



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:49 AM UTC

PDB ID : 2D9Q / pdb_00002d9q
Title : Crystal Structure of the Human GCSF-Receptor Signaling Complex
Authors : Tamada, T.; Kuroki, R.
Deposited on : 2005-12-12
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
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

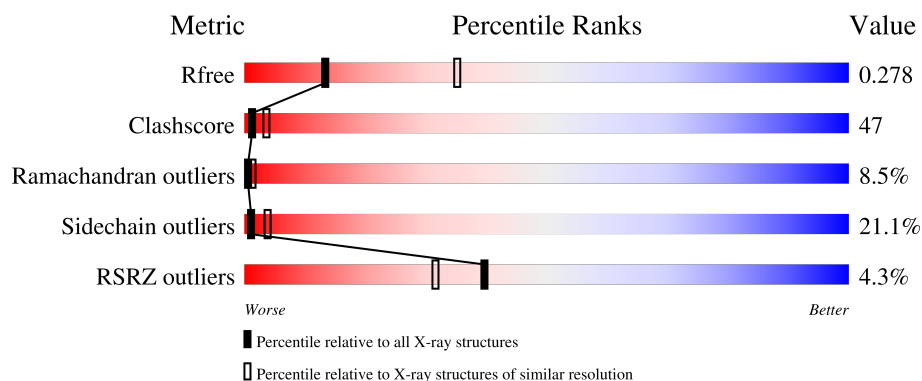
1 Overall quality at a glance

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))
R_{free}	180053	3866 (2.80-2.80)
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	174	3% 22% 46% 22% 6% .
2	B	313	4% 27% 39% 23% 6% .
3	C	2	50% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3647 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 CSF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1274	815	216	235	8			

- Molecule 2 is a protein called Granulocyte colony-stimulating factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2331	1472	410	429	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	SER	CYS	engineered mutation	UNP Q99062
B	164	SER	CYS	engineered mutation	UNP Q99062
B	229	SER	CYS	engineered mutation	UNP Q99062
B	310	ALA	-	cloning artifact	UNP Q99062
B	311	ALA	-	cloning artifact	UNP Q99062
B	312	ALA	-	cloning artifact	UNP Q99062
B	313	PRO	-	cloning artifact	UNP Q99062
B	314	ARG	-	cloning artifact	UNP Q99062

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

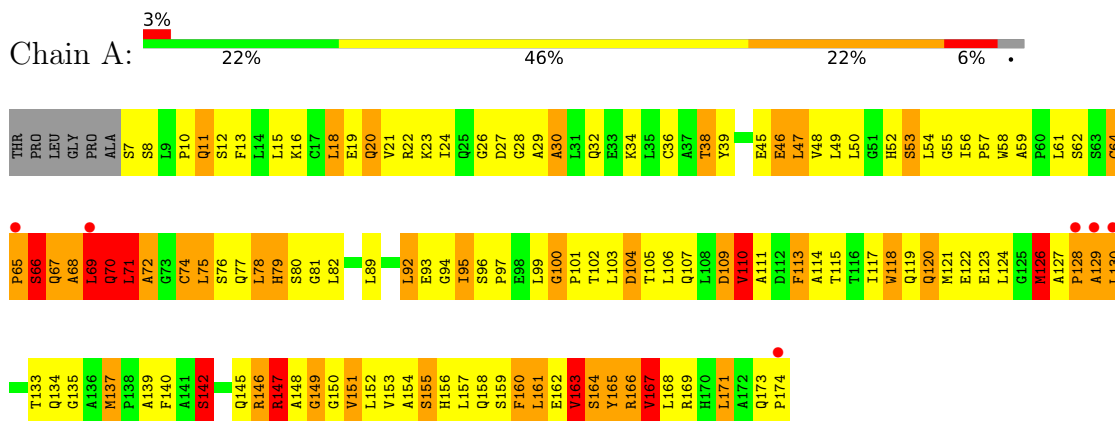
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	O 5	0	0
4	B	9	Total 9	O 9	0	0

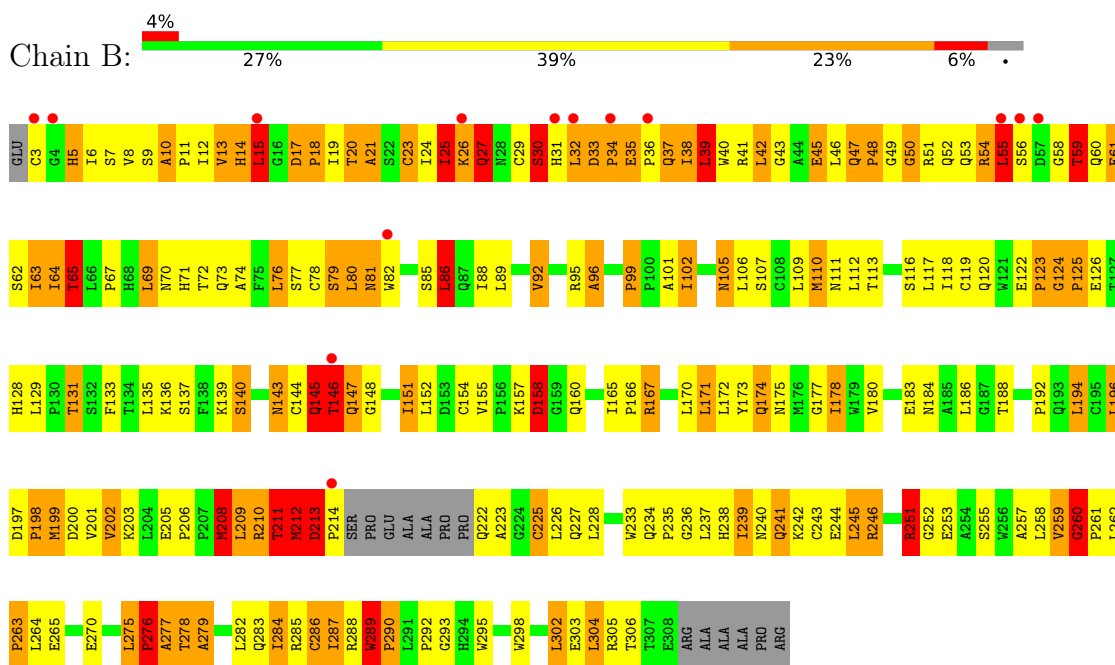
3 Residue-property plots

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: CSF3



• Molecule 2: Granulocyte colony-stimulating factor receptor



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

50%

50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.78Å 134.78Å 105.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (20.00-2.80) 90.9 (20.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.251 , 0.284 0.242 , 0.278	Depositor DCC
R_{free} test set	1266 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.07	40/1302 (3.1%)	1.70	22/1769 (1.2%)
2	B	2.08	61/2396 (2.5%)	1.83	54/3273 (1.6%)
All	All	2.08	101/3698 (2.7%)	1.79	76/5042 (1.5%)

