



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:58 AM UTC

PDB ID : 5W1M / pdb_00005w1m
Title : MACV GP1 CR1-07 Fab complex
Authors : Raymond, D.D.; Clark, L.E.; Abraham, J.
Deposited on : 2017-06-03
Resolution : 3.91 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

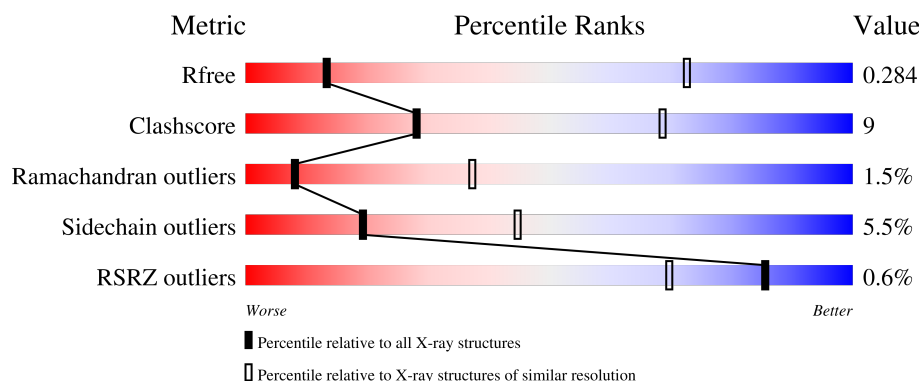
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

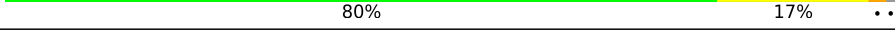
The reported resolution of this entry is 3.91 Å.

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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	221	 80% 16% .
1	C	221	 74% 24% .
1	E	221	 76% 22% .
1	G	221	 80% 17% ..
2	B	226	 69% 27% .

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Mol	Chain	Length	Quality of chain
2	D	226	
2	F	226	
2	H	226	
3	Q	152	
3	R	152	
3	S	152	
3	T	152	
4	I	2	
4	J	2	
5	K	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18425 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 CR1-07 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1708	1068	284	351	5			
1	C	221	Total	C	N	O	S	0	1	0
			1711	1070	284	352	5			
1	E	221	Total	C	N	O	S	0	0	0
			1708	1068	284	351	5			
1	G	219	Total	C	N	O	S	0	0	0
			1695	1061	282	347	5			

- Molecule 2 is a protein called CR1-07 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1658	1053	282	316	7			
2	D	220	Total	C	N	O	S	0	0	0
			1670	1059	284	319	8			
2	F	218	Total	C	N	O	S	0	0	0
			1658	1053	282	316	7			
2	H	219	Total	C	N	O	S	0	1	0
			1667	1058	283	319	7			

- Molecule 3 is a protein called Pre-glycoprotein polypeptide GP complex.

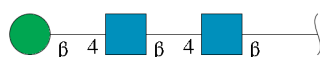
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	151	Total	C	N	O	S	0	0	0
			1209	761	209	225	14			
3	R	152	Total	C	N	O	S	0	0	0
			1218	766	211	227	14			
3	S	151	Total	C	N	O	S	0	0	0
			1209	761	209	225	14			
3	T	149	Total	C	N	O	S	0	0	0
			1194	752	206	223	13			

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



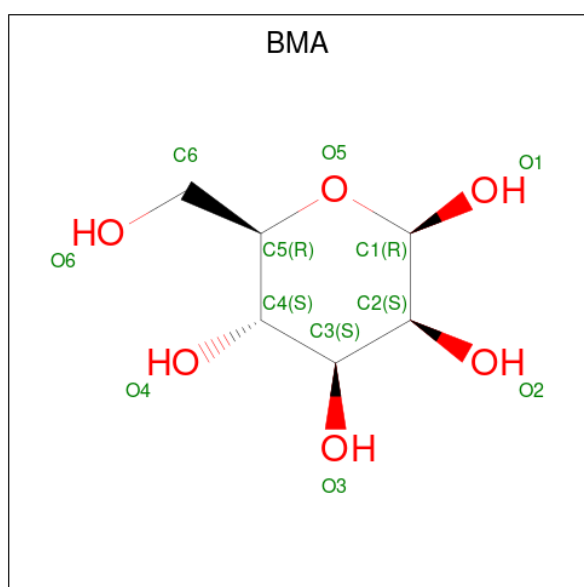
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



