



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:11 PM UTC

PDB ID : 4WZE / pdb_00004wze
Title : Crystal structure of P domain from norovirus strain Saga4 in complex with HBGA type Ley (tetraglycan)
Authors : Singh, B.K.; Hansman, G.S.
Deposited on : 2014-11-19
Resolution : 1.46 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

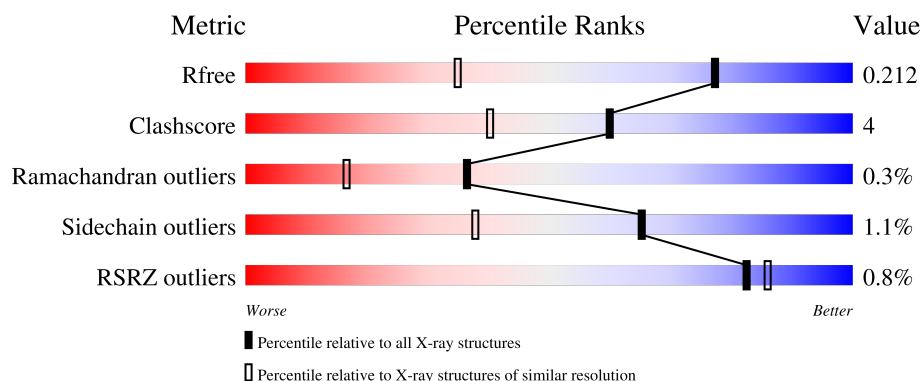
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	308	% 43% 53% 5%
1	B	308	% 43% 55% .
2	C	4	25% 50% 25%
2	D	4	25% 50% 25%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9826 atoms, of which 4383 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.

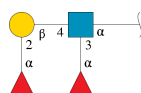
- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	2	0
			4585	1526	2186	409	454	10			
1	B	308	Total	C	H	N	O	S	0	2	0
			4599	1527	2197	410	455	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	expression tag	UNP B5BTR7
A	224	SER	-	expression tag	UNP B5BTR7
B	223	GLY	-	expression tag	UNP B5BTR7
B	224	SER	-	expression tag	UNP B5BTR7

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			46	26	1	19			
2	D	4	Total	C	N	O	0	0	0
			46	26	1	19			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

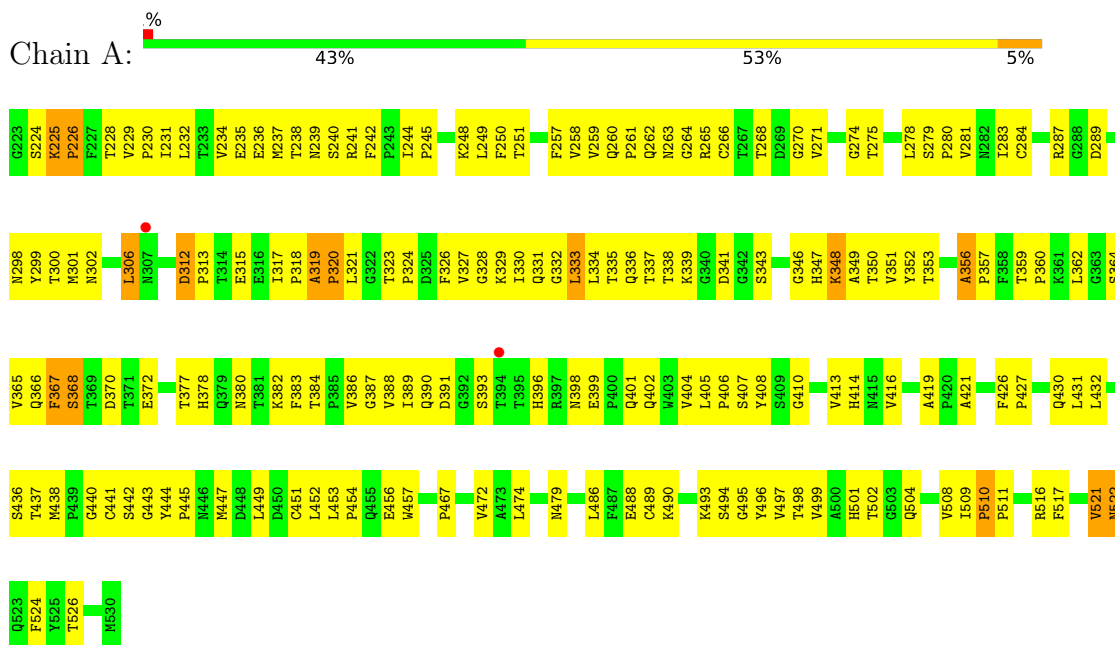
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		
4	B	272	Total	O	0	0
			272	272		

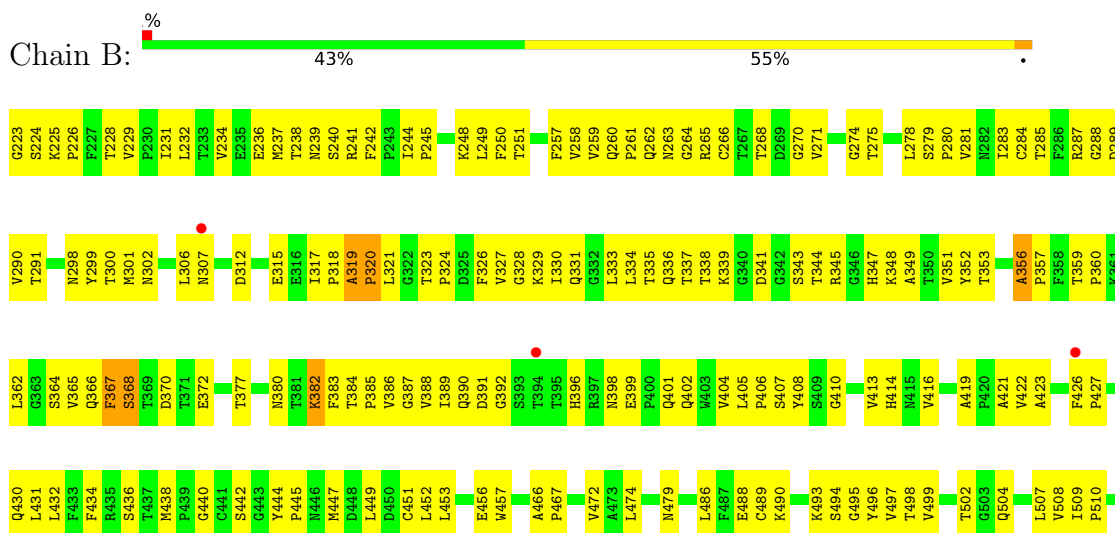
3 Residue-property plots

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: VP1



• Molecule 1: VP1





- Molecule 2: α -L-fucopyranose-(1-2)- β -D-galactopyranose-(1-4)-[α -L-fucopyranose-(1-3)]2-acetamido-2-deoxy- α -D-glucopyranose