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	208	MET	CG-SD	15.13	2.18	1.80
2	B	212	MET	SD-CE	10.16	2.04	1.79
1	A	69	LEU	CA-C	10.14	1.67	1.53
2	B	146	THR	CA-CB	9.39	1.69	1.53
2	B	202	VAL	CA-CB	-8.84	1.43	1.54
2	B	208	MET	SD-CE	8.54	2.00	1.79
2	B	286	CYS	CA-C	-8.52	1.41	1.52
2	B	92	VAL	CA-CB	-8.51	1.42	1.55
2	B	213	ASP	CA-C	8.26	1.63	1.52
1	A	75	LEU	CA-C	-8.08	1.41	1.52
2	B	122	GLU	CA-C	-8.05	1.46	1.52
2	B	290	PRO	CA-C	7.89	1.64	1.52
2	B	96	ALA	CA-CB	-7.75	1.40	1.53
2	B	199	MET	SD-CE	7.74	1.99	1.79
2	B	118	ILE	C-O	-7.55	1.16	1.24
1	A	70	GLN	CA-C	7.47	1.61	1.52
2	B	261	PRO	CA-C	7.46	1.60	1.52
2	B	278	THR	CA-CB	7.38	1.65	1.53
1	A	110	VAL	CA-CB	-7.37	1.45	1.54
2	B	26	LYS	CA-C	7.33	1.62	1.52
1	A	38	THR	CA-CB	-7.26	1.41	1.53
2	B	208	MET	CB-CG	7.19	1.74	1.52
2	B	120	GLN	C-O	-7.11	1.15	1.23
1	A	133	THR	CA-CB	7.04	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	151	ILE	CA-CB	-7.02	1.46	1.54
2	B	201	VAL	CA-CB	-6.92	1.47	1.54
2	B	237	LEU	CA-C	-6.91	1.42	1.52
2	B	211	THR	CA-CB	-6.86	1.42	1.53
2	B	178	ILE	CA-CB	-6.82	1.45	1.54
2	B	245	LEU	CA-C	-6.78	1.44	1.52
1	A	126	MET	SD-CE	6.76	1.96	1.79
2	B	86	LEU	C-O	-6.73	1.16	1.23
2	B	27	GLN	N-CA	6.72	1.54	1.46
2	B	203	LYS	CA-C	-6.64	1.44	1.52
2	B	110	MET	CA-CB	-6.56	1.43	1.53
1	A	165	TYR	CA-C	-6.52	1.44	1.52
1	A	8	SER	CA-C	6.49	1.61	1.52
2	B	245	LEU	C-O	-6.47	1.16	1.23
2	B	88	ILE	CA-CB	-6.42	1.46	1.54
1	A	147	ARG	NE-CZ	6.42	1.40	1.33
2	B	14	HIS	CA-CB	6.40	1.63	1.53
2	B	113	THR	CA-CB	-6.40	1.43	1.53
2	B	259	VAL	CA-CB	-6.36	1.46	1.54
1	A	137	MET	CG-SD	6.31	1.96	1.80
1	A	173	GLN	CA-C	6.29	1.60	1.52
2	B	106	LEU	C-O	-6.06	1.16	1.23
1	A	161	LEU	CA-C	-6.06	1.44	1.52
1	A	67	GLN	N-CA	6.02	1.53	1.46
2	B	101	ALA	CA-CB	-6.01	1.44	1.53
1	A	59	ALA	CA-C	-5.99	1.46	1.53
2	B	25	ILE	CA-CB	5.98	1.60	1.53
1	A	166	ARG	CB-CG	5.97	1.70	1.52
1	A	115	THR	CA-CB	-5.95	1.43	1.53
1	A	147	ARG	CG-CD	5.95	1.70	1.52
2	B	47	GLN	CA-C	5.92	1.59	1.52
1	A	168	LEU	CA-C	-5.92	1.45	1.52
1	A	20	GLN	C-O	5.92	1.31	1.24
2	B	13	VAL	CA-CB	-5.92	1.46	1.54
1	A	109	ASP	N-CA	-5.90	1.39	1.46
1	A	168	LEU	C-O	-5.87	1.14	1.23
2	B	111	ASN	CA-C	-5.79	1.45	1.52
1	A	47	LEU	CA-C	-5.79	1.45	1.52
2	B	17	ASP	C-O	-5.74	1.18	1.23
1	A	113	PHE	CA-C	-5.73	1.45	1.52
2	B	286	CYS	C-O	-5.66	1.16	1.23
2	B	178	ILE	C-O	-5.65	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241	GLN	C-O	-5.65	1.16	1.23
1	A	146	ARG	C-O	-5.64	1.17	1.24
2	B	251	ARG	N-CA	5.62	1.52	1.45
1	A	36	CYS	N-CA	-5.58	1.39	1.46
1	A	167	VAL	C-O	-5.57	1.17	1.24
2	B	178	ILE	N-CA	-5.57	1.39	1.46
2	B	209	LEU	CA-C	-5.56	1.45	1.52
2	B	140	SER	CA-C	-5.49	1.47	1.53
1	A	163	VAL	CA-CB	-5.44	1.47	1.54
1	A	71	LEU	N-CA	5.43	1.53	1.46
2	B	18	PRO	CA-C	-5.42	1.46	1.52
2	B	192	PRO	C-O	-5.41	1.17	1.23
2	B	194	LEU	C-O	5.37	1.30	1.23
1	A	59	ALA	CA-CB	-5.37	1.42	1.53
2	B	305	ARG	NE-CZ	5.36	1.39	1.33
1	A	11	GLN	CA-C	5.35	1.59	1.52
1	A	166	ARG	NE-CZ	5.34	1.39	1.33
1	A	32	GLN	C-O	-5.32	1.18	1.24
2	B	92	VAL	N-CA	-5.32	1.40	1.46
2	B	33	ASP	CA-C	5.29	1.59	1.53
1	A	30	ALA	CA-CB	-5.28	1.45	1.53
2	B	211	THR	CA-C	-5.28	1.45	1.53
1	A	66	SER	C-O	5.26	1.30	1.24
2	B	15	LEU	CA-CB	5.25	1.62	1.53
2	B	88	ILE	N-CA	-5.22	1.39	1.46
1	A	69	LEU	CA-CB	5.17	1.60	1.53
2	B	14	HIS	CB-CG	5.17	1.57	1.50
2	B	180	VAL	CA-CB	5.17	1.60	1.54
1	A	146	ARG	CA-CB	-5.07	1.45	1.53
1	A	66	SER	CA-C	5.04	1.59	1.52
1	A	118	TRP	C-O	-5.03	1.17	1.24
2	B	287	ILE	CA-C	-5.03	1.46	1.52
2	B	213	ASP	N-CA	5.02	1.53	1.46
1	A	153	VAL	CA-CB	-5.02	1.48	1.54
2	B	263	PRO	CA-C	5.01	1.57	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	155	VAL	CB-CA-C	-9.27	100.70	110.53
2	B	290	PRO	N-CD-CG	-8.83	89.95	103.20
2	B	145	GLN	N-CA-C	-8.33	101.89	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	GLY	N-CA-C	-8.27	101.41	112.82
2	B	55	LEU	N-CA-C	-8.11	103.53	113.50
2	B	123	PRO	N-CD-CG	-8.06	91.11	103.20
2	B	155	VAL	N-CA-C	7.86	117.32	108.05
2	B	50	GLY	CA-C-O	-7.43	114.87	121.41
2	B	102	ILE	N-CA-C	-7.42	101.68	108.95
2	B	259	VAL	N-CA-C	7.34	118.45	108.17
1	A	168	LEU	N-CA-C	-7.18	104.38	113.43
2	B	252	GLY	N-CA-C	-7.16	103.66	112.68
2	B	225	CYS	N-CA-C	7.15	120.27	109.41
1	A	75	LEU	N-CA-C	-6.83	103.07	111.33
2	B	61	GLU	N-CA-C	6.81	119.12	110.33
2	B	17	ASP	CB-CA-C	-6.72	99.87	109.96
2	B	253	GLU	N-CA-C	-6.64	96.21	108.24
2	B	259	VAL	CB-CA-C	-6.64	100.93	110.83
2	B	260	GLY	CA-C-O	-6.58	112.11	121.52
1	A	36	CYS	O-C-N	-6.50	115.22	122.12
2	B	99	PRO	N-CA-C	-6.44	102.84	110.70
2	B	208	MET	CB-CG-SD	6.43	131.99	112.70
2	B	102	ILE	N-CA-CB	-6.40	104.13	110.08
1	A	169	ARG	N-CA-C	-6.39	104.40	111.82
1	A	151	VAL	CB-CA-C	-6.26	99.84	111.79
2	B	131	THR	N-CA-C	6.25	118.58	108.34
1	A	70	GLN	CA-C-N	6.15	133.28	121.54
1	A	70	GLN	C-N-CA	6.15	133.28	121.54
2	B	39	LEU	N-CA-C	6.13	118.94	109.07
1	A	32	GLN	N-CA-C	-6.11	104.54	111.14
2	B	14	HIS	N-CA-C	-6.09	102.49	110.53
2	B	206	PRO	O-C-N	6.02	123.98	121.15
1	A	20	GLN	CA-C-N	-5.98	113.22	120.70
1	A	20	GLN	C-N-CA	-5.98	113.22	120.70
2	B	192	PRO	N-CD-CG	-5.98	94.24	103.20
2	B	239	ILE	CB-CA-C	-5.85	103.74	110.41
2	B	146	THR	CB-CA-C	5.83	122.01	110.42
1	A	162	GLU	N-CA-C	-5.82	105.02	111.71
1	A	142	SER	N-CA-C	5.82	118.21	110.53
2	B	33	ASP	CA-C-N	5.82	127.11	119.84
2	B	33	ASP	C-N-CA	5.82	127.11	119.84
2	B	23	CYS	N-CA-C	5.79	118.24	107.99
1	A	36	CYS	CA-C-N	-5.78	110.88	121.52
1	A	36	CYS	C-N-CA	-5.78	110.88	121.52
2	B	118	ILE	CG1-CB-CG2	-5.74	93.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	VAL	CB-CA-C	-5.73	103.05	110.84
1	A	38	THR	N-CA-CB	-5.69	102.22	110.47
2	B	21	ALA	N-CA-C	5.68	117.83	109.24
2	B	13	VAL	CB-CA-C	-5.62	102.07	111.29
1	A	129	ALA	N-CA-C	-5.61	105.31	111.82
2	B	293	GLY	CA-C-O	-5.60	116.13	121.62
2	B	240	ASN	N-CA-CB	5.51	118.63	109.60
1	A	165	TYR	CB-CA-C	-5.50	102.18	110.92
2	B	276	PRO	CA-C-N	5.49	132.02	121.54
2	B	276	PRO	C-N-CA	5.49	132.02	121.54
2	B	259	VAL	CA-C-N	5.46	130.44	121.87
2	B	259	VAL	C-N-CA	5.46	130.44	121.87
2	B	290	PRO	CA-C-O	5.36	127.70	119.55
2	B	65	THR	CA-C-O	5.33	126.09	120.33
1	A	70	GLN	N-CA-C	5.26	116.99	108.41
2	B	15	LEU	O-C-N	5.24	129.55	122.59
2	B	39	LEU	CA-C-O	5.22	126.07	120.38
2	B	3	CYS	CA-CB-SG	-5.18	102.48	114.40
2	B	92	VAL	CA-C-N	-5.17	115.58	122.72
2	B	92	VAL	C-N-CA	-5.17	115.58	122.72
2	B	289	TRP	N-CA-CB	5.13	119.50	110.37
1	A	38	THR	N-CA-C	5.12	119.16	113.02
2	B	14	HIS	CA-C-O	5.11	127.79	121.87
1	A	69	LEU	CB-CA-C	5.07	122.06	111.97
2	B	10	ALA	CA-C-N	5.07	124.56	119.19
2	B	10	ALA	C-N-CA	5.07	124.56	119.19
2	B	18	PRO	N-CA-C	5.07	119.27	111.57
2	B	148	GLY	CA-C-N	-5.05	113.11	122.60
2	B	148	GLY	C-N-CA	-5.05	113.11	122.60
1	A	46	GLU	CA-C-N	-5.03	114.59	122.49
1	A	46	GLU	C-N-CA	-5.03	114.59	122.49

