340	45% 42% 11% ..
1	B	340	48% 40% 9% ..
2	C	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5428 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Renin.

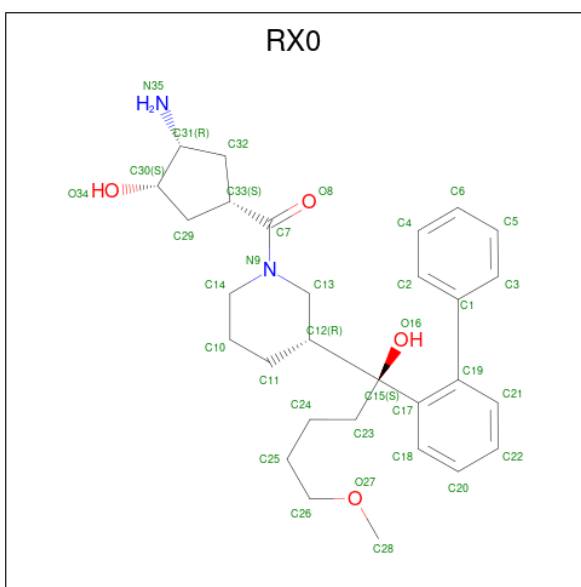
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2598	1656	421	507	14			
1	B	333	Total	C	N	O	S	0	0	0
			2566	1639	415	498	14			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is [(1S,3R,4S)-3-amino-4-hydroxycyclopentyl]{(3R)-3-[(1S)-1-(biphenyl-2-yl)-1-hydroxy-5-methoxypentyl]piperidin-1-yl}methanone (CCD ID: RX0) (formula: C₂₉H₄₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	29	2	4		
3	B	1	Total	C	N	O	0	0
			35	29	2	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

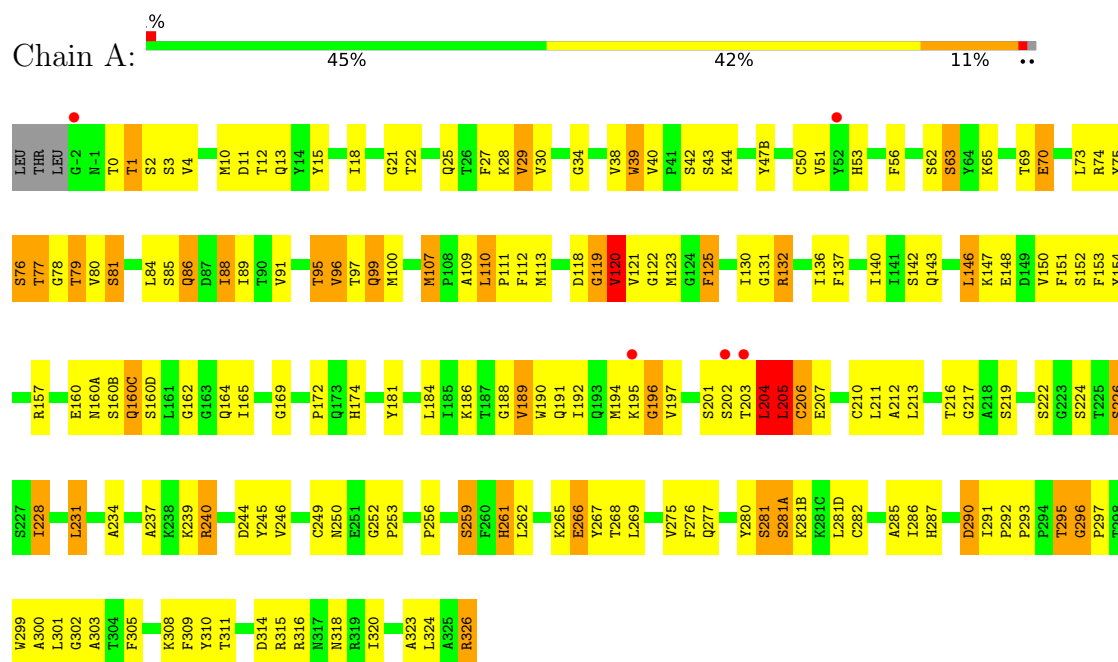
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	75	Total	O	0	0
			75	75		

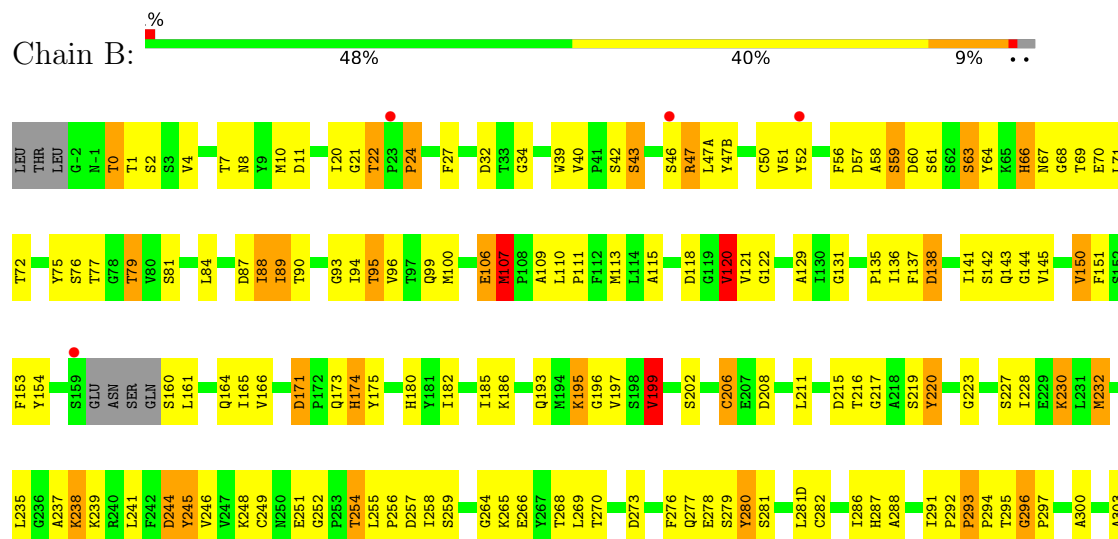
3 Residue-property plots [i](#)

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: Renin



• Molecule 1: Renin





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.25Å 97.58Å 148.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.60 46.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.36-2.60) 98.9 (46.36-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.268 0.209 , 0.266	Depositor DCC
R_{free} test set	1263 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5428	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 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, RX0, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.38	104/2658 (3.9%)	1.28	19/3604 (0.5%)
1	B	2.26	58/2625 (2.2%)	1.36	32/3558 (0.9%)
All	All	2.32	162/5283 (3.1%)	1.32	51/7162 (0.7%)