- Molecule 2: α -L-fucopyranose-(1-2)- β -D-galactopyranose-(1-4)-[α -L-fucopyranose-(1-3)]2-acetamido-2-deoxy- α -D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.02Å 58.50Å 113.86Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	31.76 – 1.46 31.76 – 1.46	Depositor EDS
% Data completeness (in resolution range)	95.0 (31.76-1.46) 95.3 (31.76-1.46)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.212 0.185 , 0.212	Depositor DCC
R_{free} test set	5112 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.029 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.032 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9826	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3307e-16. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GAL, NDG, ACT, FUC

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	2.43	170/2475 (6.9%)	1.08	7/3387 (0.2%)
1	B	2.43	169/2478 (6.8%)	1.08	7/3391 (0.2%)
All	All	2.43	339/4953 (6.8%)	1.08	14/6778 (0.2%)

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368[A]	SER	N-CA	19.82	1.70	1.46
1	B	368[B]	SER	N-CA	19.82	1.70	1.46
1	A	368[A]	SER	N-CA	19.46	1.70	1.46
1	A	368[B]	SER	N-CA	19.46	1.70	1.46
1	B	244	ILE	C-O	-15.17	1.12	1.24
1	A	244	ILE	C-O	-14.37	1.12	1.24
1	A	368[A]	SER	CA-C	13.75	1.70	1.52
1	A	368[B]	SER	CA-C	13.75	1.70	1.52
1	B	368[A]	SER	CA-C	13.74	1.70	1.52
1	B	368[B]	SER	CA-C	13.74	1.70	1.52
1	A	384	THR	C-O	-11.04	1.11	1.24
1	B	384	THR	C-O	-10.99	1.11	1.24
1	A	356	ALA	C-O	-10.19	1.14	1.24
1	A	242	PHE	C-O	-10.08	1.11	1.24
1	B	356	ALA	C-O	-10.07	1.15	1.24
1	A	453	LEU	C-O	-10.02	1.11	1.24
1	B	229	VAL	C-O	-9.95	1.14	1.24
1	B	283	ILE	C-O	-9.84	1.13	1.24
1	A	283	ILE	C-O	-9.73	1.13	1.24
1	B	453	LEU	C-O	-9.66	1.12	1.24
1	A	279	SER	C-O	-9.36	1.11	1.24
1	B	279	SER	C-O	-9.25	1.11	1.24
1	B	242	PHE	C-O	-9.23	1.12	1.24
1	B	317	ILE	C-O	-9.19	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	VAL	C-O	-9.16	1.14	1.24
1	A	317	ILE	C-O	-8.98	1.17	1.24
1	A	383	PHE	C-O	-8.97	1.13	1.24
1	B	383	PHE	C-O	-8.95	1.13	1.24
1	A	510	PRO	C-O	-8.74	1.17	1.24
1	A	489	CYS	C-O	-8.66	1.13	1.23
1	B	497	VAL	C-O	-8.61	1.15	1.24
1	A	497	VAL	C-O	-8.57	1.15	1.24
1	B	489	CYS	C-O	-8.45	1.13	1.23
1	A	239	ASN	C-O	-8.33	1.14	1.23
1	B	449	LEU	C-O	-8.06	1.14	1.23
1	B	510	PRO	C-O	-8.06	1.18	1.24
1	B	399	GLU	C-O	-7.99	1.15	1.24
1	A	337	THR	C-O	-7.92	1.15	1.24
1	A	351	VAL	C-O	-7.91	1.15	1.24
1	B	351	VAL	C-O	-7.88	1.15	1.24
1	A	318	PRO	C-O	-7.86	1.15	1.24
1	B	337	THR	C-O	-7.75	1.15	1.24
1	B	239	ASN	C-O	-7.68	1.14	1.23
1	B	323	THR	C-O	-7.65	1.14	1.24
1	A	474	LEU	C-O	-7.59	1.14	1.24
1	A	389	ILE	C-O	-7.57	1.15	1.23
1	A	386	VAL	C-O	-7.56	1.14	1.24
1	A	449	LEU	C-O	-7.56	1.15	1.23
1	B	389	ILE	C-O	-7.49	1.15	1.23
1	A	348	LYS	C-O	-7.44	1.15	1.23
1	A	438	MET	C-O	-7.43	1.14	1.24
1	B	438	MET	C-O	-7.36	1.14	1.24
1	A	399	GLU	C-O	-7.28	1.16	1.24
1	B	265	ARG	C-O	-7.28	1.15	1.24
1	B	386	VAL	C-O	-7.28	1.14	1.24
1	A	353	THR	C-O	-7.23	1.14	1.24
1	B	319	ALA	C-O	-7.19	1.15	1.24
1	B	261	PRO	C-O	-7.17	1.15	1.23
1	B	359	THR	C-O	-7.17	1.15	1.23
1	A	382	LYS	C-O	-7.16	1.15	1.23
1	B	353	THR	C-O	-7.14	1.14	1.24
1	A	380	ASN	C-O	-7.13	1.15	1.23
1	A	268	THR	C-O	-7.07	1.15	1.24
1	B	302	ASN	C-O	-7.05	1.15	1.24
1	B	457	TRP	C-O	-7.00	1.15	1.24
1	B	343	SER	C-O	-6.98	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	ALA	C-O	-6.96	1.15	1.24
1	A	331	GLN	C-O	-6.95	1.15	1.24
1	B	330	ILE	C-O	-6.90	1.16	1.24
1	A	302	ASN	C-O	-6.89	1.15	1.24
1	A	490	LYS	C-O	-6.89	1.15	1.24
1	A	265	ARG	C-O	-6.88	1.16	1.24
1	A	330	ILE	C-O	-6.85	1.16	1.24
1	B	380	ASN	C-O	-6.83	1.15	1.23
1	B	333	LEU	C-O	-6.83	1.15	1.24
1	B	367	PHE	C-O	-6.83	1.15	1.24
1	A	287	ARG	C-O	-6.80	1.15	1.23
1	B	241	ARG	C-O	-6.78	1.15	1.24
1	A	367	PHE	C-O	-6.77	1.15	1.24
1	A	323	THR	C-O	-6.74	1.15	1.24
1	B	382	LYS	C-O	-6.74	1.15	1.24
1	B	228	THR	C-O	-6.73	1.15	1.23
1	B	318	PRO	C-O	-6.73	1.16	1.24
1	A	359	THR	C-O	-6.72	1.16	1.23
1	B	499	VAL	C-O	-6.71	1.16	1.23
1	B	278	LEU	C-O	-6.71	1.15	1.24
1	B	474	LEU	C-O	-6.67	1.15	1.24
1	A	261	PRO	C-O	-6.64	1.16	1.23
1	B	268	THR	C-O	-6.64	1.15	1.24
1	A	241	ARG	C-O	-6.64	1.15	1.24
1	B	280	PRO	C-O	-6.63	1.16	1.24
1	B	327	VAL	C-O	-6.63	1.16	1.24
1	A	445	PRO	C-O	-6.62	1.16	1.23
1	A	251	THR	C-O	-6.62	1.15	1.23
1	A	467	PRO	C-O	-6.61	1.16	1.23
1	A	343	SER	C-O	-6.60	1.15	1.23
1	B	430	GLN	C-O	-6.58	1.15	1.23
1	A	387	GLY	C-O	-6.57	1.17	1.23