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	1274	0	1283	139	0
2	B	2331	0	2287	203	0
3	C	28	0	25	1	0
4	A	5	0	0	1	0
4	B	9	0	0	1	0
All	All	3647	0	3595	339	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 47.

All (339) 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)
2:B:212:MET:SD	2:B:212:MET:CE	2.05	1.45
2:B:208:MET:SD	2:B:208:MET:CG	2.18	1.31
2:B:276:PRO:O	2:B:278:THR:HG23	1.03	1.16
1:A:7:SER:HB2	1:A:174:PRO:HG2	1.25	1.12
2:B:276:PRO:O	2:B:278:THR:CG2	1.99	1.09
2:B:63:ILE:C	2:B:63:ILE:HD12	1.88	0.98
2:B:143:ASN:H	2:B:143:ASN:HD22	1.12	0.95
1:A:71:LEU:O	1:A:72:ALA:O	1.86	0.93
1:A:45:GLU:O	1:A:48:VAL:HG23	1.71	0.90
2:B:259:VAL:O	2:B:260:GLY:O	1.88	0.88
1:A:7:SER:CB	1:A:174:PRO:HG2	2.03	0.87
2:B:205:GLU:HB2	2:B:233:TRP:CE2	2.10	0.86
2:B:25:ILE:HG21	2:B:38:ILE:HG21	1.57	0.86
2:B:246:ARG:HG2	2:B:298:TRP:CZ3	2.12	0.84
1:A:38:THR:HG22	1:A:38:THR:O	1.76	0.84
1:A:71:LEU:O	1:A:74:CYS:HB3	1.76	0.83
2:B:183:GLU:HB3	2:B:188:THR:HG23	1.61	0.83
2:B:33:ASP:O	2:B:35:GLU:N	2.12	0.82
1:A:93:GLU:HB2	1:A:146:ARG:NH1	1.95	0.81
2:B:86:LEU:N	2:B:86:LEU:HD12	1.96	0.81
2:B:264:LEU:C	2:B:264:LEU:HD12	2.07	0.80
2:B:86:LEU:HD12	2:B:86:LEU:H	1.47	0.80
1:A:120:GLN:OE1	1:A:120:GLN:HA	1.83	0.79
2:B:23:CYS:HB2	2:B:40:TRP:CH2	2.18	0.79
2:B:212:MET:HA	2:B:212:MET:HE3	1.64	0.78
2:B:19:ILE:CD1	2:B:69:LEU:HD12	2.14	0.78
1:A:72:ALA:HB2	1:A:126:MET:SD	2.23	0.78
1:A:7:SER:HB2	1:A:174:PRO:CG	2.12	0.76
2:B:27:GLN:HG2	2:B:34:PRO:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ILE:HD11	2:B:69:LEU:HD12	1.67	0.76
1:A:159:SER:O	1:A:161:LEU:N	2.19	0.75
2:B:23:CYS:HB2	2:B:40:TRP:CZ2	2.22	0.74
2:B:39:LEU:HD23	2:B:39:LEU:N	2.02	0.74
2:B:275:LEU:C	2:B:277:ALA:H	1.92	0.74
1:A:20:GLN:NE2	4:A:176:HOH:O	2.19	0.74
2:B:199:MET:HE3	2:B:202:VAL:HG21	1.70	0.73
2:B:39:LEU:HB2	2:B:46:LEU:HD21	1.70	0.73
2:B:302:LEU:HD22	2:B:304:LEU:HD22	1.69	0.73
1:A:71:LEU:C	1:A:72:ALA:O	2.30	0.73
2:B:143:ASN:H	2:B:143:ASN:ND2	1.83	0.73
2:B:19:ILE:HA	4:B:405:HOH:O	1.87	0.73
1:A:79:HIS:ND1	1:A:79:HIS:C	2.47	0.72
2:B:278:THR:O	2:B:279:ALA:HB2	1.89	0.72
2:B:37:GLN:HA	2:B:52:GLN:HE21	1.54	0.72
1:A:38:THR:O	1:A:38:THR:CG2	2.37	0.72
2:B:80:LEU:HD13	2:B:89:LEU:HD11	1.71	0.71
1:A:81:GLY:O	1:A:82:LEU:C	2.32	0.71
2:B:226:LEU:HD21	2:B:304:LEU:HG	1.73	0.70
1:A:159:SER:O	1:A:160:PHE:C	2.33	0.70
2:B:137:SER:HA	2:B:177:GLY:O	1.91	0.69
1:A:82:LEU:H	1:A:82:LEU:HD22	1.57	0.69
2:B:37:GLN:HG3	2:B:52:GLN:HG3	1.74	0.69
1:A:78:LEU:O	1:A:79:HIS:C	2.36	0.68
2:B:285:ARG:HD3	2:B:298:TRP:CE2	2.29	0.68
2:B:63:ILE:C	2:B:63:ILE:CD1	2.62	0.67
2:B:184:ASN:OD1	2:B:184:ASN:C	2.37	0.67
2:B:26:LYS:HA	2:B:59:THR:HG22	1.76	0.67
2:B:37:GLN:HA	2:B:52:GLN:NE2	2.09	0.67
2:B:222:GLN:HG2	2:B:223:ALA:H	1.58	0.67
1:A:171:LEU:HD23	1:A:171:LEU:O	1.95	0.66
2:B:55:LEU:HD13	2:B:58:GLY:HA3	1.77	0.66
1:A:12:SER:OG	1:A:13:PHE:N	2.28	0.66
2:B:212:MET:HG2	2:B:227:GLN:HE21	1.60	0.65
2:B:289:TRP:HB3	2:B:290:PRO:HD3	1.78	0.65
1:A:38:THR:HG22	1:A:39:TYR:CE2	2.31	0.65
1:A:130:LEU:HD22	1:A:130:LEU:N	2.11	0.65
1:A:47:LEU:HD22	1:A:148:ALA:HB1	1.79	0.65
1:A:159:SER:C	1:A:161:LEU:N	2.55	0.65
2:B:41:ARG:HG2	2:B:45:GLU:C	2.22	0.64
2:B:251:ARG:NH1	2:B:279:ALA:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:HIS:O	2:B:129:LEU:HG	1.97	0.64
1:A:34:LYS:O	1:A:99:LEU:HD21	1.98	0.64
2:B:277:ALA:O	2:B:278:THR:C	2.41	0.63
1:A:137:MET:HE2	1:A:137:MET:HA	1.79	0.63
1:A:99:LEU:C	1:A:101:PRO:HD2	2.23	0.63
2:B:259:VAL:C	2:B:260:GLY:O	2.42	0.63
1:A:71:LEU:O	1:A:72:ALA:C	2.42	0.62
2:B:239:ILE:HG23	2:B:288:ARG:HG3	1.81	0.62
2:B:80:LEU:C	2:B:80:LEU:HD23	2.25	0.62
2:B:143:ASN:HD22	2:B:143:ASN:N	1.90	0.61
2:B:275:LEU:C	2:B:277:ALA:N	2.56	0.61
2:B:211:THR:HG22	2:B:212:MET:H	1.64	0.61
2:B:8:VAL:HG12	2:B:21:ALA:HB2	1.82	0.60