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	CA-C	-8.49	1.46	1.52
1	A	40	VAL	C-O	-7.71	1.18	1.24
1	A	65	LYS	C-O	-7.49	1.15	1.24
1	A	286	ILE	C-O	-7.19	1.16	1.24
1	B	40	VAL	C-O	-7.18	1.18	1.24
1	A	293	PRO	C-O	-7.15	1.18	1.24
1	B	286	ILE	C-O	-7.00	1.17	1.24
1	B	282	CYS	C-O	-6.95	1.15	1.24
1	B	34	GLY	C-O	-6.81	1.17	1.24
1	A	15	TYR	C-O	-6.78	1.15	1.23
1	A	311	THR	C-O	-6.76	1.16	1.24
1	A	213	LEU	C-O	-6.66	1.16	1.24
1	B	305	PHE	C-O	-6.65	1.16	1.24
1	A	290	ASP	C-O	-6.65	1.15	1.24
1	A	309	PHE	C-O	-6.65	1.16	1.24
1	A	234	ALA	CA-CB	-6.64	1.42	1.53
1	A	42	SER	C-O	-6.63	1.15	1.24
1	A	302	GLY	C-O	-6.57	1.17	1.23
1	B	245	TYR	C-O	-6.52	1.16	1.24
1	A	89	ILE	C-O	-6.51	1.17	1.24
1	A	107	MET	C-O	-6.48	1.19	1.25
1	B	237	ALA	CA-CB	-6.40	1.42	1.53
1	A	30	VAL	C-O	-6.37	1.16	1.24
1	A	210	CYS	C-O	-6.36	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	PHE	C-O	-6.35	1.16	1.24
1	B	235	LEU	C-O	-6.33	1.15	1.24
1	A	123	MET	C-O	-6.33	1.15	1.24
1	A	122	GLY	C-O	-6.32	1.18	1.24
1	A	267	TYR	C-O	-6.32	1.16	1.24
1	B	32	ASP	C-O	-6.32	1.16	1.24
1	A	13	GLN	C-O	-6.28	1.17	1.24
1	B	215	ASP	C-O	-6.28	1.16	1.24
1	B	115	ALA	CA-CB	-6.28	1.44	1.53
1	A	77	THR	CA-CB	-6.27	1.43	1.53
1	A	84	LEU	C-O	-6.27	1.16	1.23
1	B	182	ILE	C-O	-6.27	1.17	1.24
1	A	237	ALA	CA-CB	-6.25	1.43	1.53
1	B	288	ALA	CA-CB	-6.21	1.44	1.53
1	A	28	LYS	C-O	-6.21	1.16	1.24
1	B	150	VAL	C-O	-6.16	1.17	1.24
1	A	219	SER	C-O	-6.12	1.17	1.24
1	B	241	LEU	C-O	-6.08	1.17	1.23
1	A	34	GLY	C-O	-6.08	1.17	1.24
1	A	50	CYS	CB-SG	-6.03	1.61	1.81
1	A	99	GLN	C-O	-6.03	1.16	1.23
1	A	244	ASP	C-O	-5.98	1.16	1.23
1	A	22	THR	C-O	-5.98	1.17	1.25
1	A	85	SER	C-O	-5.98	1.16	1.23
1	A	194	MET	C-O	-5.97	1.16	1.24
1	A	154	TYR	C-O	-5.96	1.16	1.24
1	B	171	ASP	C-O	-5.95	1.19	1.25
1	B	7	THR	C-O	-5.92	1.17	1.23
1	A	38	VAL	C-O	-5.91	1.17	1.24
1	A	96	VAL	C-O	-5.91	1.18	1.24
1	A	285	ALA	CA-CB	-5.90	1.45	1.52
1	A	320	ILE	C-O	-5.88	1.17	1.24
1	A	137	PHE	C-O	-5.87	1.17	1.24
1	B	166	VAL	C-O	-5.87	1.17	1.24
1	A	121	VAL	C-O	-5.87	1.17	1.24
1	B	219	SER	C-O	-5.87	1.17	1.24
1	A	296	GLY	C-O	-5.85	1.16	1.24
1	B	211	LEU	C-O	-5.85	1.16	1.24
1	B	196	GLY	C-O	-5.83	1.17	1.24
1	B	279	SER	C-O	-5.82	1.16	1.23
1	B	129	ALA	CA-CB	-5.80	1.43	1.53
1	A	47(B)	TYR	C-O	-5.75	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	VAL	C-O	-5.74	1.18	1.24
1	A	4	VAL	C-O	-5.73	1.18	1.24
1	A	119	GLY	C-O	-5.73	1.17	1.23
1	B	118	ASP	C-O	-5.73	1.16	1.23
1	A	39	TRP	C-O	-5.72	1.16	1.23
1	B	300	ALA	C-O	-5.65	1.17	1.24
1	A	216	THR	C-O	-5.65	1.16	1.24
1	A	153	PHE	C-O	-5.63	1.17	1.24
1	B	227	SER	C-O	-5.61	1.17	1.24
1	B	228	ILE	C-O	-5.61	1.17	1.24
1	A	222	SER	C-O	-5.61	1.16	1.23
1	A	130	ILE	C-O	-5.59	1.18	1.24
1	A	120	VAL	C-O	-5.55	1.18	1.24
1	A	259	SER	C-O	-5.55	1.17	1.24
1	A	136	ILE	C-O	-5.54	1.17	1.24
1	A	88	ILE	CA-CB	-5.54	1.47	1.54
1	B	138	ASP	C-O	-5.54	1.17	1.24
1	A	125	PHE	C-O	-5.54	1.16	1.23
1	A	56	PHE	C-O	-5.53	1.17	1.24
1	A	79	THR	C-O	-5.52	1.17	1.24
1	A	190	TRP	C-O	-5.52	1.17	1.23
1	A	142	SER	C-O	-5.51	1.17	1.24
1	B	252	GLY	C-O	-5.50	1.18	1.24
1	B	308	LYS	C-O	-5.49	1.17	1.24
1	A	300	ALA	C-O	-5.49	1.17	1.24
1	B	185	ILE	CA-CB	-5.46	1.47	1.54
1	A	81	SER	C-O	-5.46	1.17	1.23
1	A	226	SER	C-O	-5.44	1.17	1.24
1	A	12	THR	C-O	-5.43	1.17	1.24
1	A	192	ILE	C-O	-5.43	1.17	1.23
1	A	95	THR	C-O	-5.42	1.17	1.24
1	A	86	GLN	C-O	-5.42	1.17	1.23
1	A	269	LEU	C-O	-5.39	1.17	1.24
1	A	27	PHE	C-O	-5.37	1.17	1.23
1	A	287	HIS	C-O	-5.36	1.17	1.23
1	B	154	TYR	C-O	-5.36	1.17	1.24
1	A	293	PRO	CA-CB	-5.35	1.49	1.54
1	A	217	GLY	C-O	-5.33	1.17	1.24
1	A	276	PHE	C-O	-5.32	1.17	1.23
1	B	217	GLY	C-O	-5.32	1.17	1.24
1	B	270	THR	C-O	-5.32	1.16	1.23
1	B	303	ALA	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	TYR	C-O	-5.28	1.17	1.24
1	B	320	ILE	C-O	-5.28	1.18	1.24
1	A	212	ALA	C-O	-5.27	1.18	1.24
1	A	224	SER	C-O	-5.27	1.16	1.23
1	B	293	PRO	C-O	-5.27	1.20	1.24
1	A	70	GLU	C-O	-5.24	1.17	1.23
1	A	50	CYS	CA-C	-5.23	1.45	1.52
1	B	120	VAL	C-O	-5.22	1.18	1.24
1	B	268	THR	C-O	-5.22	1.17	1.24
1	A	164	GLN	C-O	-5.20	1.17	1.23
1	A	323	ALA	CA-CB	-5.20	1.44	1.54
1	B	174	HIS	C-O	-5.19	1.16	1.24
1	B	246	VAL	C-O	-5.19	1.18	1.24
1	B	244	ASP	C-O	-5.17	1.17	1.23
1	A	25	GLN	C-O	-5.17	1.17	1.24
1	B	230	LYS	C-O	-5.16	1.18	1.24
1	B	95	THR	C-O	-5.16	1.18	1.24
1	A	43	SER	C-O	-5.16	1.17	1.24
1	B	296	GLY	C-O	-5.16	1.17	1.24
1	A	206	CYS	CB-SG	-5.15	1.64	1.81
1	A	69	THR	C-O	-5.14	1.17	1.23
1	A	295	THR	C-O	-5.14	1.18	1.24
1	A	299	TRP	C-O	-5.14	1.17	1.23
1	B	89	ILE	C-O	-5.13	1.18	1.24
1	B	238	LYS	C-O	-5.12	1.17	1.23
1	B	107	MET	C-O	-5.12	1.20	1.24
1	A	18	ILE	C-O	-5.12	1.18	1.23
1	A	205	LEU	C-O	-5.12	1.17	1.23
1	A	63	SER	C-O	-5.12	1.17	1.24
1	A	151	PHE	C-O	-5.11	1.17	1.23
1	A	303	ALA	C-O	-5.11	1.17	1.24
1	A	305	PHE	C-O	-5.11	1.18	1.24
1	A	256	PRO	C-O	-5.10	1.18	1.23
1	B	197	VAL	C-O	-5.09	1.18	1.24
1	A	196	GLY	C-O	-5.08	1.18	1.24
1	A	301	LEU	C-O	-5.07	1.17	1.23
1	B	199	VAL	CB-CG1	-5.07	1.35	1.52
1	A	97	THR	C-O	-5.06	1.18	1.24
1	B	257	ASP	C-O	-5.05	1.17	1.23
1	A	261	HIS	C-O	-5.04	1.17	1.23
1	A	281(D)	LEU	C-O	-5.04	1.17	1.24
1	B	281(D)	LEU	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	C-O	-5.04	1.19	1.24
1	A	240	ARG	C-O	-5.04	1.17	1.23
1	B	220	TYR	C-O	-5.03	1.17	1.23
1	A	281	SER	C-O	-5.03	1.17	1.23
1	A	275	VAL	C-O	-5.03	1.18	1.24
1	B	151	PHE	C-O	-5.03	1.17	1.23
1	B	258	ILE	C-O	-5.02	1.18	1.24
1	A	73	LEU	C-O	-5.02	1.18	1.24
1	A	197	VAL	C-O	-5.02	1.18	1.24
1	A	172	PRO	C-O	-5.02	1.18	1.24
1	B	8	ASN	C-O	-5.01	1.18	1.24
1	B	164	GLN	C-O	-5.00	1.18	1.23