1	A	396	HIS	C-O	-6.57	1.16	1.23
1	B	287	ARG	C-O	-6.57	1.15	1.23
1	A	499	VAL	C-O	-6.56	1.16	1.23
1	A	440	GLY	C-O	-6.55	1.15	1.23
1	A	327	VAL	C-O	-6.54	1.17	1.24
1	A	496	TYR	C-O	-6.54	1.16	1.23
1	A	335	THR	C-O	-6.51	1.15	1.23
1	A	402	GLN	C-O	-6.51	1.15	1.24
1	A	280	PRO	C-O	-6.51	1.16	1.24
1	B	467	PRO	C-O	-6.50	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	PRO	C-O	-6.48	1.16	1.23
1	B	348	LYS	C-O	-6.48	1.16	1.23
1	B	517	PHE	C-O	-6.47	1.16	1.24
1	A	334	LEU	C-O	-6.47	1.16	1.24
1	B	260	GLN	C-O	-6.44	1.16	1.24
1	A	240	SER	C-O	-6.43	1.15	1.24
1	B	496	TYR	C-O	-6.43	1.16	1.23
1	B	251	THR	C-O	-6.42	1.16	1.23
1	B	344	THR	C-O	-6.42	1.15	1.23
1	A	488	GLU	C-O	-6.41	1.15	1.23
1	B	328	GLY	C-O	-6.41	1.17	1.23
1	A	444	TYR	C-O	-6.41	1.16	1.24
1	A	321	LEU	C-O	-6.40	1.16	1.23
1	A	430	GLN	C-O	-6.40	1.15	1.23
1	B	444	TYR	C-O	-6.40	1.16	1.24
1	B	526	THR	C-O	-6.39	1.16	1.24
1	B	335	THR	C-O	-6.39	1.15	1.23
1	B	232	LEU	C-O	-6.38	1.16	1.23
1	B	341	ASP	C-O	-6.37	1.15	1.24
1	A	231	ILE	C-O	-6.36	1.17	1.24
1	B	440	GLY	C-O	-6.34	1.15	1.23
1	A	333	LEU	C-O	-6.33	1.15	1.24
1	B	445	PRO	C-O	-6.33	1.16	1.23
1	A	341	ASP	C-O	-6.33	1.15	1.24
1	A	365	VAL	C-O	-6.28	1.17	1.23
1	A	300	THR	C-O	-6.27	1.16	1.24
1	A	232	LEU	C-O	-6.26	1.16	1.23
1	A	368[A]	SER	C-O	-6.25	1.16	1.24
1	A	368[B]	SER	C-O	-6.25	1.16	1.24
1	A	238	THR	C-O	-6.25	1.16	1.24
1	A	260	GLN	C-O	-6.25	1.16	1.24
1	B	300	THR	C-O	-6.24	1.16	1.24
1	B	516	ARG	C-O	-6.23	1.17	1.23
1	A	328	GLY	C-O	-6.22	1.17	1.23
1	A	526	THR	C-O	-6.22	1.16	1.24
1	B	413	VAL	N-CA	-6.21	1.38	1.46
1	B	432	LEU	C-O	-6.20	1.16	1.24
1	B	231	ILE	C-O	-6.20	1.17	1.24
1	B	240	SER	C-O	-6.19	1.15	1.24
1	A	237	MET	C-O	-6.19	1.15	1.23
1	B	396	HIS	C-O	-6.19	1.16	1.23
1	B	321	LEU	C-O	-6.18	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	GLU	C-O	-6.16	1.16	1.23
1	B	406	PRO	C-O	-6.16	1.16	1.23
1	A	324	PRO	C-O	-6.15	1.16	1.23
1	B	336	GLN	C-O	-6.15	1.16	1.23
1	B	360	PRO	C-O	-6.14	1.16	1.24
1	A	278	LEU	C-O	-6.13	1.16	1.24
1	A	419	ALA	C-O	-6.13	1.16	1.24
1	A	457	TRP	C-O	-6.12	1.16	1.24
1	B	326	PHE	C-O	-6.12	1.16	1.23
1	A	228	THR	C-O	-6.12	1.16	1.23
1	B	398	ASN	C-O	-6.11	1.15	1.23
1	B	419	ALA	C-O	-6.11	1.16	1.24
1	B	237	MET	C-O	-6.11	1.15	1.23
1	A	336	GLN	C-O	-6.11	1.16	1.23
1	B	365	VAL	C-O	-6.09	1.17	1.23
1	B	452	LEU	C-O	-6.08	1.16	1.24
1	A	408	TYR	C-O	-6.07	1.16	1.24
1	B	245	PRO	C-O	-6.06	1.16	1.23
1	A	432	LEU	C-O	-6.05	1.16	1.24
1	A	360	PRO	C-O	-6.04	1.16	1.24
1	A	263	ASN	C-O	-6.04	1.16	1.23
1	A	352	TYR	C-O	-6.03	1.16	1.24
1	B	324	PRO	C-O	-6.03	1.16	1.23
1	B	225	LYS	C-O	-6.03	1.16	1.24
1	A	364	SER	C-O	-6.03	1.16	1.23
1	B	498	THR	C-O	-6.02	1.16	1.23
1	B	490	LYS	C-O	-6.01	1.16	1.24
1	A	493	LYS	C-O	-5.99	1.16	1.24
1	B	338	THR	C-O	-5.98	1.16	1.24
1	B	387	GLY	C-O	-5.95	1.17	1.23
1	B	266	CYS	C-O	-5.94	1.16	1.23
1	B	401	GLN	C-O	-5.94	1.17	1.24
1	A	398	ASN	C-O	-5.93	1.15	1.23
1	A	264	GLY	C-O	-5.93	1.17	1.24
1	A	258	VAL	C-O	-5.92	1.17	1.24
1	A	349	ALA	C-O	-5.92	1.16	1.23
1	B	364	SER	C-O	-5.92	1.16	1.23
1	A	517	PHE	C-O	-5.91	1.16	1.24
1	A	271	VAL	C-O	-5.91	1.17	1.24
1	B	258	VAL	C-O	-5.91	1.17	1.24
1	A	454	PRO	C-O	-5.90	1.16	1.23
1	B	388	VAL	C-O	-5.90	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	GLN	C-O	-5.90	1.16	1.24
1	A	442	SER	C-O	-5.90	1.16	1.24
1	A	516	ARG	C-O	-5.88	1.17	1.23
1	B	290	VAL	C-O	-5.88	1.17	1.24
1	B	493	LYS	C-O	-5.88	1.16	1.24
1	B	390	GLN	C-O	-5.88	1.17	1.24
1	B	331	GLN	C-O	-5.88	1.16	1.24
1	A	390	GLN	C-O	-5.88	1.17	1.24
1	B	416	VAL	C-O	-5.87	1.17	1.23
1	A	413	VAL	N-CA	-5.87	1.39	1.46
1	B	408	TYR	C-O	-5.85	1.16	1.24
1	B	456	GLU	C-O	-5.85	1.16	1.24
1	A	312	ASP	C-O	-5.84	1.17	1.24
1	B	466	ALA	C-O	-5.84	1.16	1.24
1	A	299	TYR	C-O	-5.84	1.16	1.23
1	A	416	VAL	C-O	-5.83	1.17	1.23
1	B	414[A]	HIS	N-CA	-5.83	1.38	1.45
1	B	414[B]	HIS	N-CA	-5.83	1.38	1.45
1	A	451	CYS	C-O	-5.82	1.16	1.23
1	A	347	HIS	C-O	-5.81	1.16	1.23
1	B	494	SER	C-O	-5.80	1.16	1.24
1	A	401	GLN	C-O	-5.80	1.17	1.24
1	B	349	ALA	C-O	-5.80	1.16	1.23
1	A	479	ASN	C-O	-5.76	1.18	1.24
1	B	263	ASN	C-O	-5.76	1.17	1.23
1	A	404	VAL	C-O	-5.75	1.17	1.24
1	B	451	CYS	C-O	-5.74	1.16	1.23
1	B	339	LYS	C-O	-5.74	1.17	1.24
1	B	248	LYS	C-O	-5.73	1.17	1.23
1	B	472	VAL	C-O	-5.73	1.18	1.24
1	A	338	THR	C-O	-5.73	1.17	1.24
1	A	326	PHE	C-O	-5.70	1.16	1.23
1	B	236	GLU	C-O	-5.70	1.16	1.24
1	A	388	VAL	C-O	-5.69	1.17	1.23
1	B	250	PHE	C-O	-5.68	1.17	1.23
1	A	225	LYS	C-O	-5.67	1.16	1.24