2:B:14:HIS:HB3	2:B:15:LEU:HG	1.84	0.60
2:B:64:ILE:HD12	2:B:65:THR:H	1.67	0.60
1:A:95:ILE:HG21	1:A:99:LEU:HD12	1.83	0.60
1:A:20:GLN:O	1:A:24:ILE:HG13	2.00	0.60
2:B:145:GLN:O	2:B:147:GLN:N	2.34	0.60
2:B:212:MET:CE	2:B:212:MET:HA	2.32	0.60
2:B:287:ILE:O	2:B:287:ILE:HG23	2.02	0.59
1:A:82:LEU:HD22	1:A:82:LEU:N	2.16	0.59
1:A:10:PRO:O	1:A:11:GLN:C	2.41	0.59
1:A:167:VAL:HG12	1:A:167:VAL:O	2.03	0.59
2:B:63:ILE:HD12	2:B:63:ILE:O	2.02	0.59
1:A:61:LEU:HD23	1:A:163:VAL:CG1	2.33	0.59
2:B:6:ILE:HD11	2:B:78:CYS:CB	2.34	0.58
2:B:80:LEU:HD23	2:B:81:ASN:N	2.18	0.58
1:A:13:PHE:C	1:A:13:PHE:CD2	2.81	0.58
2:B:278:THR:HA	2:B:306:THR:H	1.67	0.58
1:A:93:GLU:C	1:A:95:ILE:H	2.12	0.58
1:A:99:LEU:O	1:A:101:PRO:HD2	2.03	0.58
1:A:16:LYS:O	1:A:20:GLN:HG3	2.04	0.58
1:A:69:LEU:O	1:A:70:GLN:OE1	2.21	0.58
1:A:92:LEU:HD11	1:A:150:GLY:HA2	1.85	0.58
2:B:233:TRP:CD2	2:B:235:PRO:HG2	2.39	0.58
2:B:233:TRP:CE2	2:B:235:PRO:HG2	2.39	0.57
2:B:6:ILE:HD11	2:B:78:CYS:HB2	1.85	0.57
1:A:34:LYS:HG2	1:A:99:LEU:HD23	1.86	0.57
2:B:26:LYS:HD3	2:B:59:THR:HG23	1.86	0.57
1:A:39:TYR:CE1	1:A:147:ARG:HD2	2.39	0.57
1:A:119:GLN:O	1:A:120:GLN:C	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:C	1:A:161:LEU:H	2.13	0.57
2:B:41:ARG:HG2	2:B:45:GLU:O	2.04	0.57
1:A:34:LYS:O	1:A:34:LYS:HG3	2.05	0.56
1:A:99:LEU:O	1:A:101:PRO:CD	2.53	0.56
1:A:52:HIS:O	1:A:54:LEU:N	2.38	0.56
2:B:17:ASP:HB3	2:B:18:PRO:HD2	1.86	0.56
2:B:304:LEU:N	2:B:304:LEU:HD23	2.21	0.56
1:A:77:GLN:O	1:A:78:LEU:O	2.24	0.56
1:A:64:CYS:O	1:A:66:SER:N	2.39	0.56
2:B:80:LEU:HD13	2:B:89:LEU:CD1	2.36	0.55
2:B:26:LYS:CD	2:B:59:THR:HG23	2.36	0.55
2:B:116:SER:HB2	2:B:166:PRO:HA	1.87	0.55
2:B:278:THR:O	2:B:279:ALA:CB	2.55	0.55
2:B:173:TYR:O	2:B:174:GLN:OE1	2.25	0.55
2:B:173:TYR:CE1	2:B:199:MET:HG2	2.42	0.54
1:A:23:LYS:HB2	2:B:238:HIS:ND1	2.22	0.54
2:B:12:ILE:C	2:B:13:VAL:HG13	2.32	0.54
2:B:196:LEU:C	2:B:196:LEU:HD12	2.33	0.54
2:B:197:ASP:O	2:B:199:MET:N	2.41	0.54
2:B:24:ILE:O	2:B:24:ILE:HG22	2.08	0.54
1:A:124:LEU:O	1:A:126:MET:HE3	2.08	0.54
2:B:6:ILE:HD13	2:B:76:LEU:CD1	2.37	0.54
2:B:20:THR:OG1	2:B:65:THR:OG1	2.26	0.54
1:A:99:LEU:O	1:A:101:PRO:N	2.41	0.54
1:A:148:ALA:C	1:A:150:GLY:N	2.66	0.54
2:B:157:LYS:HB2	2:B:160:GLN:NE2	2.23	0.54
2:B:284:ILE:HG12	2:B:285:ARG:N	2.22	0.54
1:A:56:ILE:HD12	1:A:152:LEU:HD23	1.90	0.54
1:A:151:VAL:HG12	1:A:151:VAL:O	2.07	0.53
2:B:41:ARG:HH21	2:B:79:SER:CB	2.22	0.53
2:B:262:LEU:HB3	2:B:263:PRO:HD2	1.90	0.53
1:A:56:ILE:HG21	1:A:58:TRP:CH2	2.43	0.53
1:A:93:GLU:C	1:A:95:ILE:N	2.65	0.53
2:B:197:ASP:C	2:B:199:MET:N	2.65	0.53
2:B:275:LEU:H	2:B:275:LEU:HD23	1.74	0.53
1:A:13:PHE:CE1	1:A:120:GLN:HB2	2.44	0.53
2:B:72:THR:HA	2:B:96:ALA:O	2.09	0.53
1:A:19:GLU:HA	1:A:22:ARG:NH2	2.24	0.53
2:B:54:ARG:NE	2:B:60:GLN:NE2	2.57	0.53
2:B:239:ILE:CG2	2:B:288:ARG:HG3	2.38	0.53
2:B:209:LEU:C	2:B:210:ARG:HG3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:HG22	1:A:96:SER:N	2.22	0.52
1:A:134:GLN:HG3	1:A:135:GLY:H	1.74	0.52
1:A:61:LEU:HD23	1:A:163:VAL:HG12	1.91	0.52
2:B:19:ILE:HD12	2:B:69:LEU:HD12	1.89	0.52
1:A:45:GLU:O	1:A:47:LEU:N	2.43	0.52
2:B:123:PRO:HB3	2:B:133:PHE:CE2	2.43	0.52
2:B:275:LEU:O	2:B:277:ALA:N	2.43	0.52
1:A:50:LEU:HD13	1:A:54:LEU:HD12	1.92	0.52
1:A:148:ALA:O	1:A:149:GLY:C	2.53	0.52
1:A:38:THR:O	1:A:39:TYR:CG	2.63	0.52
2:B:172:LEU:HD22	2:B:199:MET:SD	2.50	0.52
1:A:130:LEU:HD22	1:A:130:LEU:H	1.72	0.51
2:B:38:ILE:HD11	2:B:62:SER:CB	2.40	0.51
2:B:107:SER:O	2:B:119:CYS:HA	2.10	0.51
2:B:109:LEU:O	2:B:117:LEU:HD12	2.10	0.51
2:B:110:MET:HB3	2:B:202:VAL:HA	1.93	0.51
2:B:285:ARG:HD3	2:B:298:TRP:CZ2	2.46	0.51
1:A:24:ILE:CD1	1:A:110:VAL:HA	2.41	0.51
1:A:20:GLN:NE2	1:A:113:PHE:HA	2.26	0.50
2:B:63:ILE:HD12	2:B:64:ILE:N	2.26	0.50
2:B:139:LYS:HD2	2:B:171:LEU:HB2	1.91	0.50
2:B:234:GLN:N	2:B:235:PRO:HD2	2.27	0.50