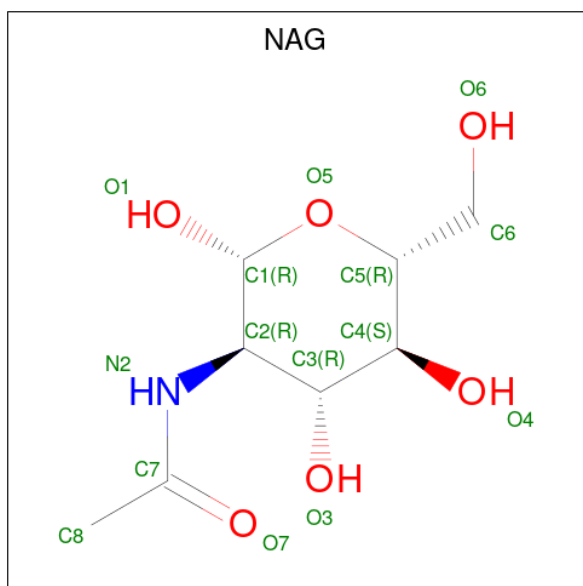
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Q	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

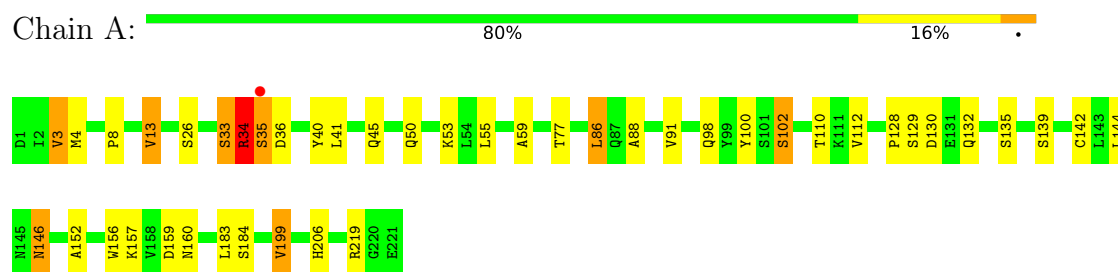


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	T	1	Total	C	N	O	0	0
			14	8	1	5		

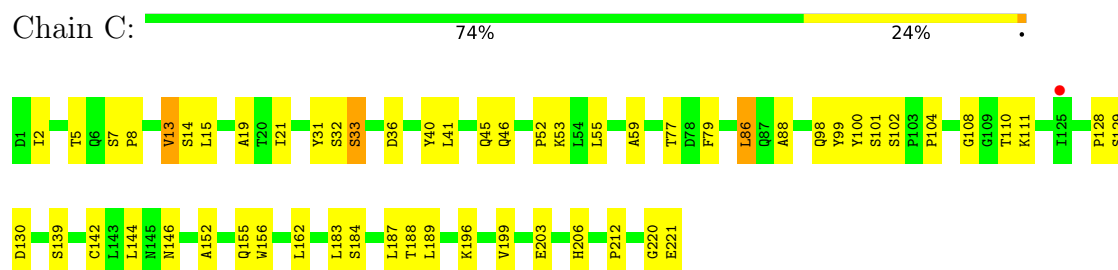
3 Residue-property plots

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.