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	VAL	N-CA-C	12.04	122.88	110.72
1	B	185	ILE	N-CA-C	10.03	119.96	110.53
1	A	118	ASP	N-CA-C	9.86	121.79	111.14
1	B	308	LYS	N-CA-C	7.79	119.85	111.36
1	A	204	LEU	N-CA-C	7.77	119.83	111.36
1	B	76	SER	CA-C-N	7.42	131.59	120.31
1	B	76	SER	C-N-CA	7.42	131.59	120.31
1	B	293	PRO	N-CA-C	-7.37	102.69	110.58
1	B	131	GLY	N-CA-C	-7.28	105.68	115.36
1	B	185	ILE	CB-CA-C	-7.27	102.50	112.02
1	B	47	ARG	N-CA-C	-7.20	104.38	113.02
1	A	240	ARG	N-CA-C	-6.83	99.03	109.41
1	A	305	PHE	N-CA-C	6.77	118.45	111.14
1	B	143	GLN	N-CA-C	-6.77	104.12	112.38
1	A	244	ASP	N-CA-C	6.71	119.14	109.14
1	B	43	SER	N-CA-C	-6.40	104.36	111.71
1	B	315	ARG	N-CA-C	6.38	118.31	111.36
1	A	281(D)	LEU	CA-C-N	-6.30	113.48	122.94
1	A	281(D)	LEU	C-N-CA	-6.30	113.48	122.94
1	B	122	GLY	N-CA-C	6.28	119.81	111.03
1	B	141	ILE	CA-C-N	6.27	128.68	120.28
1	B	141	ILE	C-N-CA	6.27	128.68	120.28
1	A	76	SER	N-CA-C	-6.20	104.58	111.71
1	B	51	VAL	N-CA-C	5.96	117.50	111.00
1	A	315	ARG	N-CA-C	5.92	117.82	111.36
1	B	94	ILE	N-CA-C	5.83	117.15	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	SER	N-CA-C	5.80	118.55	111.82
1	B	0	THR	N-CA-C	5.78	118.66	109.24
1	A	308	LYS	N-CA-C	5.77	117.65	111.36
1	A	51	VAL	N-CA-C	5.67	116.45	110.72
1	B	47(A)	LEU	N-CA-C	-5.61	106.41	113.20
1	B	120	VAL	N-CA-C	5.50	116.39	108.48
1	B	75	TYR	CA-C-N	5.49	127.64	120.28
1	B	75	TYR	C-N-CA	5.49	127.64	120.28
1	B	52	TYR	CB-CA-C	5.43	119.78	110.01
1	B	280	TYR	N-CA-C	-5.42	105.30	112.94
1	A	281(A)	SER	N-CA-C	-5.40	106.72	113.15
1	A	136	ILE	N-CA-C	5.37	116.10	110.62
1	A	2	SER	N-CA-C	5.34	117.76	110.55
1	A	162	GLY	N-CA-C	5.29	119.07	112.73
1	A	137	PHE	N-CA-C	5.20	117.03	111.36
1	B	295	THR	N-CA-C	5.17	116.92	111.28
1	B	216	THR	N-CA-C	5.12	117.76	111.82
1	A	295	THR	N-CA-C	5.11	116.85	111.28
1	B	223	GLY	N-CA-C	-5.08	101.07	110.73
1	B	71	LEU	N-CA-C	5.05	117.63	108.69
1	B	208	ASP	N-CA-C	-5.04	106.87	112.57
1	B	24	PRO	CB-CA-C	-5.03	104.97	111.46
1	A	21	GLY	N-CA-C	5.02	121.37	112.83
1	B	273	ASP	N-CA-C	5.02	117.64	111.82
1	B	153	PHE	N-CA-C	5.00	117.05	108.90

There are no chirality outliers.

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	2598	0	2525	77	0
1	B	2566	0	2499	78	0
2	C	28	0	25	0	0
3	A	35	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	40	2	0
4	A	12	0	16	0	0
5	B	14	0	13	3	0
6	A	65	0	0	3	0
6	B	75	0	0	3	0
All	All	5428	0	5158	158	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 15.