1	B	407	SER	C-O	-5.66	1.16	1.23
1	A	339	LYS	C-O	-5.66	1.17	1.24
1	A	332	GLY	C-O	-5.65	1.16	1.23
1	B	301	MET	C-O	-5.65	1.17	1.24
1	B	352	TYR	C-O	-5.65	1.17	1.24
1	A	436	SER	C-O	-5.63	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	THR	C-O	-5.63	1.17	1.24
1	B	479	ASN	C-O	-5.63	1.18	1.24
1	A	498	THR	C-O	-5.62	1.16	1.23
1	A	266	CYS	C-O	-5.61	1.16	1.23
1	A	472	VAL	C-O	-5.60	1.18	1.24
1	A	248	LYS	C-O	-5.60	1.17	1.23
1	A	284	CYS	C-O	-5.59	1.14	1.24
1	A	414[A]	HIS	N-CA	-5.59	1.38	1.45
1	A	414[B]	HIS	N-CA	-5.59	1.38	1.45
1	B	404	VAL	C-O	-5.58	1.18	1.24
1	B	436	SER	C-O	-5.58	1.16	1.23
1	B	271	VAL	C-O	-5.58	1.18	1.24
1	B	281	VAL	C-O	-5.57	1.18	1.24
1	B	299	TYR	C-O	-5.57	1.17	1.23
1	A	301	MET	C-O	-5.56	1.17	1.24
1	A	236	GLU	C-O	-5.56	1.16	1.24
1	B	320	PRO	C-O	-5.56	1.17	1.23
1	B	421	ALA	C-O	-5.56	1.16	1.23
1	A	366	GLN	C-O	-5.54	1.16	1.24
1	B	262	GLN	C-O	-5.51	1.17	1.23
1	B	291	THR	C-O	-5.50	1.17	1.24
1	B	414[A]	HIS	C-O	-5.50	1.17	1.23
1	B	414[B]	HIS	C-O	-5.50	1.17	1.23
1	B	502	THR	C-O	-5.50	1.17	1.24
1	A	235	GLU	C-O	-5.47	1.17	1.24
1	A	452	LEU	C-O	-5.47	1.17	1.24
1	B	509	ILE	C-O	-5.46	1.17	1.24
1	A	441	CYS	C-O	-5.46	1.17	1.24
1	B	238	THR	C-O	-5.46	1.17	1.24
1	B	495	GLY	C-O	-5.45	1.16	1.23
1	A	509	ILE	C-O	-5.45	1.17	1.24
1	A	346	GLY	C-O	-5.45	1.16	1.23
1	A	270	GLY	C-O	-5.44	1.17	1.24
1	A	456	GLU	C-O	-5.42	1.17	1.24
1	B	377	THR	C-O	-5.42	1.16	1.23
1	B	504	GLN	C-O	-5.42	1.17	1.24
1	B	442	SER	C-O	-5.41	1.16	1.23
1	A	495	GLY	C-O	-5.40	1.16	1.23
1	B	249	LEU	C-O	-5.37	1.17	1.23
1	B	447	MET	C-O	-5.37	1.16	1.23
1	B	366	GLN	C-O	-5.35	1.17	1.24
1	A	281	VAL	C-O	-5.35	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	THR	C-O	-5.34	1.16	1.23
1	A	421	ALA	C-O	-5.34	1.17	1.23
1	A	504	GLN	C-O	-5.33	1.17	1.24
1	B	362	LEU	C-O	-5.33	1.17	1.24
1	A	437	THR	C-O	-5.33	1.18	1.24
1	A	494	SER	C-O	-5.33	1.16	1.24
1	A	245	PRO	C-O	-5.31	1.17	1.23
1	B	508	VAL	C-O	-5.31	1.18	1.24
1	A	250	PHE	C-O	-5.31	1.17	1.23
1	B	298	ASN	C-O	-5.31	1.17	1.23
1	A	407	SER	C-O	-5.29	1.17	1.23
1	B	285	THR	C-O	-5.28	1.17	1.23
1	B	347	HIS	C-O	-5.27	1.17	1.23
1	A	234	VAL	C-O	-5.26	1.18	1.24
1	A	447	MET	C-O	-5.26	1.16	1.23
1	B	274	GLY	C-O	-5.25	1.17	1.24
1	B	312	ASP	C-O	-5.24	1.18	1.24
1	A	362	LEU	C-O	-5.23	1.17	1.24
1	A	298	ASN	C-O	-5.23	1.17	1.23
1	B	410	GLY	C-O	-5.22	1.17	1.23
1	B	486	LEU	C-O	-5.22	1.18	1.24
1	B	270	GLY	C-O	-5.21	1.17	1.24
1	A	259	VAL	C-O	-5.18	1.17	1.23
1	A	226	PRO	C-O	-5.16	1.18	1.23
1	B	275	THR	C-O	-5.16	1.17	1.24
1	A	262	GLN	C-O	-5.16	1.17	1.23
1	A	320	PRO	C-O	-5.15	1.17	1.23
1	A	508	VAL	C-O	-5.15	1.18	1.24
1	B	368[A]	SER	C-O	-5.14	1.17	1.24
1	B	368[B]	SER	C-O	-5.14	1.17	1.24
1	B	259	VAL	C-O	-5.14	1.17	1.23
1	A	230	PRO	C-O	-5.13	1.17	1.23
1	B	224	SER	C-O	-5.13	1.17	1.23
1	A	378	HIS	C-O	-5.13	1.17	1.23
1	A	410	GLY	C-O	-5.13	1.17	1.23
1	A	431	LEU	C-O	-5.13	1.17	1.23
1	A	501	HIS	C-O	-5.12	1.17	1.23
1	A	413	VAL	CA-C	5.12	1.58	1.52
1	B	234	VAL	C-O	-5.11	1.18	1.24
1	A	274	GLY	C-O	-5.10	1.17	1.24
1	B	431	LEU	C-O	-5.10	1.17	1.23
1	A	350	THR	C-O	-5.10	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	LEU	C-O	-5.10	1.17	1.24
1	A	443	GLY	C-O	-5.09	1.16	1.23
1	B	288	GLY	C-O	-5.09	1.17	1.24
1	A	521	VAL	C-O	-5.09	1.18	1.24
1	B	264	GLY	C-O	-5.08	1.17	1.24
1	A	249	LEU	C-O	-5.08	1.18	1.23
1	A	405	LEU	C-O	-5.06	1.17	1.24
1	B	423	ALA	C-O	-5.06	1.18	1.24
1	A	224	SER	C-O	-5.05	1.18	1.23
1	B	226	PRO	C-O	-5.05	1.18	1.23
1	B	507	LEU	C-O	-5.05	1.17	1.23
1	A	275	THR	C-O	-5.04	1.17	1.24
1	B	345	ARG	C-O	-5.04	1.17	1.23
1	A	306	LEU	C-O	-5.03	1.17	1.24
1	B	385	PRO	C-O	-5.03	1.18	1.23
1	A	289	ASP	C-O	-5.02	1.17	1.23
1	B	434	PHE	C-O	-5.01	1.18	1.24
1	B	334	LEU	C-O	-5.01	1.18	1.24
1	B	284	CYS	C-O	-5.01	1.15	1.24
1	B	422	VAL	C-O	-5.00	1.18	1.24
1	A	524	PHE	C-O	-5.00	1.17	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	VAL	O-C-N	-7.93	114.85	123.18
1	A	413	VAL	O-C-N	-7.86	114.93	123.18
1	B	392	GLY	CA-C-N	6.25	128.66	120.28
1	B	392	GLY	C-N-CA	6.25	128.66	120.28
1	A	486	LEU	N-CA-C	5.74	117.34	111.14
1	A	393	SER	N-CA-C	5.70	118.43	111.82
1	B	486	LEU	N-CA-C	5.54	117.12	111.14
1	B	522	ASN	N-CA-C	5.45	116.26	108.74
1	A	279	SER	CA-C-O	5.44	124.12	119.66
1	A	522	ASN	N-CA-C	5.27	116.01	108.74
1	A	367	PHE	CA-C-N	5.04	129.11	122.30
1	A	367	PHE	C-N-CA	5.04	129.11	122.30
1	B	279	SER	CA-C-O	5.03	123.79	119.66
1	B	472	VAL	N-CA-C	5.00	115.47	108.17