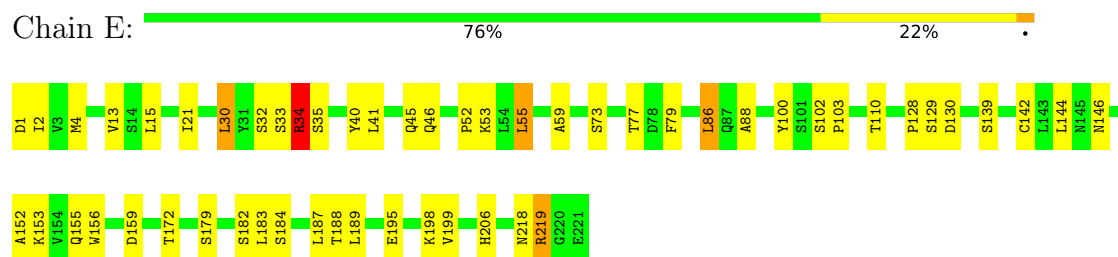
• Molecule 1: CR1-07 Fab light chain



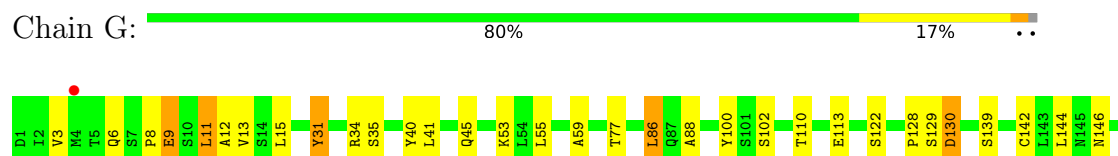
• Molecule 1: CR1-07 Fab light chain



• Molecule 1: CR1-07 Fab light chain



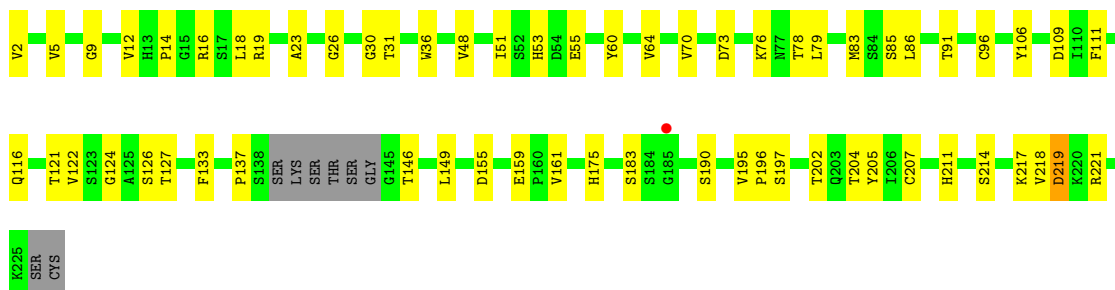
• Molecule 1: CR1-07 Fab light chain





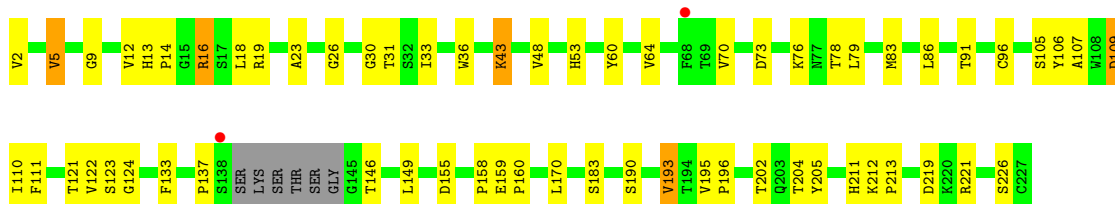
• Molecule 2: CR1-07 Fab heavy chain

Chain B: 69% 27%



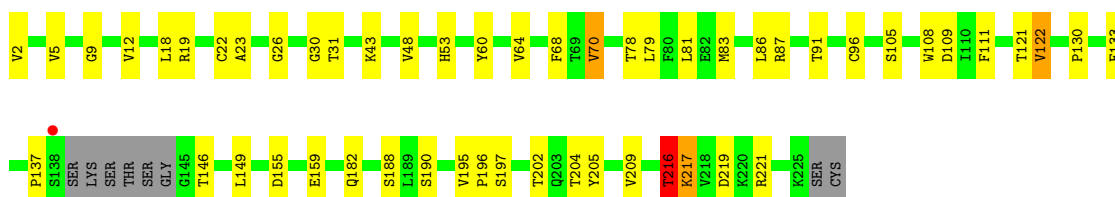
• Molecule 2: CR1-07 Fab heavy chain

Chain D: 70% 25%



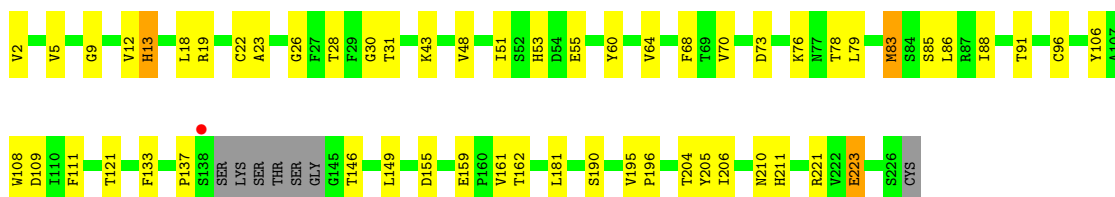
• Molecule 2: CR1-07 Fab heavy chain

Chain F: 73% 22%

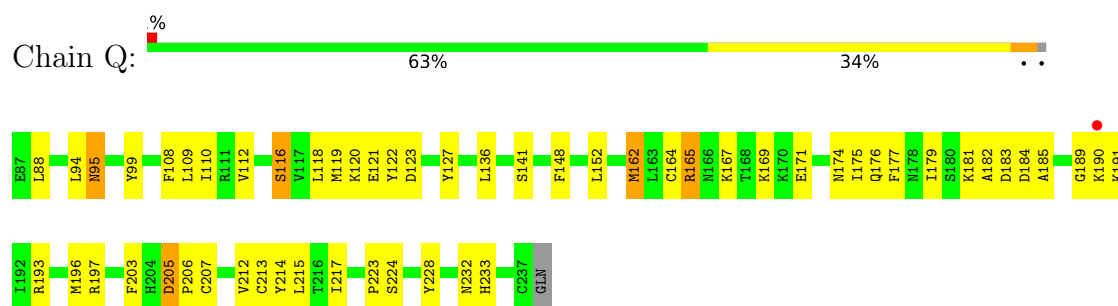


• Molecule 2: CR1-07 Fab heavy chain

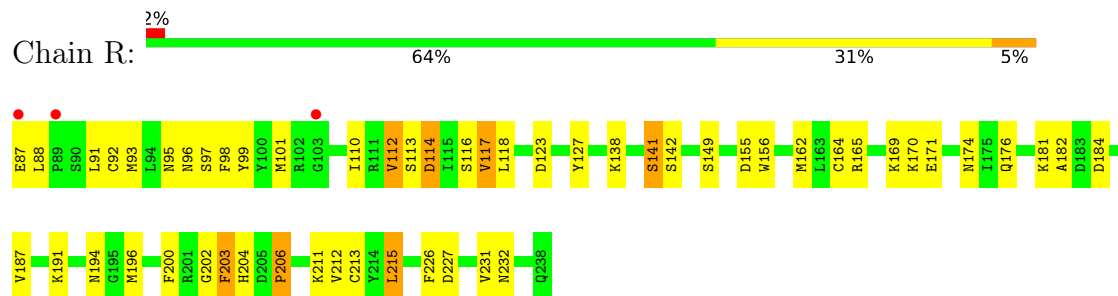
Chain H: 72% 23%



• Molecule 3: Pre-glycoprotein polypeptide GP complex



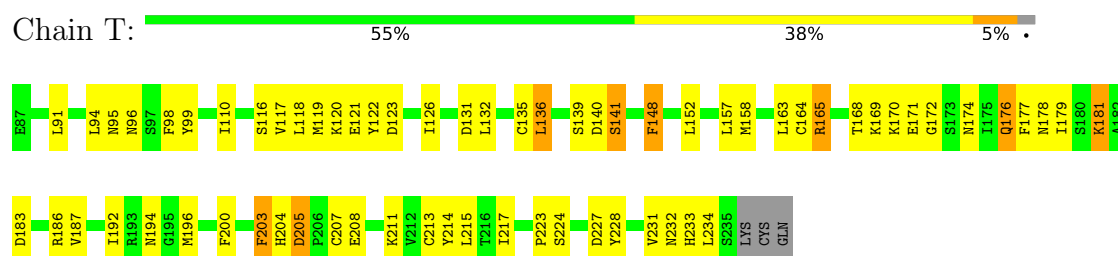
- Molecule 3: Pre-glycoprotein polyprotein GP complex



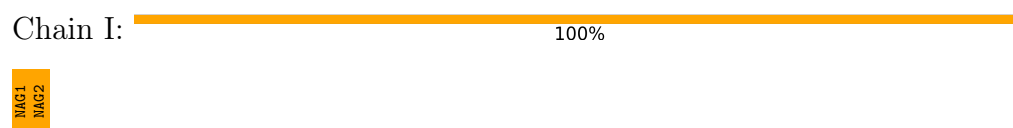
- Molecule 3: Pre-glycoprotein polyprotein GP complex



- Molecule 3: Pre-glycoprotein polyprotein GP complex