All (158) 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:B:22:THR:OG1	1:B:63:SER:OG	1.65	1.12
1:A:77:THR:HG23	1:A:78:GLY:N	1.51	1.12
1:A:1:THR:HG22	1:A:1:THR:O	1.53	1.06
1:A:77:THR:CG2	1:A:78:GLY:N	2.19	1.05
1:A:160(C):GLN:NE2	1:A:160(C):GLN:HA	1.68	1.05
1:A:77:THR:CG2	1:A:78:GLY:H	1.71	1.00
1:A:259:SER:OG	1:A:268:THR:OG1	1.84	0.95
1:A:202:SER:OG	1:A:204:LEU:HD21	1.69	0.92
1:B:206:CYS:SG	1:B:206:CYS:O	2.36	0.84
1:B:27:PHE:CZ	1:B:56:PHE:HB2	2.13	0.82
1:B:266:GLU:OE1	6:B:364:HOH:O	2.00	0.80
1:A:160(C):GLN:NE2	1:A:160(C):GLN:CA	2.43	0.79
1:A:202:SER:OG	1:A:204:LEU:CD2	2.32	0.78
1:B:100:MET:HE1	5:B:600:NAG:O5	1.82	0.78
1:A:160(C):GLN:HA	1:A:160(C):GLN:HE21	1.50	0.76
1:A:77:THR:HG23	1:A:78:GLY:H	1.24	0.76
1:B:27:PHE:HZ	1:B:56:PHE:HB2	1.50	0.75
1:B:180:HIS:CD2	1:B:265:LYS:HE3	2.22	0.75
1:A:206:CYS:SG	1:A:206:CYS:O	2.44	0.74
1:A:95:THR:O	1:A:143:GLN:NE2	2.21	0.74
1:B:180:HIS:NE2	1:B:265:LYS:HE3	2.02	0.74
1:B:20:ILE:HG12	1:B:89:ILE:HG12	1.71	0.72
1:B:67:ASN:OD1	1:B:67:ASN:C	2.32	0.72
1:B:39:TRP:NE1	1:B:120:VAL:HG13	2.06	0.71
1:B:248:LYS:HB2	1:B:251:GLU:HG3	1.72	0.71
1:A:174:HIS:HA	1:A:326:ARG:OXT	1.90	0.71
1:A:160(C):GLN:CA	1:A:160(C):GLN:HE21	2.03	0.70
1:B:232:MET:HG3	1:B:245:TYR:CD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HE1	1:A:112:PHE:O	1.75	0.69
1:A:249:CYS:O	1:A:277:GLN:NE2	2.25	0.69
1:B:232:MET:HG3	1:B:245:TYR:CE1	2.28	0.69
1:B:66:HIS:ND1	1:B:66:HIS:C	2.51	0.68
1:B:70:GLU:O	6:B:378:HOH:O	2.12	0.67
1:A:77:THR:HG22	1:A:78:GLY:H	1.60	0.65
3:B:500:RX0:C2	3:B:500:RX0:H23	2.27	0.65
1:B:69:THR:HB	1:B:84:LEU:HD12	1.78	0.64
1:A:203:THR:O	1:A:203:THR:HG22	1.97	0.64
3:B:500:RX0:H23	3:B:500:RX0:H2	1.80	0.63
1:B:87:ASP:OD1	1:B:88:ILE:N	2.26	0.61
1:B:277:GLN:HG2	1:B:280:TYR:CE1	2.34	0.61
1:A:202:SER:HG	1:A:204:LEU:HD21	1.65	0.60
1:B:174:HIS:HA	1:B:326:ARG:OXT	2.01	0.59
1:A:125:PHE:CB	1:A:188:GLY:HA2	2.33	0.59
1:A:202:SER:O	1:A:204:LEU:HD23	2.04	0.58
1:B:88:ILE:CG2	1:B:95:THR:HG22	2.33	0.58
1:B:2:SER:HB2	1:B:93:GLY:H	1.70	0.57
1:A:140:ILE:O	1:A:143:GLN:HB2	2.06	0.56
1:A:250:ASN:OD1	1:A:281(A):SER:HA	2.05	0.56
1:A:125:PHE:CG	1:A:188:GLY:HA2	2.40	0.56
1:A:291:ILE:O	1:A:296:GLY:HA3	2.06	0.56
1:A:110:LEU:HG	1:A:110:LEU:O	2.06	0.56
1:B:88:ILE:CG2	1:B:95:THR:CG2	2.85	0.55
1:A:277:GLN:HG2	1:A:280:TYR:CE1	2.42	0.55
1:B:64:TYR:OH	1:B:66:HIS:HB2	2.06	0.55
1:A:246:VAL:HA	1:A:282:CYS:O	2.07	0.55
1:B:66:HIS:ND1	1:B:67:ASN:N	2.55	0.55
1:A:205:LEU:HD11	1:A:231:LEU:HB2	1.89	0.55
1:A:268:THR:HB	6:A:365:HOH:O	2.07	0.54
1:B:67:ASN:OD1	1:B:69:THR:N	2.36	0.54
1:B:67:ASN:CG	5:B:600:NAG:O7	2.51	0.54
1:A:10:MET:O	1:A:11:ASP:HB2	2.08	0.54
1:B:296:GLY:HA2	1:B:297:PRO:C	2.32	0.54
1:B:46:SER:OG	1:B:47:ARG:N	2.38	0.53
1:B:195:LYS:NZ	1:B:264:GLY:H	2.06	0.53
1:A:204:LEU:HD23	1:A:204:LEU:N	2.23	0.53
1:B:57:ASP:OD1	1:B:59:SER:N	2.40	0.53
1:A:207:GLU:OE1	1:A:207:GLU:N	2.30	0.52
1:B:67:ASN:OD1	1:B:68:GLY:N	2.42	0.52
1:A:150:VAL:HG12	1:A:314:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.91	0.52
1:B:150:VAL:HG12	1:B:314:ASP:HA	1.91	0.52
1:A:239:LYS:HG3	1:A:245:TYR:CE1	2.44	0.52
1:A:246:VAL:HG12	1:A:282:CYS:O	2.10	0.51
1:A:316:ARG:NH1	6:A:391:HOH:O	2.43	0.51
1:A:281:SER:C	1:A:281(B):LYS:H	2.17	0.51
1:B:220:TYR:HB2	1:B:287:HIS:HD2	1.75	0.51
1:A:189:VAL:HG22	1:A:191:GLN:HB2	1.93	0.51
1:B:106:GLU:O	1:B:106:GLU:CG	2.58	0.50
1:B:1:THR:O	1:B:1:THR:OG1	2.30	0.50
1:A:109:ALA:O	1:A:113:MET:HB2	2.12	0.50
1:A:160(C):GLN:HE21	1:A:160(C):GLN:N	2.09	0.50
1:A:88:ILE:CG2	1:A:95:THR:CG2	2.91	0.49
1:A:88:ILE:CG2	1:A:95:THR:HG23	2.43	0.49
1:A:131:GLY:C	1:A:132:ARG:HG3	2.37	0.49
1:A:184:LEU:HG	1:A:318:ASN:O	2.13	0.49
1:A:113:MET:HE3	1:B:113:MET:HE3	1.94	0.49
1:A:152:SER:OG	1:A:169:GLY:O	2.22	0.49
1:B:249:CYS:HB2	1:B:281:SER:O	2.13	0.49
1:B:66:HIS:CE1	1:B:67:ASN:O	2.67	0.48
1:A:296:GLY:HA2	1:A:297:PRO:C	2.38	0.48
1:A:53:HIS:CE1	1:A:112:PHE:O	2.61	0.48
1:B:293:PRO:HA	1:B:294:PRO:C	2.39	0.48
1:B:21:GLY:O	1:B:24:PRO:HA	2.14	0.48
1:B:142:SER:C	1:B:144:GLY:N	2.69	0.47
1:A:0:THR:O	1:A:146:LEU:HA	2.13	0.47
1:A:110:LEU:HA	1:A:111:PRO:HA	1.59	0.47
1:B:135:PRO:HD2	1:B:138:ASP:OD2	2.13	0.47
1:A:228:ILE:HD12	1:A:228:ILE:HA	1.67	0.47
1:A:246:VAL:HG12	1:A:282:CYS:C	2.39	0.47
1:A:148:GLU:HA	1:A:148:GLU:OE1	2.14	0.47
3:A:500:RX0:H33	3:A:500:RX0:H13	1.62	0.47
1:A:196:GLY:C	1:A:261:HIS:HD2	2.23	0.47
1:B:99:GLN:OE1	1:B:136:ILE:HA	2.15	0.47
1:A:75:TYR:C	1:A:77:THR:N	2.71	0.47
1:A:99:GLN:HG3	1:A:100:MET:N	2.28	0.47
1:B:100:MET:HE1	5:B:600:NAG:C1	2.44	0.47
1:A:196:GLY:O	1:A:261:HIS:HD2	1.98	0.46
1:A:152:SER:HB2	1:A:310:TYR:CE1	2.51	0.46
1:A:261:HIS:CE1	1:A:266:GLU:HG2	2.51	0.46
1:B:39:TRP:HE1	1:B:120:VAL:HG13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:SER:HB3	1:B:266:GLU:HG3	1.98	0.46
1:A:29:VAL:HA	1:A:119:GLY:O	2.16	0.45
3:A:500:RX0:H12	3:A:500:RX0:C1	2.46	0.45
1:B:110:LEU:HA	1:B:111:PRO:HA	1.69	0.45
1:B:22:THR:O	1:B:61:SER:HA	2.17	0.45
1:B:171:ASP:OD1	1:B:173:GLN:HB2	2.17	0.45
1:A:252:GLY:N	1:A:253:PRO:CD	2.79	0.45
1:A:75:TYR:O	1:A:76:SER:C	2.59	0.45
1:A:77:THR:HG21	1:A:111:PRO:HG3	1.99	0.45
1:A:207:GLU:H	1:A:207:GLU:CD	2.21	0.44
1:B:57:ASP:OD1	1:B:59:SER:HB2	2.17	0.44
1:B:316:ARG:HH11	1:B:317:ASN:HD21	1.65	0.44
1:B:326:ARG:OXT	1:B:326:ARG:CG	2.65	0.44
1:B:58:ALA:C	1:B:60:ASP:N	2.73	0.44
1:B:136:ILE:HG23	1:B:137:PHE:N	2.33	0.44
1:A:261:HIS:CE1	1:A:266:GLU:CG	3.01	0.43
1:A:204:LEU:CD2	1:A:204:LEU:N	2.82	0.43
1:A:204:LEU:HD23	1:A:204:LEU:H	1.83	0.43
1:A:39:TRP:NE1	1:A:120:VAL:HG13	2.34	0.43
1:B:195:LYS:HE3	1:B:195:LYS:HB2	1.77	0.43
1:A:239:LYS:HG3	1:A:245:TYR:CZ	2.53	0.43
1:B:220:TYR:HB2	1:B:287:HIS:CD2	2.54	0.42
1:B:72:THR:HG23	1:B:79:THR:HG23	2.01	0.42
1:B:121:VAL:O	1:B:121:VAL:HG12	2.19	0.42
1:B:254:THR:H	1:B:254:THR:HG23	1.59	0.42
1:B:56:PHE:CD2	1:B:56:PHE:C	2.97	0.42
1:B:314:ASP:OD1	1:B:314:ASP:C	2.61	0.42
1:A:96:VAL:O	1:A:96:VAL:HG13	2.20	0.42
1:B:39:TRP:CH2	1:B:107:MET:HE3	2.55	0.42
1:B:239:LYS:HD3	1:B:245:TYR:CZ	2.54	0.41
1:B:248:LYS:CB	1:B:251:GLU:HG3	2.47	0.41
1:A:202:SER:C	1:A:204:LEU:HD23	2.45	0.41
1:B:57:ASP:OD1	1:B:57:ASP:C	2.62	0.41
1:B:106:GLU:O	1:B:106:GLU:HG2	2.21	0.41
1:A:86:GLN:NE2	6:A:362:HOH:O	2.21	0.41
1:B:47(B):TYR:CE2	1:B:106:GLU:HA	2.55	0.41
1:B:109:ALA:O	1:B:113:MET:HB2	2.20	0.41
1:B:10:MET:O	1:B:11:ASP:HB2	2.20	0.41
1:A:250:ASN:HB3	1:A:280:TYR:O	2.19	0.41
1:B:175:TYR:CD2	1:B:175:TYR:C	2.99	0.41
1:B:291:ILE:HA	1:B:292:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.87	0.41
1:B:244:ASP:HB2	6:B:396:HOH:O	2.21	0.41
1:B:39:TRP:HH2	1:B:107:MET:HE3	1.86	0.40
1:B:199:VAL:O	1:B:199:VAL:HG12	2.18	0.40
1:A:196:GLY:HA2	1:A:206:CYS:O	2.21	0.40
1:B:88:ILE:HG22	1:B:95:THR:CG2	2.52	0.40
1:B:64:TYR:HH	1:B:66:HIS:HB2	1.86	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	335/340 (98%)	330 (98%)	5 (2%)	0	100	100
1	B	329/340 (97%)	322 (98%)	7 (2%)	0	100	100
All	All	664/680 (98%)	652 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	287/290 (99%)	247 (86%)	40 (14%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	283/290 (98%)	249 (88%)	34 (12%)	5	10
All	All	570/580 (98%)	496 (87%)	74 (13%)	4	8