1:A:167:VAL:O	1:A:171:LEU:HB2	2.11	0.50
2:B:157:LYS:O	2:B:158:ASP:C	2.55	0.50
1:A:93:GLU:O	1:A:95:ILE:N	2.45	0.50
2:B:60:GLN:O	2:B:60:GLN:HG2	2.12	0.50
1:A:82:LEU:H	1:A:82:LEU:CD2	2.24	0.50
2:B:33:ASP:O	2:B:35:GLU:HG3	2.12	0.50
2:B:245:LEU:HD12	2:B:246:ARG:H	1.76	0.50
1:A:154:ALA:O	1:A:158:GLN:HB2	2.10	0.50
2:B:38:ILE:HD11	2:B:62:SER:HB3	1.92	0.50
1:A:72:ALA:C	1:A:74:CYS:H	2.19	0.49
1:A:64:CYS:O	1:A:65:PRO:C	2.56	0.49
2:B:80:LEU:HD22	2:B:89:LEU:HD11	1.94	0.49
2:B:49:GLY:O	2:B:50:GLY:C	2.54	0.49
1:A:45:GLU:C	1:A:47:LEU:H	2.21	0.49
2:B:29:CYS:O	2:B:30:SER:CB	2.58	0.49
2:B:197:ASP:O	2:B:198:PRO:C	2.54	0.49
2:B:226:LEU:CD2	2:B:304:LEU:HG	2.41	0.49
2:B:200:ASP:HB3	2:B:292:PRO:HB2	1.94	0.49
2:B:239:ILE:O	2:B:239:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HD23	2:B:303:GLU:N	2.28	0.48
2:B:288:ARG:HD3	2:B:292:PRO:O	2.13	0.48
1:A:52:HIS:O	1:A:53:SER:C	2.56	0.48
2:B:226:LEU:O	2:B:270:GLU:HA	2.13	0.48
1:A:38:THR:CG2	1:A:39:TYR:CE2	2.96	0.48
1:A:100:GLY:O	1:A:104:ASP:HB2	2.13	0.48
2:B:86:LEU:N	2:B:86:LEU:CD1	2.69	0.48
2:B:234:GLN:HB2	2:B:235:PRO:CD	2.43	0.48
2:B:276:PRO:C	2:B:278:THR:N	2.71	0.48
2:B:27:GLN:NE2	2:B:33:ASP:HB3	2.29	0.48
1:A:55:GLY:O	1:A:57:PRO:HD3	2.14	0.48
2:B:39:LEU:HD23	2:B:39:LEU:H	1.77	0.48
1:A:27:ASP:OD1	1:A:109:ASP:OD2	2.31	0.47
1:A:38:THR:HG22	1:A:39:TYR:CZ	2.49	0.47
1:A:50:LEU:HD13	1:A:54:LEU:CD1	2.44	0.47
1:A:156:HIS:O	1:A:157:LEU:C	2.58	0.47
1:A:24:ILE:HD13	1:A:110:VAL:CG2	2.44	0.47
2:B:304:LEU:N	2:B:304:LEU:CD2	2.77	0.47
1:A:13:PHE:CE1	1:A:120:GLN:CB	2.98	0.47
1:A:52:HIS:C	1:A:54:LEU:N	2.71	0.47
1:A:106:LEU:O	1:A:107:GLN:C	2.56	0.47
2:B:42:LEU:HD13	2:B:74:ALA:HB1	1.97	0.47
2:B:175:ASN:HA	2:B:196:LEU:O	2.15	0.47
2:B:246:ARG:NH1	2:B:283:GLN:OE1	2.44	0.47
1:A:123:GLU:O	1:A:124:LEU:HD22	2.15	0.47
1:A:163:VAL:HG12	1:A:164:SER:N	2.28	0.47
2:B:6:ILE:HG22	2:B:7:SER:N	2.30	0.47
2:B:242:LYS:HE3	2:B:289:TRP:NE1	2.30	0.47
2:B:245:LEU:HD12	2:B:246:ARG:N	2.29	0.47
2:B:146:THR:O	2:B:147:GLN:C	2.57	0.47
2:B:209:LEU:O	2:B:210:ARG:HG3	2.14	0.47
1:A:119:GLN:O	1:A:122:GLU:N	2.48	0.47
1:A:68:ALA:C	1:A:69:LEU:HG	2.40	0.46
1:A:77:GLN:O	1:A:78:LEU:C	2.59	0.46
2:B:6:ILE:HD13	2:B:76:LEU:HD13	1.96	0.46
2:B:55:LEU:O	2:B:55:LEU:HD23	2.15	0.46
2:B:205:GLU:HB2	2:B:233:TRP:CD2	2.51	0.46
1:A:24:ILE:HD13	1:A:110:VAL:HA	1.96	0.46
1:A:164:SER:O	1:A:165:TYR:C	2.49	0.46
1:A:21:VAL:O	1:A:22:ARG:C	2.58	0.46
2:B:12:ILE:C	2:B:13:VAL:CG1	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:O	2:B:172:LEU:C	2.56	0.46
2:B:264:LEU:HD12	2:B:265:GLU:N	2.31	0.46
1:A:13:PHE:CE1	1:A:120:GLN:HG2	2.51	0.46
1:A:29:ALA:O	1:A:30:ALA:C	2.56	0.45
1:A:117:ILE:O	1:A:118:TRP:C	2.60	0.45
2:B:197:ASP:C	2:B:199:MET:H	2.23	0.45
1:A:130:LEU:N	1:A:130:LEU:CD2	2.77	0.45
2:B:126:GLU:HG3	2:B:128:HIS:H	1.81	0.45
2:B:276:PRO:C	2:B:278:THR:H	2.24	0.45
1:A:145:GLN:O	1:A:149:GLY:N	2.44	0.45
2:B:131:THR:HB	2:B:184:ASN:HB3	1.98	0.45
2:B:55:LEU:CD1	2:B:58:GLY:HA3	2.46	0.45
2:B:233:TRP:O	2:B:234:GLN:C	2.60	0.45
2:B:173:TYR:CZ	2:B:199:MET:HG2	2.52	0.45
2:B:245:LEU:HD12	2:B:283:GLN:O	2.17	0.45
1:A:18:LEU:HB3	1:A:22:ARG:HH12	1.82	0.45
2:B:41:ARG:HA	2:B:45:GLU:O	2.15	0.45
1:A:61:LEU:HD23	1:A:163:VAL:HG11	1.97	0.44
1:A:119:GLN:O	1:A:121:MET:N	2.50	0.44
2:B:133:PHE:CD1	2:B:133:PHE:N	2.82	0.44
1:A:74:CYS:C	1:A:76:SER:N	2.67	0.44
2:B:119:CYS:HB2	2:B:135:LEU:CD2	2.48	0.44
2:B:205:GLU:OE1	3:C:1:NAG:H81	2.18	0.44
2:B:242:LYS:HE3	2:B:289:TRP:CD1	2.53	0.44
1:A:93:GLU:HB2	1:A:146:ARG:HH11	1.75	0.44
2:B:82:TRP:O	2:B:85:SER:OG	2.36	0.44
2:B:287:ILE:O	2:B:287:ILE:CG2	2.64	0.44
2:B:196:LEU:C	2:B:196:LEU:CD1	2.90	0.44
1:A:167:VAL:O	1:A:167:VAL:CG1	2.63	0.44
2:B:25:ILE:HG21	2:B:38:ILE:CG2	2.40	0.44
2:B:32:LEU:HB3	2:B:36:PRO:HG3	2.00	0.44
2:B:178:ILE:HD13	2:B:178:ILE:HG21	1.68	0.44