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



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

Chain J:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	206.97Å 206.97Å 238.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.91 49.12 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.12-3.91) 98.5 (49.12-3.91)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.248 , 0.264 (Not available) , 0.284	Depositor DCC
R_{free} test set	2332 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	183.6	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18425	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, BMA

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	0.84	0/1745	1.31	13/2369 (0.5%)
1	C	0.83	1/1751 (0.1%)	1.25	11/2377 (0.5%)
1	E	0.83	0/1745	1.26	10/2369 (0.4%)
1	G	0.79	0/1732	1.23	6/2352 (0.3%)
2	B	0.80	0/1702	1.26	10/2316 (0.4%)
2	D	0.87	1/1714 (0.1%)	1.32	9/2332 (0.4%)
2	F	0.92	2/1702 (0.1%)	1.29	9/2316 (0.4%)
2	H	0.83	0/1714	1.27	5/2332 (0.2%)
3	Q	1.08	0/1239	1.59	21/1670 (1.3%)
3	R	1.24	5/1248 (0.4%)	1.70	34/1682 (2.0%)
3	S	1.31	10/1239 (0.8%)	1.71	35/1670 (2.1%)
3	T	1.32	4/1224 (0.3%)	1.85	39/1651 (2.4%)
All	All	0.96	23/18755 (0.1%)	1.40	202/25436 (0.8%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	181	LYS	CA-C	6.40	1.62	1.52
3	S	126	ILE	CG1-CD1	-6.23	1.27	1.51
3	R	231	VAL	CA-C	6.11	1.60	1.52
3	S	162	MET	SD-CE	-6.07	1.64	1.79
3	S	205	ASP	C-N	6.02	1.39	1.33
3	T	96	ASN	CA-C	6.00	1.61	1.52
3	S	225	SER	C-N	5.89	1.39	1.33
3	R	232	ASN	CA-C	5.55	1.60	1.52
2	F	216	THR	CA-C	5.53	1.60	1.52
3	S	96	ASN	CA-C	5.50	1.60	1.52
3	R	92	CYS	CA-C	5.49	1.59	1.52
2	D	212	LYS	C-N	5.39	1.40	1.33
3	S	138	LYS	CA-C	5.35	1.59	1.52
3	T	234	LEU	CA-C	5.22	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	179	ILE	CG1-CD1	-5.18	1.31	1.51
3	S	87	GLU	C-N	5.15	1.39	1.33
3	T	231	VAL	CA-C	5.12	1.59	1.52
3	T	136	LEU	CA-C	-5.11	1.46	1.52
2	F	217	LYS	CA-C	5.08	1.59	1.52
1	C	33	SER	CA-C	5.08	1.59	1.52
3	R	101	MET	SD-CE	-5.04	1.67	1.79
3	S	231	VAL	CA-C	5.01	1.59	1.52
3	S	88	LEU	CA-C	5.00	1.57	1.52