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	SER
1	A	44	LYS
1	A	63	SER
1	A	70	GLU
1	A	74	ARG
1	A	79	THR
1	A	81	SER
1	A	91	VAL
1	A	107	MET
1	A	110	LEU
1	A	120	VAL
1	A	132	ARG
1	A	146	LEU
1	A	147	LYS
1	A	157	ARG
1	A	160	GLU
1	A	160(A)	ASN
1	A	160(B)	SER
1	A	160(C)	GLN
1	A	160(D)	SER
1	A	165	ILE
1	A	186	LYS
1	A	189	VAL
1	A	195	LYS
1	A	201	SER
1	A	204	LEU
1	A	205	LEU
1	A	211	LEU
1	A	226	SER
1	A	228	ILE
1	A	231	LEU
1	A	240	ARG
1	A	262	LEU
1	A	265	LYS
1	A	266	GLU

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Mol	Chain	Res	Type
1	A	290	ASP
1	A	295	THR
1	A	324	LEU
1	A	326	ARG
1	B	0	THR
1	B	4	VAL
1	B	22	THR
1	B	42	SER
1	B	43	SER
1	B	50	CYS
1	B	59	SER
1	B	63	SER
1	B	66	HIS
1	B	77	THR
1	B	79	THR
1	B	81	SER
1	B	88	ILE
1	B	90	THR
1	B	96	VAL
1	B	106	GLU
1	B	107	MET
1	B	120	VAL
1	B	160	SER
1	B	161	LEU
1	B	165	ILE
1	B	186	LYS
1	B	193	GLN
1	B	195	LYS
1	B	199	VAL
1	B	202	SER
1	B	206	CYS
1	B	230	LYS
1	B	232	MET
1	B	238	LYS
1	B	254	THR
1	B	269	LEU
1	B	278	GLU
1	B	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	128	GLN
1	A	160(C)	GLN
1	A	164	GLN
1	A	183	ASN
1	A	191	GLN
1	A	317	ASN
1	B	139	ASN
1	B	143	GLN
1	B	164	GLN
1	B	191	GLN
1	B	261	HIS
1	B	287	HIS
1	B	317	ASN
1	B	318	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 ⓘ

2 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	C	1	2,1	14,14,15	0.56	0	17,19,21	1.70	4 (23%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.08	1 (5%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	3.89	128.12	122.90
2	C	1	NAG	O5-C5-C6	2.98	113.47	107.66
2	C	1	NAG	O7-C7-N2	2.58	126.53	121.98
2	C	2	NAG	O5-C5-C6	2.43	112.39	107.66
2	C	1	NAG	O7-C7-C8	-2.28	118.00	122.05