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	2399	2186	2300	18	0
1	B	2402	2197	2304	16	0
2	C	46	0	39	3	0
2	D	46	0	39	3	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	270	0	0	5	0
4	B	272	0	0	8	0
All	All	5443	4383	4688	40	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 4.

All (40) 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:370:ASP:OD2	4:A:941:HOH:O	1.78	0.99
1:B:370:ASP:OD2	4:B:941:HOH:O	1.81	0.96
4:B:971:HOH:O	2:D:2:GAL:O4	2.00	0.74
1:A:306:LEU:HD13	4:A:913:HOH:O	1.94	0.66
1:B:306:LEU:HD13	4:B:917:HOH:O	1.97	0.65
4:A:970:HOH:O	2:C:2:GAL:O4	2.04	0.62
1:B:223:GLY:N	4:B:701:HOH:O	2.35	0.59
1:A:356:ALA:N	1:A:357:PRO:CD	2.67	0.57
1:B:356:ALA:N	1:B:357:PRO:CD	2.69	0.56
1:A:329:LYS:NZ	1:A:391:ASP:OD2	2.38	0.52
2:D:1:NDG:H6C1	2:D:2:GAL:C1	2.41	0.50
1:A:356:ALA:HB3	1:A:357:PRO:HD3	1.93	0.50
2:C:1:NDG:H6C1	2:C:2:GAL:C1	2.41	0.50
1:B:356:ALA:HB3	1:B:357:PRO:HD3	1.95	0.47
1:B:426:PHE:CD2	1:B:427:PRO:HD2	2.50	0.47
1:B:319:ALA:HB1	1:B:320:PRO:HD2	1.97	0.46
1:A:367:PHE:C	1:A:368[A]:SER:CA	2.72	0.46
1:A:319:ALA:HB1	1:A:320:PRO:HD2	1.97	0.46
1:B:367:PHE:C	1:B:368[A]:SER:CA	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.90	0.44
1:A:225:LYS:HA	1:A:226:PRO:HD3	1.81	0.42
1:B:257:PHE:O	4:B:789:HOH:O	2.22	0.42
2:D:1:NDG:H6C2	2:D:3:FUC:H3	2.01	0.42
1:A:257:PHE:O	4:A:788:HOH:O	2.21	0.42
1:A:315:GLU:HG3	4:A:906:HOH:O	2.20	0.42
1:B:329:LYS:NZ	1:B:391:ASP:OD2	2.46	0.42
2:C:1:NDG:H6C2	2:C:3:FUC:H3	2.01	0.42
1:B:382:LYS:NZ	4:B:794:HOH:O	2.54	0.41
1:A:510:PRO:HA	1:A:511:PRO:HD3	1.94	0.40
1:A:426:PHE:CD2	1:A:427:PRO:HD2	2.56	0.40
1:B:315:GLU:HG3	4:B:912:HOH:O	2.20	0.40
1:A:367:PHE:C	1:A:368[B]:SER:CA	2.74	0.40
1:B:391:ASP:HB3	4:B:970:HOH:O	2.22	0.40
1:A:333:LEU:HD23	1:A:348:LYS:HA	2.03	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	308/308 (100%)	303 (98%)	4 (1%)	1 (0%)	36	16
1	B	308/308 (100%)	304 (99%)	3 (1%)	1 (0%)	36	16
All	All	616/616 (100%)	607 (98%)	7 (1%)	2 (0%)	36	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	VAL
1	B	521	VAL