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	172	GLY	N-CA-C	9.26	120.91	111.56
3	T	174	ASN	CA-C-N	8.84	136.23	122.70
3	T	174	ASN	C-N-CA	8.84	136.23	122.70
3	S	121	GLU	CB-CG-CD	8.71	127.41	112.60
3	T	186	ARG	CA-C-N	8.34	131.12	120.70
3	T	186	ARG	C-N-CA	8.34	131.12	120.70
3	T	95	ASN	CA-CB-CG	8.19	120.79	112.60
3	R	227	ASP	CA-CB-CG	8.12	120.72	112.60
3	T	211	LYS	CA-C-N	8.11	132.53	120.69
3	T	211	LYS	C-N-CA	8.11	132.53	120.69
3	Q	141	SER	N-CA-C	-7.97	102.33	112.93
3	S	95	ASN	CA-CB-CG	7.97	120.57	112.60
3	T	187	VAL	CA-C-N	7.90	130.71	120.44
3	T	187	VAL	C-N-CA	7.90	130.71	120.44
3	R	155	ASP	CA-C-N	7.88	131.18	120.38
3	R	155	ASP	C-N-CA	7.88	131.18	120.38
3	Q	95	ASN	CA-CB-CG	7.86	120.46	112.60
3	T	214	TYR	CA-C-N	7.62	134.41	123.14
3	T	214	TYR	C-N-CA	7.62	134.41	123.14
3	S	88	LEU	N-CA-C	7.53	116.98	108.25
3	S	232	ASN	CA-CB-CG	7.46	120.06	112.60
3	T	123	ASP	CA-C-N	7.31	131.44	120.77
3	T	123	ASP	C-N-CA	7.31	131.44	120.77
3	R	232	ASN	CA-CB-CG	7.13	119.73	112.60
3	S	205	ASP	CA-CB-CG	7.10	119.70	112.60
3	T	232	ASN	CA-CB-CG	7.01	119.61	112.60
3	R	141	SER	N-CA-C	-6.97	102.58	112.13
3	T	181	LYS	CA-C-N	6.97	131.47	121.50
3	T	181	LYS	C-N-CA	6.97	131.47	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	121	GLU	CB-CG-CD	6.88	124.30	112.60
3	Q	174	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	34	ARG	N-CA-C	-6.83	96.24	110.80
3	S	141	SER	N-CA-C	-6.79	96.33	110.80
1	A	34	ARG	CA-C-N	6.77	134.47	121.54
1	A	34	ARG	C-N-CA	6.77	134.47	121.54
2	H	111	PHE	CA-C-N	6.64	129.41	120.65
2	H	111	PHE	C-N-CA	6.64	129.41	120.65
3	R	203	PHE	CA-C-N	6.59	132.82	122.94
3	R	203	PHE	C-N-CA	6.59	132.82	122.94
3	S	116	SER	CA-C-N	6.54	129.42	120.46
3	S	116	SER	C-N-CA	6.54	129.42	120.46
3	S	122	TYR	N-CA-C	-6.51	105.49	113.50
3	S	150	ASN	N-CA-C	-6.44	103.54	111.40
3	R	114	ASP	N-CA-C	-6.44	105.35	113.72
2	D	111	PHE	CA-C-N	6.37	129.05	120.65
2	D	111	PHE	C-N-CA	6.37	129.05	120.65
1	G	88	ALA	CA-C-N	6.36	128.80	120.28
1	G	88	ALA	C-N-CA	6.36	128.80	120.28
3	R	116	SER	CA-C-N	6.35	128.47	120.72
3	R	116	SER	C-N-CA	6.35	128.47	120.72
2	F	111	PHE	CA-C-N	6.33	129.01	120.65
2	F	111	PHE	C-N-CA	6.33	129.01	120.65
3	T	233	HIS	CA-C-N	6.31	133.67	121.18
3	T	233	HIS	C-N-CA	6.31	133.67	121.18
2	H	109	ASP	CA-CB-CG	6.31	118.91	112.60