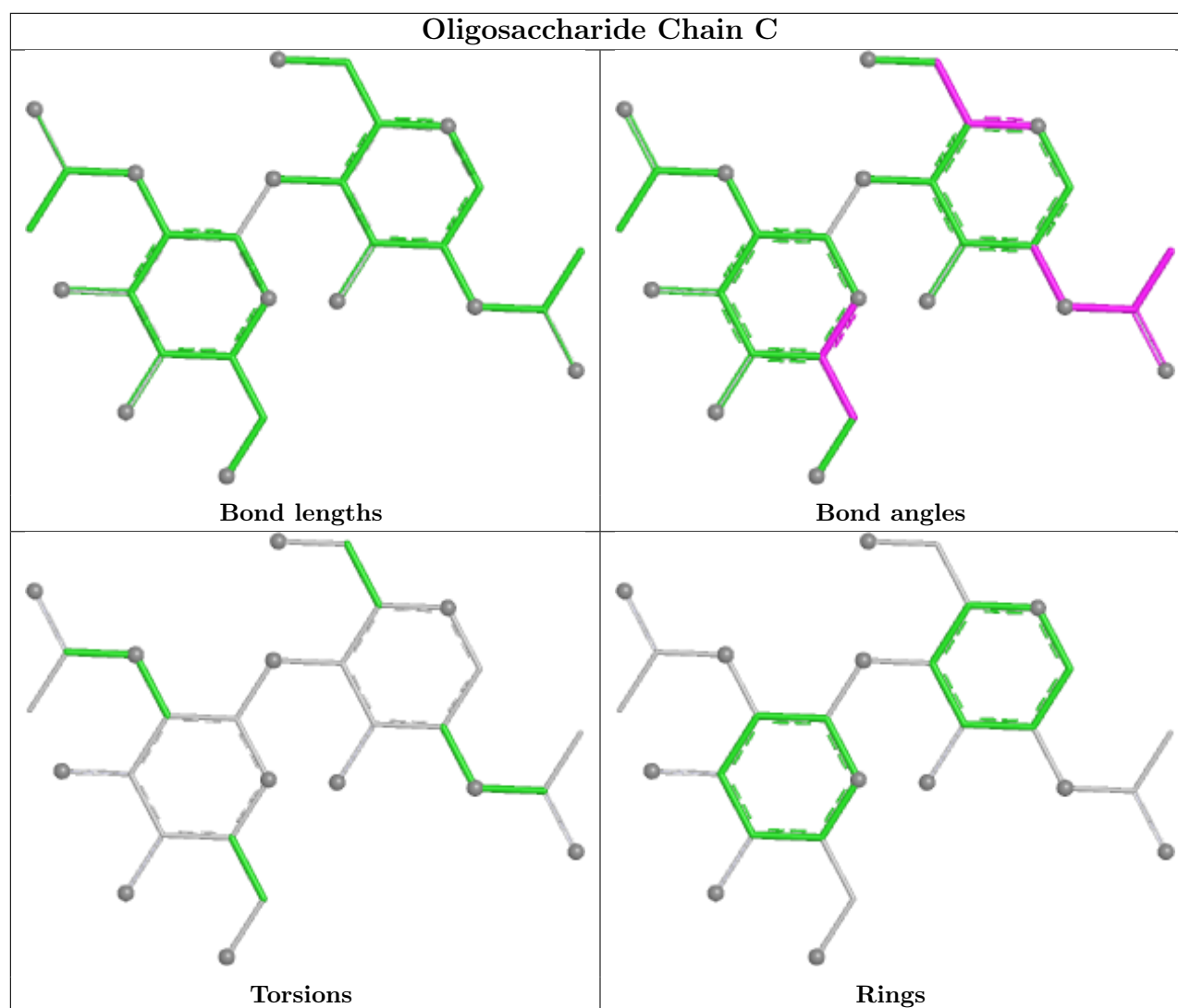
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

5 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	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.61	0
3	RX0	A	500	-	37,38,38	1.04	2 (5%)	43,53,53	1.87	13 (30%)
4	GOL	A	341	-	5,5,5	0.47	0	5,5,5	1.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	RX0	B	500	-	37,38,38	1.14	1 (2%)	43,53,53	1.88	9 (20%)
5	NAG	B	600	1	14,14,15	0.63	0	17,19,21	1.43	2 (11%)

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	GOL	A	502	-	-	1/4/4/4	-
3	RX0	A	500	-	-	1/31/53/53	0/4/4/4
4	GOL	A	341	-	-	4/4/4/4	-
3	RX0	B	500	-	-	2/31/53/53	0/4/4/4
5	NAG	B	600	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	RX0	C7-N9	4.53	1.41	1.35
3	A	500	RX0	C7-N9	3.29	1.39	1.35
3	A	500	RX0	C13-N9	3.15	1.50	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	RX0	O16-C15-C23	-6.72	98.75	108.26
3	B	500	RX0	O8-C7-C33	-4.43	114.34	120.86
3	A	500	RX0	C29-C33-C7	4.08	118.73	110.91
3	B	500	RX0	C29-C30-C31	3.96	108.00	103.19
3	A	500	RX0	C29-C30-C31	3.82	107.83	103.19
3	A	500	RX0	O8-C7-N9	-3.52	117.41	121.61
3	A	500	RX0	O16-C15-C23	-3.51	103.29	108.26
3	A	500	RX0	C14-N9-C13	3.37	119.57	113.07
3	A	500	RX0	C18-C17-C15	-3.34	116.90	120.79
3	A	500	RX0	C33-C7-N9	3.23	121.84	118.80
5	B	600	NAG	C1-O5-C5	3.08	116.32	112.19
3	B	500	RX0	O8-C7-N9	2.74	124.89	121.61
5	B	600	NAG	C3-C4-C5	2.65	115.04	110.23
3	A	500	RX0	C13-N9-C7	-2.58	113.59	122.14
3	B	500	RX0	C21-C19-C1	-2.52	113.69	118.70
3	A	500	RX0	C11-C10-C14	-2.50	107.46	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	RX0	C14-N9-C7	-2.49	113.95	123.30
3	B	500	RX0	O34-C30-C29	-2.48	102.27	110.88
3	B	500	RX0	C10-C11-C12	-2.44	108.00	112.21
3	A	500	RX0	C11-C12-C13	-2.39	104.30	108.65
3	B	500	RX0	C18-C17-C15	-2.37	118.03	120.79
3	A	500	RX0	C21-C19-C1	-2.30	114.13	118.70
3	B	500	RX0	O16-C15-C17	2.14	111.72	107.54
3	A	500	RX0	C20-C18-C17	2.06	123.68	119.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	341	GOL	O1-C1-C2-C3
4	A	341	GOL	C1-C2-C3-O3
4	A	341	GOL	O2-C2-C3-O3
3	B	500	RX0	C25-C26-O27-C28
3	A	500	RX0	O8-C7-N9-C14
4	A	341	GOL	O1-C1-C2-O2
3	B	500	RX0	C33-C7-N9-C13
5	B	600	NAG	C1-C2-N2-C7
4	A	502	GOL	O1-C1-C2-O2

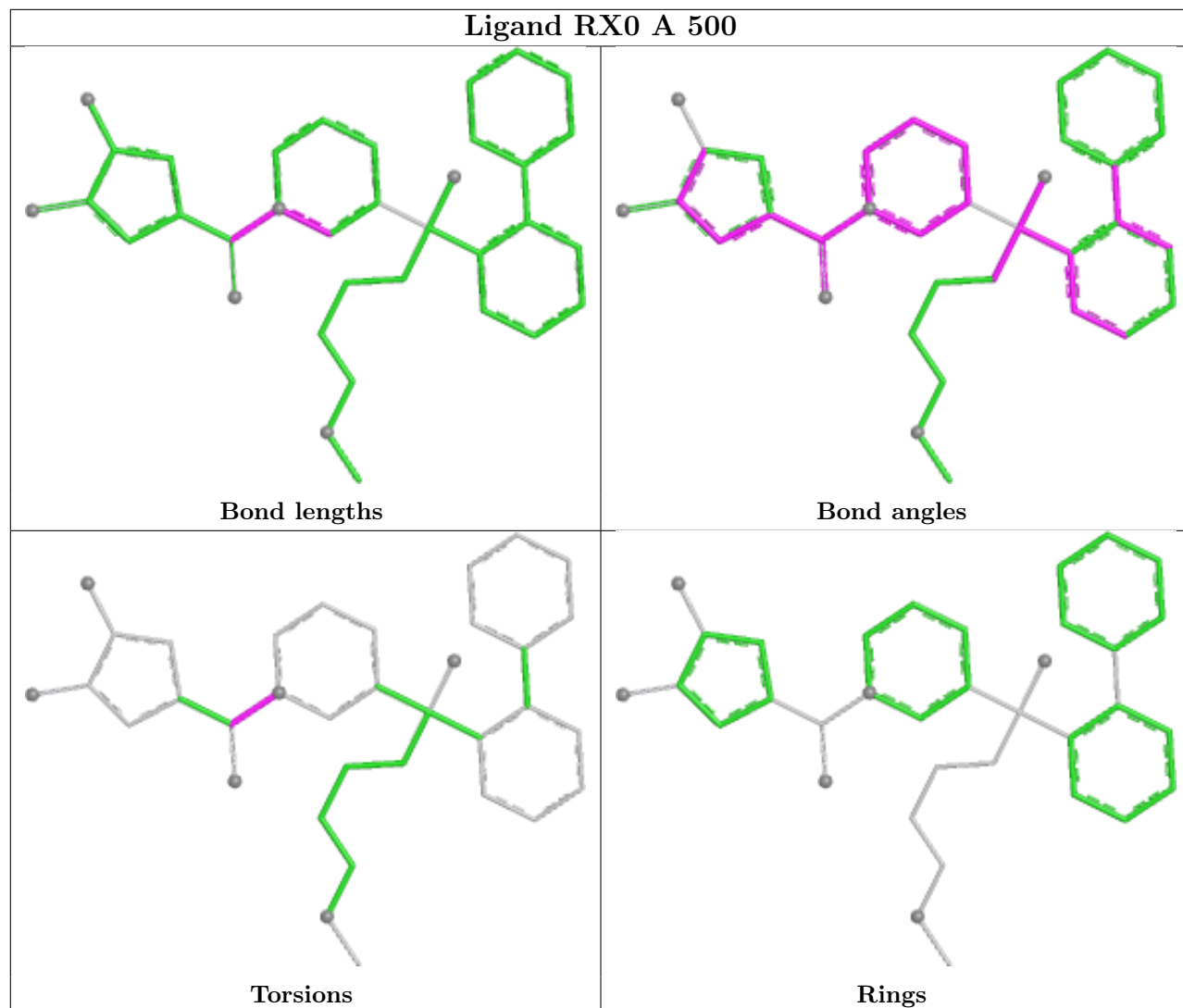
There are no ring outliers.