1:A:52:HIS:C	1:A:54:LEU:H	2.26	0.43
2:B:99:PRO:HB3	2:B:186:LEU:HB3	2.00	0.43
2:B:105:ASN:N	2:B:105:ASN:HD22	2.16	0.43
1:A:94:GLY:HA2	1:A:103:LEU:HD23	2.00	0.43
2:B:123:PRO:HB3	2:B:133:PHE:CZ	2.52	0.43
2:B:213:ASP:HB2	2:B:214:PRO:HD3	1.98	0.43
2:B:241:GLN:HE21	2:B:286:CYS:HB3	1.83	0.43
1:A:151:VAL:O	1:A:155:SER:HB3	2.18	0.43
1:A:19:GLU:OE1	2:B:173:TYR:OH	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ILE:O	2:B:38:ILE:CG1	2.67	0.43
1:A:78:LEU:O	1:A:80:SER:N	2.52	0.43
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.77	0.43
2:B:124:GLY:O	2:B:125:PRO:C	2.60	0.43
2:B:47:GLN:O	2:B:48:PRO:O	2.37	0.43
2:B:275:LEU:HD23	2:B:275:LEU:N	2.34	0.43
2:B:17:ASP:HB3	2:B:18:PRO:CD	2.45	0.43
2:B:167:ARG:NH1	2:B:172:LEU:CD1	2.81	0.43
2:B:19:ILE:HD11	2:B:69:LEU:CD1	2.42	0.43
2:B:86:LEU:H	2:B:86:LEU:CD1	2.26	0.43
1:A:67:GLN:O	1:A:68:ALA:HB2	2.19	0.42
2:B:25:ILE:HG13	2:B:34:PRO:HG3	2.00	0.42
2:B:275:LEU:HB2	2:B:277:ALA:HB2	2.01	0.42
2:B:244:GLU:HG2	2:B:295:TRP:CH2	2.53	0.42
1:A:34:LYS:HG2	1:A:99:LEU:CD2	2.50	0.42
1:A:62:SER:HA	1:A:65:PRO:HD2	2.01	0.42
2:B:117:LEU:HB2	2:B:170:LEU:HD11	2.02	0.42
2:B:53:GLN:HG3	2:B:54:ARG:H	1.85	0.42
2:B:167:ARG:NH1	2:B:172:LEU:HD12	2.35	0.42
1:A:26:GLY:O	1:A:27:ASP:C	2.62	0.42
1:A:148:ALA:O	1:A:150:GLY:N	2.52	0.42
2:B:69:LEU:CD2	2:B:71:HIS:H	2.32	0.42
1:A:45:GLU:C	1:A:47:LEU:N	2.76	0.42
1:A:74:CYS:O	1:A:75:LEU:C	2.59	0.42
2:B:225:CYS:N	2:B:306:THR:HG22	2.34	0.42
2:B:236:GLY:C	2:B:238:HIS:N	2.76	0.42
2:B:241:GLN:HG2	2:B:264:LEU:HD23	2.02	0.42
1:A:27:ASP:O	1:A:28:GLY:C	2.63	0.41
1:A:142:SER:OG	1:A:145:GLN:HG3	2.20	0.41
2:B:32:LEU:HD22	2:B:36:PRO:HD3	2.00	0.41
2:B:143:ASN:C	2:B:145:GLN:H	2.28	0.41
1:A:129:ALA:HB3	1:A:130:LEU:HD22	2.01	0.41
1:A:67:GLN:O	1:A:67:GLN:HG2	2.19	0.41
2:B:186:LEU:HA	2:B:186:LEU:HD23	1.71	0.41
2:B:243:CYS:HB3	2:B:285:ARG:O	2.19	0.41
1:A:103:LEU:O	1:A:107:GLN:HG3	2.20	0.41
2:B:212:MET:HG2	2:B:227:GLN:NE2	2.32	0.41
1:A:50:LEU:O	1:A:53:SER:OG	2.26	0.41
1:A:74:CYS:SG	1:A:75:LEU:N	2.89	0.41
1:A:111:ALA:O	1:A:114:ALA:HB3	2.21	0.41
2:B:183:GLU:O	2:B:183:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:LEU:HD11	2:B:282:LEU:HB3	2.02	0.41
2:B:246:ARG:HA	2:B:257:ALA:O	2.21	0.41
1:A:140:PHE:HB3	1:A:146:ARG:HG2	2.02	0.41
2:B:26:LYS:HA	2:B:59:THR:CG2	2.48	0.41
2:B:54:ARG:NE	2:B:60:GLN:HE21	2.17	0.41
1:A:39:TYR:CG	1:A:147:ARG:HG2	2.56	0.41
2:B:5:HIS:C	2:B:5:HIS:ND1	2.78	0.41
1:A:20:GLN:HG2	2:B:173:TYR:CE2	2.55	0.41
2:B:10:ALA:HA	2:B:11:PRO:HD2	1.83	0.41
2:B:29:CYS:O	2:B:29:CYS:SG	2.78	0.41
2:B:46:LEU:HA	2:B:46:LEU:HD23	1.65	0.41
2:B:73:GLN:HG2	2:B:74:ALA:N	2.35	0.41
2:B:259:VAL:HG12	2:B:260:GLY:N	2.35	0.41
2:B:209:LEU:HD22	2:B:228:LEU:CD1	2.51	0.40
2:B:264:LEU:C	2:B:264:LEU:CD1	2.82	0.40
2:B:13:VAL:O	2:B:14:HIS:C	2.64	0.40
1:A:79:HIS:HB2	1:A:117:ILE:HG21	2.04	0.40
1:A:146:ARG:O	1:A:147:ARG:C	2.63	0.40
1:A:148:ALA:O	1:A:151:VAL:N	2.55	0.40
1:A:89:LEU:O	1:A:92:LEU:HB2	2.21	0.40
1:A:99:LEU:O	1:A:100:GLY:C	2.63	0.40
1:A:127:ALA:O	1:A:128:PRO:C	2.64	0.40
1:A:130:LEU:H	1:A:130:LEU:CD2	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	166/174 (95%)	125 (75%)	23 (14%)	18 (11%)	0	1
2	B	295/313 (94%)	241 (82%)	33 (11%)	21 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	461/487 (95%)	366 (79%)	56 (12%)	39 (8%)	0 1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ALA
1	A	71	LEU
1	A	72	ALA
1	A	78	LEU
1	A	79	HIS
1	A	100	GLY
2	B	15	LEU
2	B	34	PRO
2	B	48	PRO
2	B	56	SER
2	B	260	GLY
2	B	277	ALA
2	B	279	ALA
1	A	66	SER
1	A	139	ALA
1	A	149	GLY
1	A	160	PHE
2	B	30	SER
2	B	124	GLY
2	B	289	TRP
1	A	46	GLU
1	A	53	SER
1	A	120	GLN
1	A	128	PRO
2	B	31	HIS
2	B	67	PRO
2	B	69	LEU
2	B	158	ASP
2	B	213	ASP
1	A	95	ILE
2	B	59	THR
2	B	144	CYS
2	B	146	THR
2	B	276	PRO
1	A	167	VAL
1	A	64	CYS
1	A	65	PRO