3	S	227	ASP	CA-CB-CG	6.30	118.90	112.60
3	T	176	GLN	N-CA-C	6.27	118.64	108.41
3	R	98	PHE	CA-CB-CG	-6.26	107.54	113.80
1	E	30	LEU	CA-C-N	6.22	130.92	122.84
1	E	30	LEU	C-N-CA	6.22	130.92	122.84
3	R	174	ASN	CA-CB-CG	6.20	118.80	112.60
1	E	34	ARG	CA-C-N	6.17	133.32	121.54
1	E	34	ARG	C-N-CA	6.17	133.32	121.54
1	G	130	ASP	CA-C-N	6.14	128.43	120.44
1	G	130	ASP	C-N-CA	6.14	128.43	120.44
3	S	186	ARG	CA-C-N	6.12	133.00	121.97
3	S	186	ARG	C-N-CA	6.12	133.00	121.97
2	B	111	PHE	CA-C-N	6.06	129.21	120.79
2	B	111	PHE	C-N-CA	6.06	129.21	120.79
1	C	130	ASP	CA-C-N	6.04	128.69	120.54
1	C	130	ASP	C-N-CA	6.04	128.69	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	205	ASP	CA-CB-CG	6.00	118.60	112.60
3	Q	185	ALA	N-CA-C	-5.99	104.16	112.30
3	T	183	ASP	CA-C-N	5.93	128.48	120.65
3	T	183	ASP	C-N-CA	5.93	128.48	120.65
1	A	219	ARG	CA-C-N	5.91	126.49	119.94
1	A	219	ARG	C-N-CA	5.91	126.49	119.94
2	H	13	HIS	N-CA-C	-5.89	102.62	109.93
1	E	88	ALA	CA-C-N	5.88	128.75	120.28
1	E	88	ALA	C-N-CA	5.88	128.75	120.28
3	T	141	SER	N-CA-C	-5.88	105.19	112.72
1	A	35	SER	CA-C-N	5.84	129.05	120.82
1	A	35	SER	C-N-CA	5.84	129.05	120.82
2	B	109	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	130	ASP	CA-C-N	5.77	128.34	120.54
1	A	130	ASP	C-N-CA	5.77	128.34	120.54
3	S	176	GLN	CA-C-N	5.76	130.44	122.77
3	S	176	GLN	C-N-CA	5.76	130.44	122.77
1	E	130	ASP	CA-C-N	5.76	128.32	120.54
1	E	130	ASP	C-N-CA	5.76	128.32	120.54
1	E	32	SER	CA-C-N	5.74	132.50	121.54
1	E	32	SER	C-N-CA	5.74	132.50	121.54
3	R	226	PHE	CA-C-N	5.73	129.01	120.31
3	R	226	PHE	C-N-CA	5.73	129.01	120.31
3	R	95	ASN	CA-C-N	5.71	128.72	120.38
3	R	95	ASN	C-N-CA	5.71	128.72	120.38
3	S	130	GLU	CB-CG-CD	5.71	122.30	112.60
2	F	70	VAL	N-CA-CB	5.69	118.06	110.26
1	G	217	PHE	CA-CB-CG	5.68	119.48	113.80
1	C	88	ALA	CA-C-N	5.66	128.43	120.28
1	C	88	ALA	C-N-CA	5.66	128.43	120.28
3	Q	121	GLU	CB-CG-CD	5.64	122.19	112.60
3	R	114	ASP	CA-CB-CG	5.63	118.23	112.60
3	T	231	VAL	CA-C-N	5.63	128.09	120.44
3	T	231	VAL	C-N-CA	5.63	128.09	120.44
3	T	122	TYR	N-CA-C	-5.60	106.81	113.97
3	R	206	PRO	CA-C-N	5.59	129.20	120.75
3	R	206	PRO	C-N-CA	5.59	129.20	120.75
3	R	211	LYS	CA-C-N	5.58	128.19	120.49
3	R	211	LYS	C-N-CA	5.58	128.19	120.49
3	T	140	ASP	CA-CB-CG	5.54	118.14	112.60