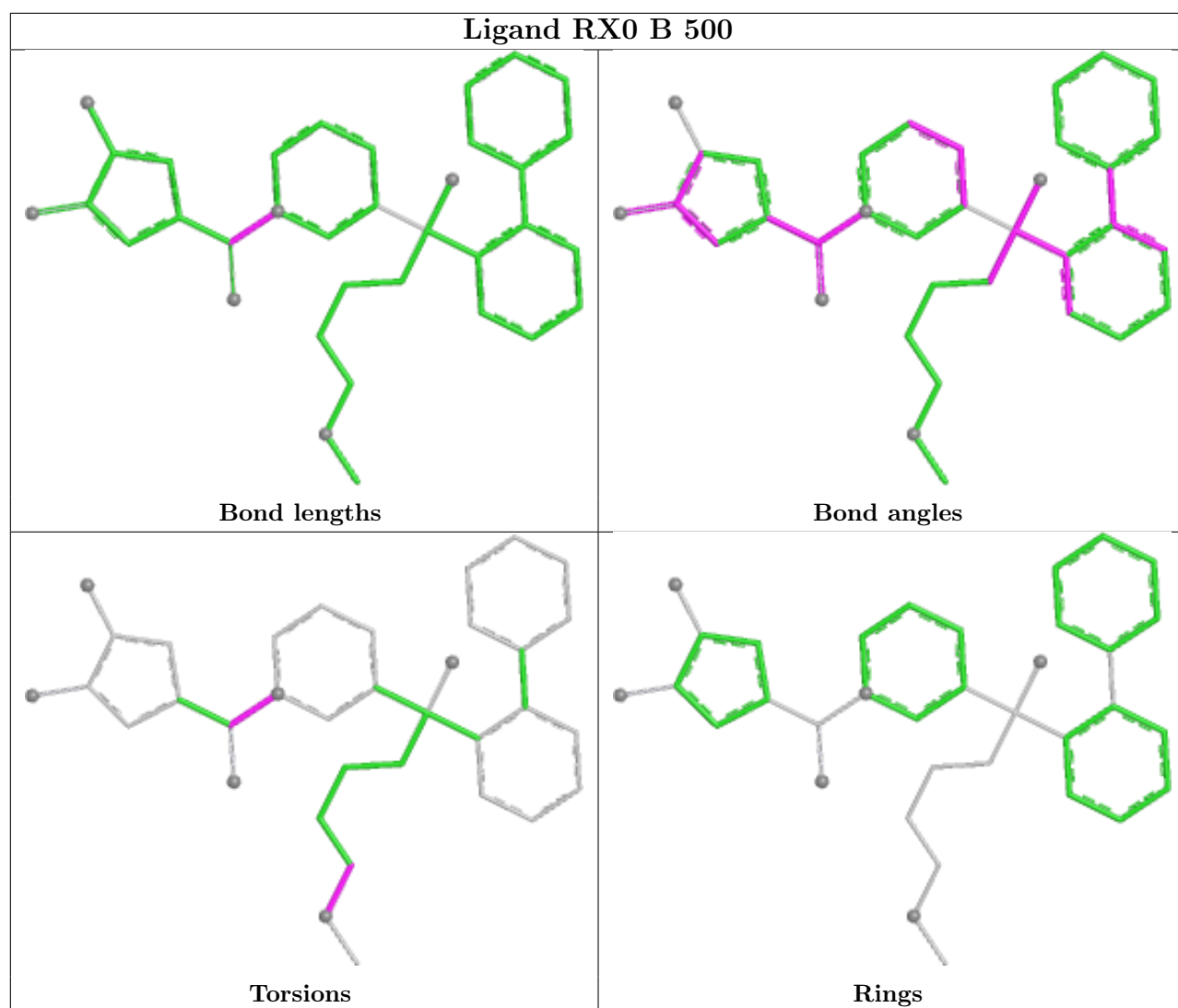
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	RX0	2	0
3	B	500	RX0	2	0
5	B	600	NAG	3	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	337/340 (99%)	-0.18	5 (1%) 72 68	13, 27, 46, 60	0
1	B	333/340 (97%)	-0.01	4 (1%) 76 73	15, 33, 56, 65	0
All	All	670/680 (98%)	-0.10	9 (1%) 75 71	13, 30, 54, 65	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	SER	3.9
1	A	203	THR	3.3
1	B	159	SER	2.9
1	A	-2	GLY	2.9
1	B	52	TYR	2.6
1	B	46	SER	2.4
1	A	195	LYS	2.3
1	B	23	PRO	2.2
1	A	52	TYR	2.0

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.

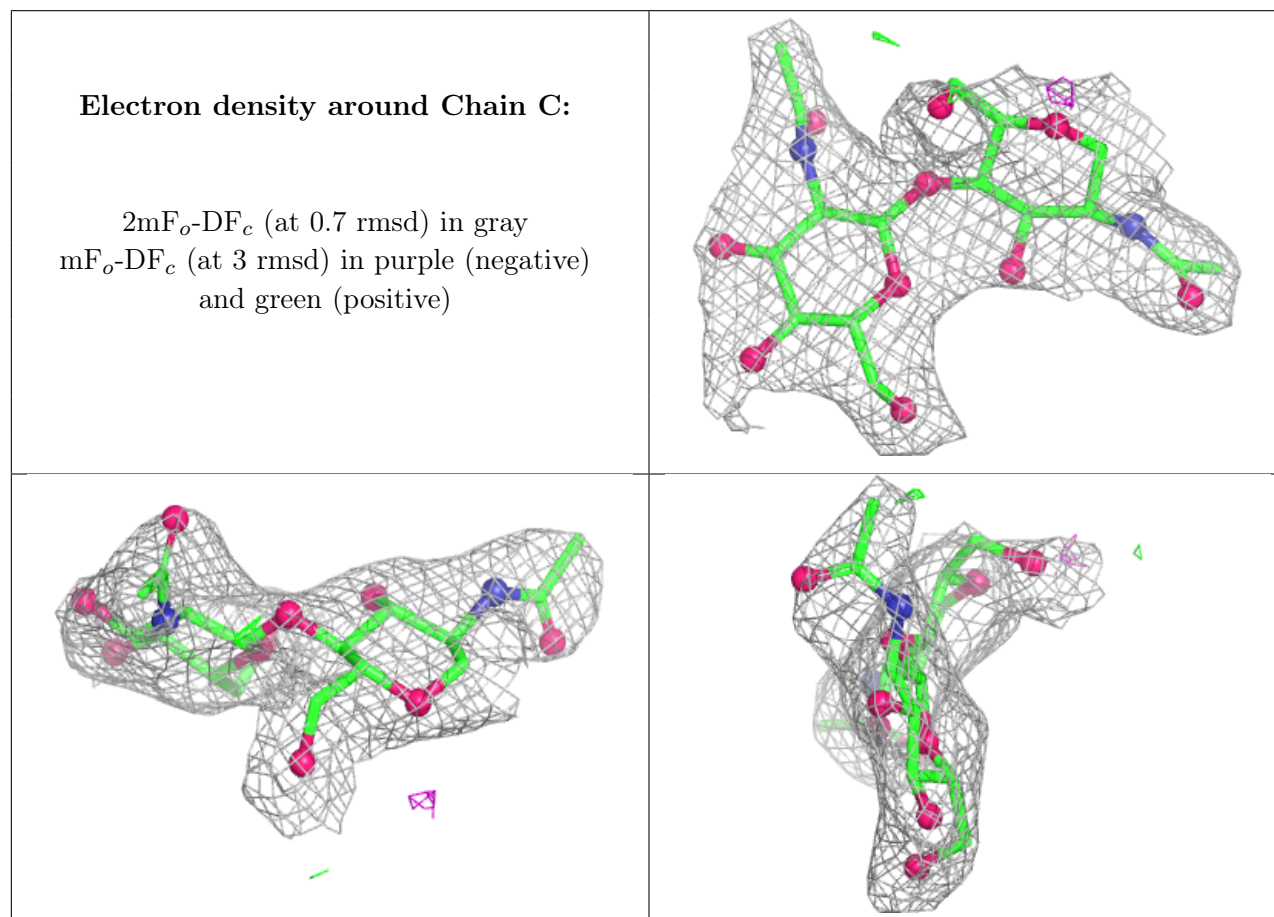
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.71	0.14	66,67,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	1	14/15	0.86	0.13	44,52,56,62	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](#)