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Mol	Chain	Res	Type
2	B	35	GLU
2	B	43	GLY

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	137/141 (97%)	114 (83%)	23 (17%)	2	8
2	B	265/274 (97%)	203 (77%)	62 (23%)	1	3
All	All	402/415 (97%)	317 (79%)	85 (21%)	1	4

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	LEU
1	A	49	LEU
1	A	66	SER
1	A	69	LEU
1	A	70	GLN
1	A	71	LEU
1	A	74	CYS
1	A	92	LEU
1	A	97	PRO
1	A	102	THR
1	A	104	ASP
1	A	105	THR
1	A	110	VAL
1	A	126	MET
1	A	130	LEU
1	A	142	SER
1	A	147	ARG
1	A	155	SER
1	A	163	VAL
1	A	164	SER

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Mol	Chain	Res	Type
1	A	166	ARG
1	A	171	LEU
2	B	5	HIS
2	B	9	SER
2	B	15	LEU
2	B	20	THR
2	B	25	ILE
2	B	27	GLN
2	B	30	SER
2	B	32	LEU
2	B	37	GLN
2	B	38	ILE
2	B	39	LEU
2	B	42	LEU
2	B	45	GLU
2	B	51	ARG
2	B	54	ARG
2	B	55	LEU
2	B	59	THR
2	B	61	GLU
2	B	63	ILE
2	B	64	ILE
2	B	65	THR
2	B	70	ASN
2	B	76	LEU
2	B	77	SER
2	B	79	SER
2	B	80	LEU
2	B	81	ASN
2	B	86	LEU
2	B	92	VAL
2	B	95	ARG
2	B	102	ILE
2	B	105	ASN
2	B	112	LEU
2	B	125	PRO
2	B	136	LYS
2	B	140	SER
2	B	143	ASN
2	B	145	GLN
2	B	147	GLN
2	B	151	ILE

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Mol	Chain	Res	Type
2	B	152	LEU
2	B	154	CYS
2	B	158	ASP
2	B	165	ILE
2	B	167	ARG
2	B	171	LEU
2	B	174	GLN
2	B	194	LEU
2	B	196	LEU
2	B	198	PRO
2	B	208	MET
2	B	210	ARG
2	B	211	THR
2	B	212	MET
2	B	246	ARG
2	B	251	ARG
2	B	255	SER
2	B	258	LEU
2	B	275	LEU
2	B	284	ILE
2	B	302	LEU
2	B	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	52	HIS
1	A	67	GLN
2	B	27	GLN
2	B	31	HIS
2	B	37	GLN
2	B	52	GLN
2	B	81	ASN
2	B	87	GLN
2	B	105	ASN
2	B	120	GLN
2	B	128	HIS
2	B	143	ASN
2	B	160	GLN
2	B	175	ASN
2	B	227	GLN

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Mol	Chain	Res	Type
2	B	241	GLN

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
3	NAG	C	1	2,3	14,14,15	1.32	2 (14%)	17,19,21	2.60	8 (47%)
3	NAG	C	2	3	14,14,15	1.94	2 (14%)	17,19,21	2.69	7 (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
3	NAG	C	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	4.25	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C2-N2	3.99	1.52	1.46
3	C	1	NAG	O7-C7	3.15	1.30	1.23
3	C	1	NAG	O5-C1	-2.37	1.39	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-C2-N2	5.96	119.82	110.43
3	C	1	NAG	C1-O5-C5	-5.72	104.52	112.19
3	C	2	NAG	O5-C5-C6	5.12	117.62	107.66
3	C	2	NAG	C2-N2-C7	4.67	129.16	122.90
3	C	1	NAG	O5-C1-C2	-4.54	104.27	111.29
3	C	1	NAG	O6-C6-C5	-3.83	98.28	111.33
3	C	2	NAG	C4-C3-C2	3.64	116.35	111.02
3	C	1	NAG	C6-C5-C4	-3.26	105.02	113.02
3	C	1	NAG	C8-C7-N2	-2.94	111.24	116.12
3	C	1	NAG	O3-C3-C4	2.56	116.41	110.38
3	C	2	NAG	C3-C4-C5	2.34	114.48	110.23
3	C	2	NAG	O7-C7-C8	-2.30	117.95	122.05
3	C	1	NAG	O7-C7-N2	2.23	125.93	121.98
3	C	1	NAG	O3-C3-C2	2.23	114.04	109.40
3	C	2	NAG	O4-C4-C5	-2.12	104.10	109.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7