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	267/267 (100%)	265 (99%)	2 (1%)	76	54
1	B	268/267 (100%)	264 (98%)	4 (2%)	57	25
All	All	535/534 (100%)	529 (99%)	6 (1%)	65	38

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	GLU
1	A	522	ASN
1	B	289	ASP
1	B	307	ASN
1	B	372	GLU
1	B	522	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	HIS
1	A	417	HIS
1	B	412	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 ⓘ

8 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	NDG	C	1	2	15,15,15	0.65	0	21,21,21	0.82	1 (4%)
2	GAL	C	2	2	11,11,12	0.51	0	15,15,17	0.83	0
2	FUC	C	3	2	10,10,11	0.73	0	14,14,16	0.74	0
2	FUC	C	4	2	10,10,11	0.72	0	14,14,16	0.63	0
2	NDG	D	1	2	15,15,15	0.67	0	21,21,21	0.82	1 (4%)
2	GAL	D	2	2	11,11,12	0.53	0	15,15,17	0.85	0
2	FUC	D	3	2	10,10,11	0.73	0	14,14,16	0.75	0
2	FUC	D	4	2	10,10,11	0.72	0	14,14,16	0.64	0

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	NDG	C	1	2	-	2/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NDG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NDG	C1-C2-N2	2.55	113.68	110.73
2	C	1	NDG	C1-C2-N2	2.43	113.54	110.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

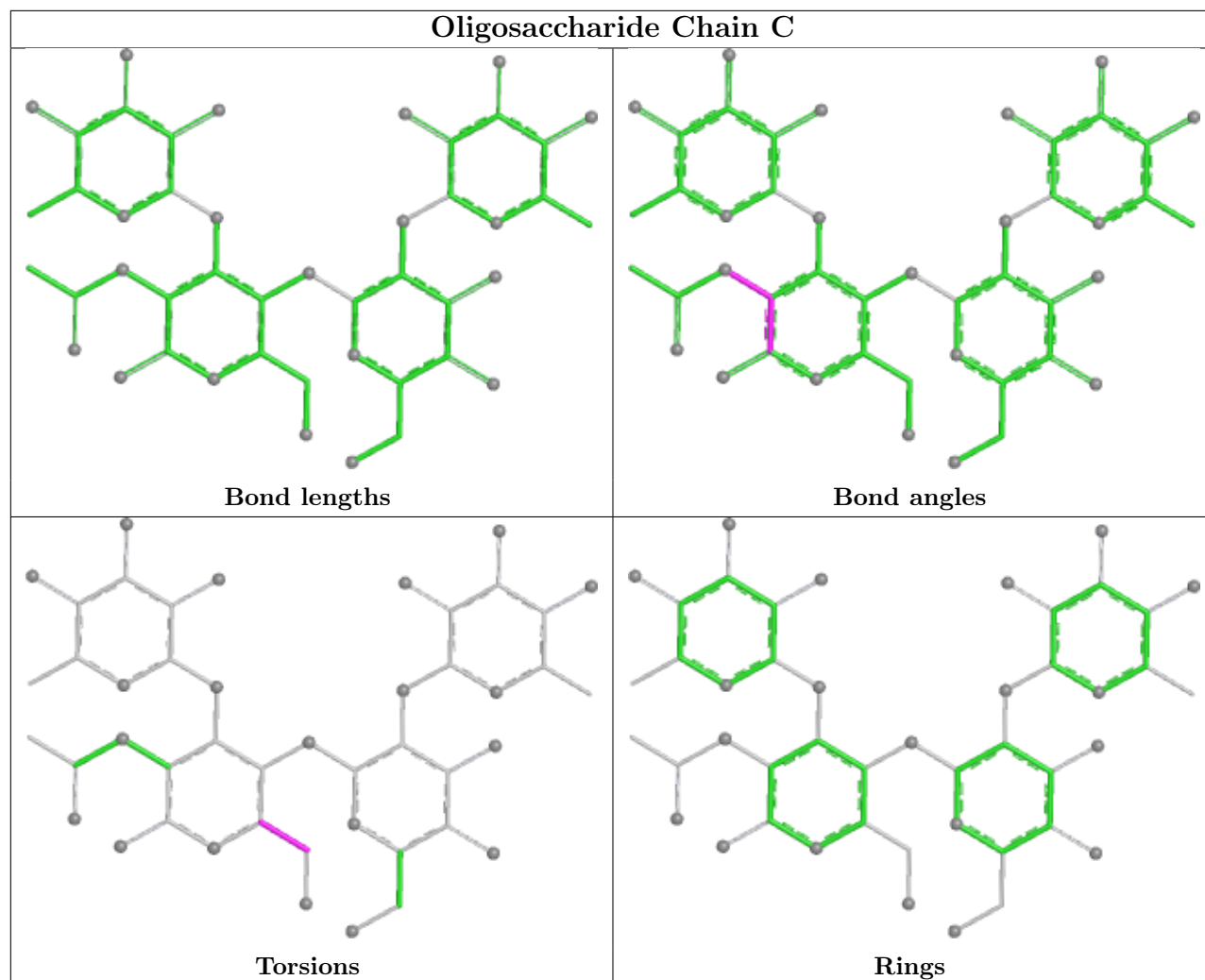
Mol	Chain	Res	Type	Atoms
2	C	1	NDG	O5-C5-C6-O6
2	D	1	NDG	O5-C5-C6-O6
2	C	1	NDG	C4-C5-C6-O6
2	D	1	NDG	C4-C5-C6-O6