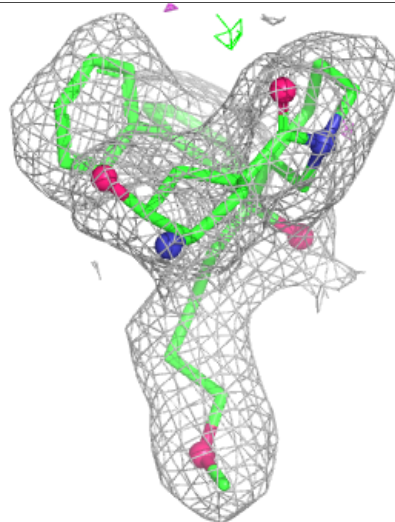
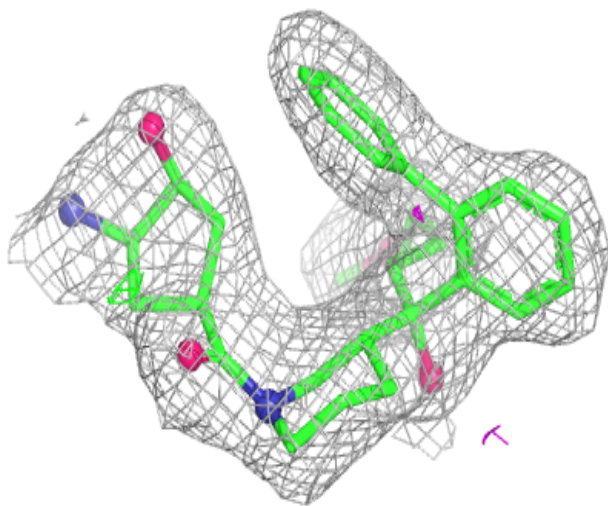
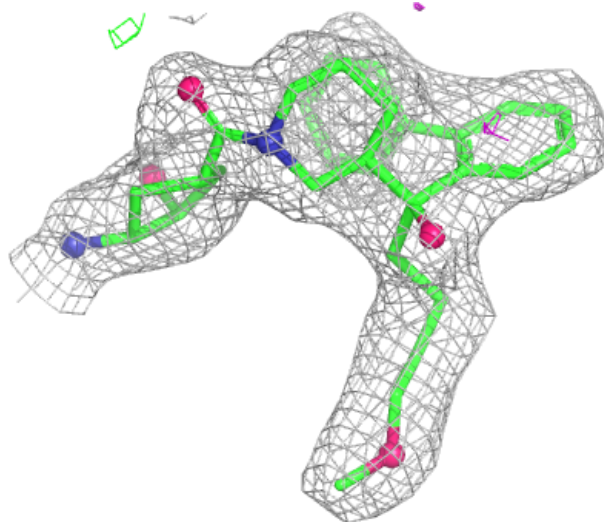
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	600	14/15	0.12	0.31	73,79,80,81	0
4	GOL	A	502	6/6	0.84	0.17	52,53,54,55	0
4	GOL	A	341	6/6	0.88	0.16	44,45,47,47	0
3	RX0	B	500	35/35	0.95	0.07	15,21,25,26	0
3	RX0	A	500	35/35	0.96	0.07	9,18,23,26	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.

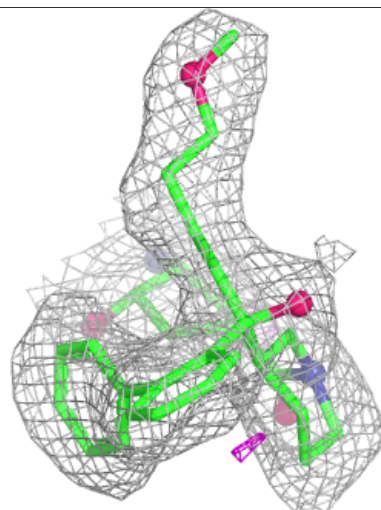
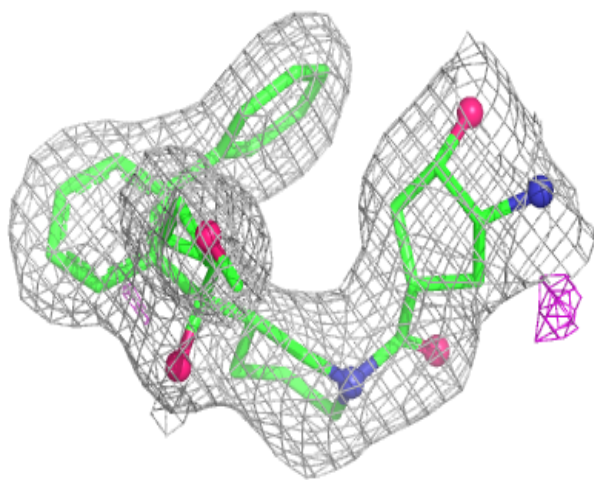
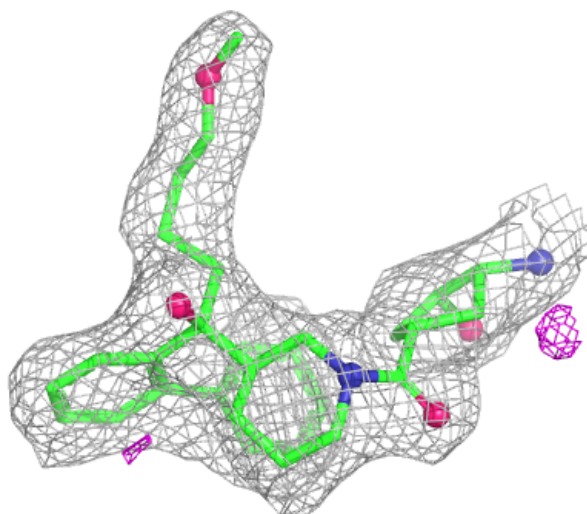
Electron density around RX0 B 500:

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



Electron density around RX0 A 500:

$2mF_o-DF_c$ (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.