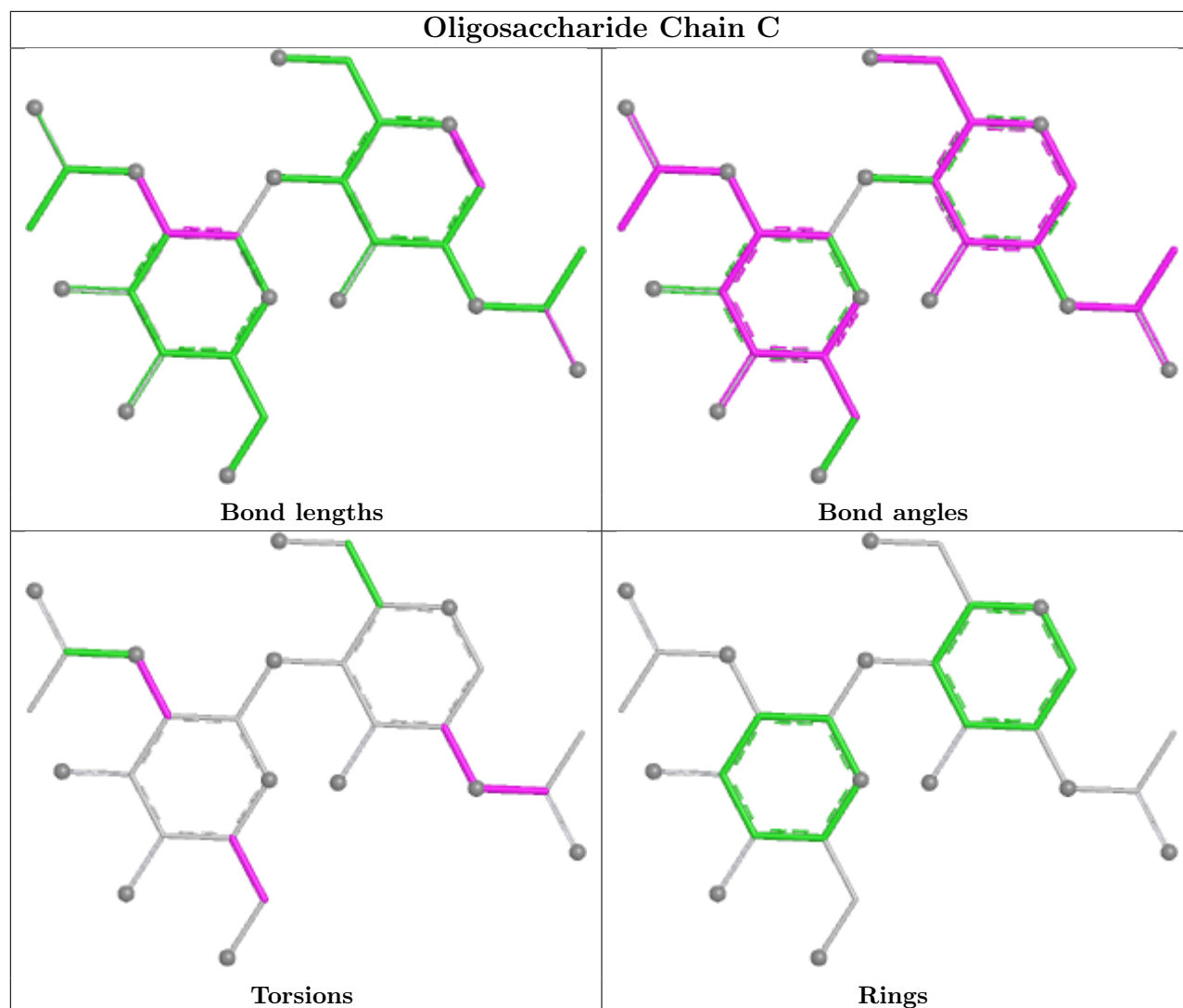
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	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](#)

There are no ligands in this entry.

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	168/174 (96%)	-0.27	6 (3%)	46 37	31, 68, 120, 128	0
2	B	299/313 (95%)	-0.13	14 (4%)	36 29	33, 64, 125, 140	0
All	All	467/487 (95%)	-0.18	20 (4%)	40 31	31, 66, 121, 140	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	32	LEU	7.8
2	B	55	LEU	4.7
1	A	69	LEU	3.9
2	B	3	CYS	3.8
2	B	214	PRO	3.6
2	B	57	ASP	3.6
2	B	31	HIS	3.3
1	A	130	LEU	3.3
2	B	146	THR	3.2
2	B	56	SER	3.2
2	B	26	LYS	2.8
1	A	174	PRO	2.6
1	A	128	PRO	2.5
1	A	129	ALA	2.5
1	A	65	PRO	2.4
2	B	82	TRP	2.3
2	B	4	GLY	2.3
2	B	36	PRO	2.2
2	B	15	LEU	2.2
2	B	34	PRO	2.1

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

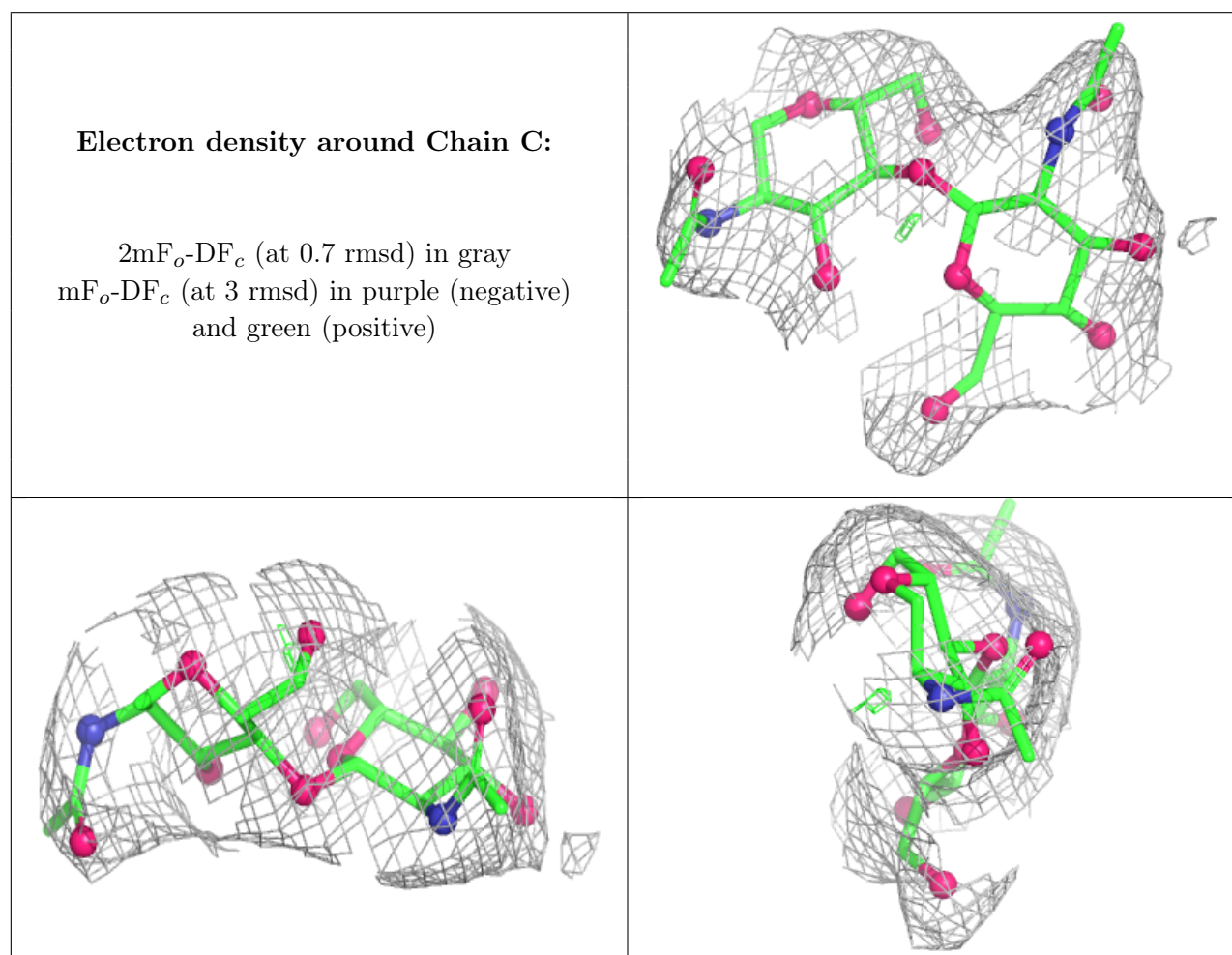
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
3	NAG	C	2	14/15	0.89	0.07	94,96,97,98	0
3	NAG	C	1	14/15	0.92	0.08	73,82,86,89	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.