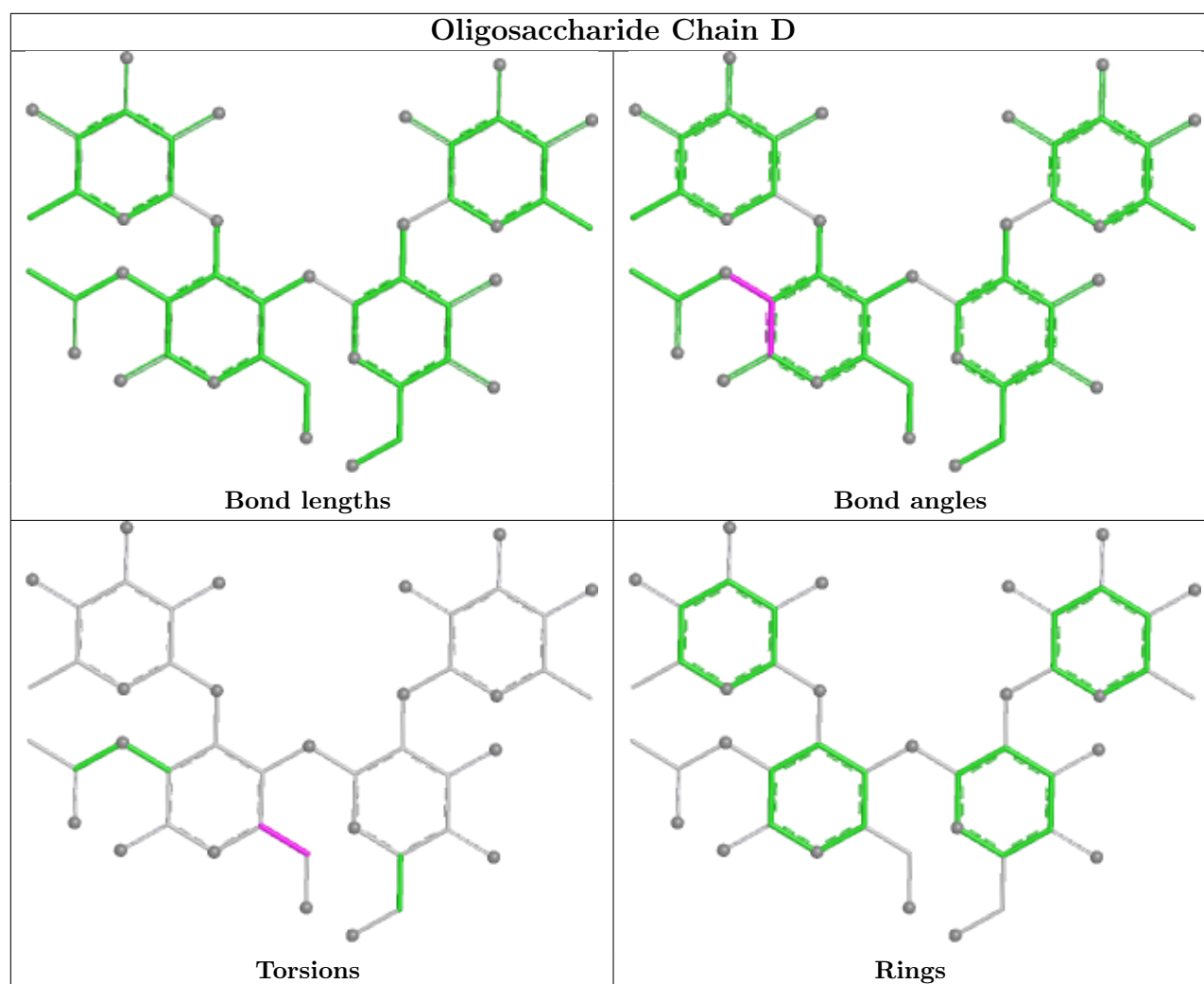
There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NDG	2	0
2	C	1	NDG	2	0
2	C	3	FUC	1	0
2	C	2	GAL	2	0
2	D	2	GAL	2	0
2	D	3	FUC	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](#)

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	$\# Z > 2$
3	ACT	A	601	-	3,3,3	0.83	0	3,3,3	1.30	0
3	ACT	B	601	-	3,3,3	0.80	0	3,3,3	1.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	308/308 (100%)	-0.51	2 (0%) 85 89	10, 23, 41, 64	2 (0%)
1	B	308/308 (100%)	-0.50	3 (0%) 79 83	10, 23, 42, 64	2 (0%)
All	All	616/616 (100%)	-0.50	5 (0%) 82 86	10, 23, 42, 64	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	PHE	2.7
1	A	307	ASN	2.7
1	B	307	ASN	2.5
1	B	394	THR	2.4
1	A	394	THR	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.

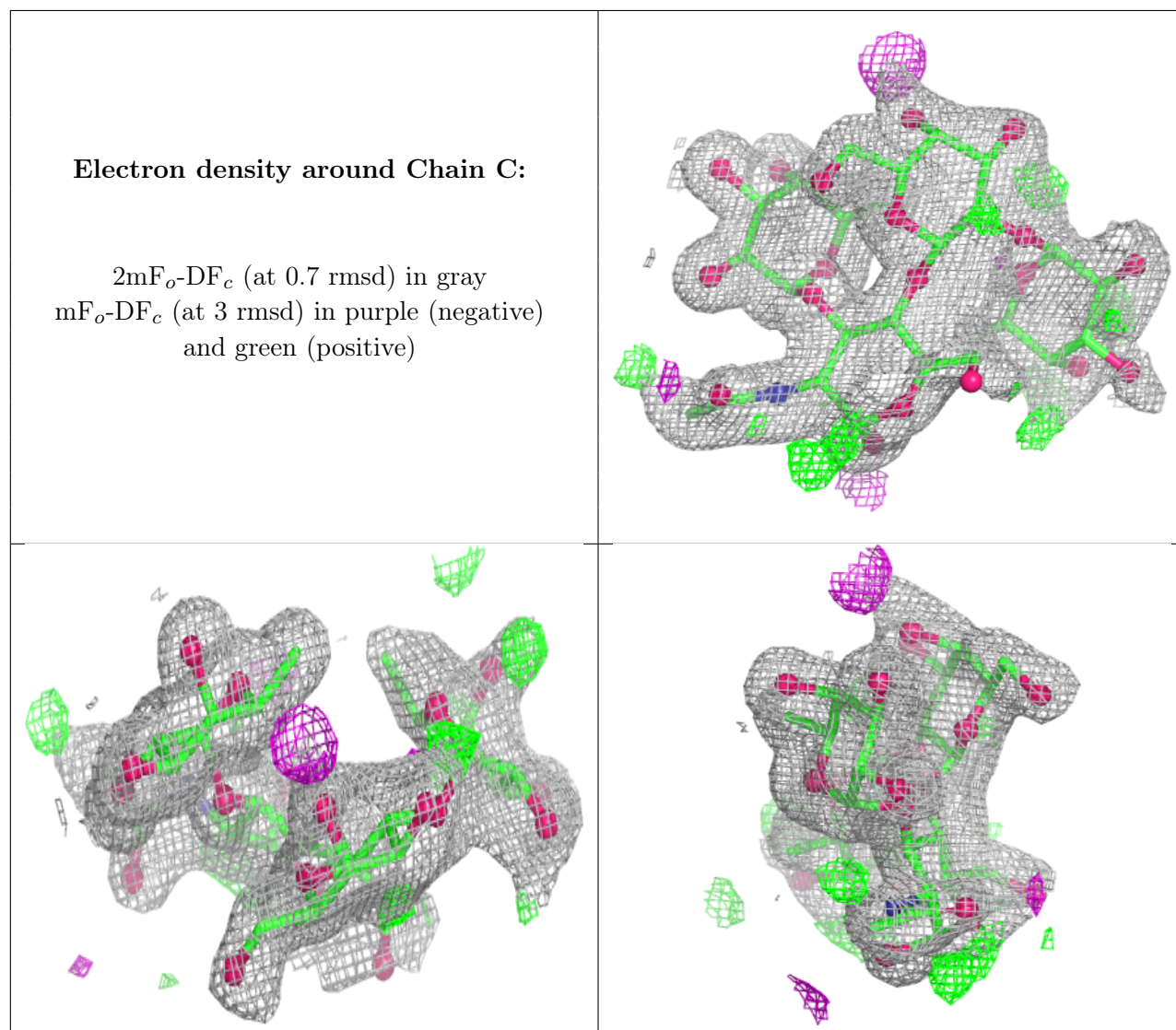
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	C	3	10/11	0.78	0.13	43,60,74,75	0
2	FUC	D	3	10/11	0.78	0.13	43,60,74,76	0
2	GAL	D	2	11/12	0.87	0.10	33,43,54,55	0
2	GAL	C	2	11/12	0.88	0.10	34,42,55,55	0

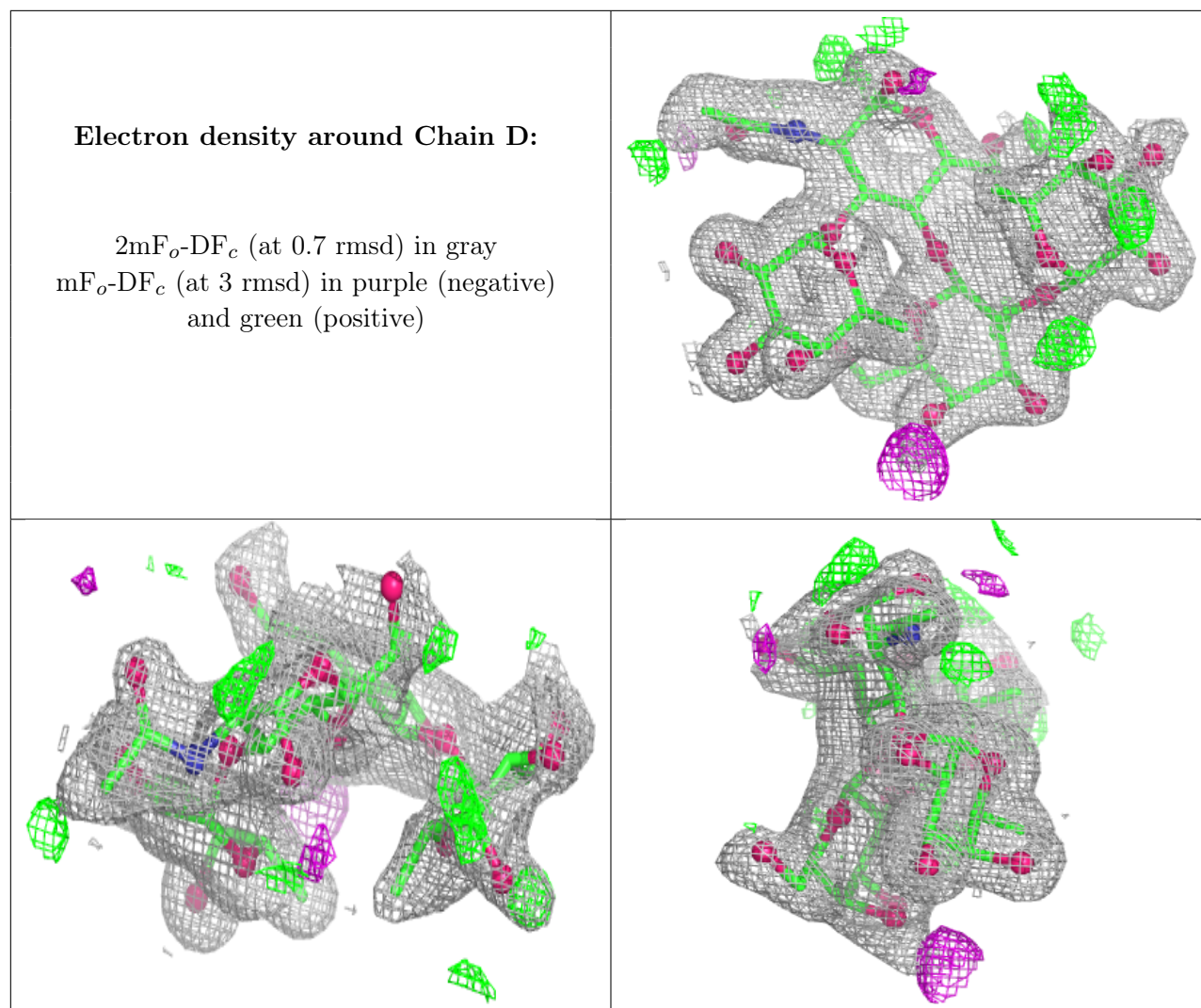
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDG	C	1	15/15	0.91	0.10	21,31,53,56	0
2	NDG	D	1	15/15	0.91	0.10	21,31,53,57	0
2	FUC	C	4	10/11	0.97	0.05	19,20,23,23	0
2	FUC	D	4	10/11	0.97	0.05	19,20,23,23	0

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
3	ACT	A	601	4/4	0.86	0.15	31,41,50,68	0
3	ACT	B	601	4/4	0.87	0.15	30,41,49,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.