3	Q	223	PRO	CA-C-N	5.53	128.24	120.28
3	Q	223	PRO	C-N-CA	5.53	128.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	181	LYS	CA-C-N	5.52	129.73	121.72
3	S	181	LYS	C-N-CA	5.52	129.73	121.72
1	G	34	ARG	N-CA-C	-5.50	105.20	111.14
2	F	109	ASP	CA-CB-CG	5.49	118.09	112.60
2	D	109	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	88	ALA	CA-C-N	5.48	128.17	120.28
1	A	88	ALA	C-N-CA	5.48	128.17	120.28
2	B	197	SER	CA-C-N	5.45	127.59	120.28
2	B	197	SER	C-N-CA	5.45	127.59	120.28
3	Q	123	ASP	CA-C-N	5.44	128.71	120.77
3	Q	123	ASP	C-N-CA	5.44	128.71	120.77
3	T	116	SER	CA-C-N	5.43	127.35	120.72
3	T	116	SER	C-N-CA	5.43	127.35	120.72
3	S	231	VAL	CA-C-N	5.42	127.99	120.29
3	S	231	VAL	C-N-CA	5.42	127.99	120.29
1	C	220	GLY	CA-C-N	5.41	131.44	121.70
1	C	220	GLY	C-N-CA	5.41	131.44	121.70
1	C	33	SER	CA-C-N	5.41	127.53	120.28
1	C	33	SER	C-N-CA	5.41	127.53	120.28
3	Q	176	GLN	N-CA-C	5.39	117.75	109.07
3	R	123	ASP	CA-C-N	5.38	129.25	121.18
3	R	123	ASP	C-N-CA	5.38	129.25	121.18
3	R	156	TRP	CA-C-N	5.36	127.90	120.29
3	R	156	TRP	C-N-CA	5.36	127.90	120.29
3	S	182	ALA	CA-C-N	5.36	131.77	121.54
3	S	182	ALA	C-N-CA	5.36	131.77	121.54
3	Q	116	SER	CA-C-N	5.34	127.77	120.46
3	Q	116	SER	C-N-CA	5.34	127.77	120.46
3	Q	120	LYS	CA-C-N	5.32	131.70	121.54
3	Q	120	LYS	C-N-CA	5.32	131.70	121.54
3	R	95	ASN	CA-CB-CG	5.31	117.91	112.60
2	F	197	SER	CA-C-N	5.31	127.93	120.28
2	F	197	SER	C-N-CA	5.31	127.93	120.28
3	S	141	SER	CA-C-N	5.29	127.62	120.38
3	S	141	SER	C-N-CA	5.29	127.62	120.38
2	D	123	SER	N-CA-C	5.27	122.03	110.80
3	T	139	SER	N-CA-C	-5.26	107.03	113.50
1	A	33	SER	CA-C-N	5.25	131.58	121.54
1	A	33	SER	C-N-CA	5.25	131.58	121.54
3	R	142	SER	CA-C-N	5.25	127.32	120.28
3	R	142	SER	C-N-CA	5.25	127.32	120.28
3	R	117	VAL	CA-C-N	5.22	129.82	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	117	VAL	C-N-CA	5.22	129.82	122.09
2	B	217	LYS	N-CA-C	-5.21	99.46	108.69
3	Q	232	ASN	CA-CB-CG	5.21	117.81	112.60
2	F	219	ASP	CA-CB-CG	5.21	117.81	112.60
3	R	227	ASP	CA-C-N	5.20	129.00	120.63
3	R	227	ASP	C-N-CA	5.20	129.00	120.63
3	T	227	ASP	CA-C-N	5.19	128.99	120.63
3	T	227	ASP	C-N-CA	5.19	128.99	120.63
3	S	187	VAL	CA-C-N	5.19	127.66	120.29
3	S	187	VAL	C-N-CA	5.19	127.66	120.29
2	B	202	THR	CA-C-N	5.18	128.21	120.90
2	B	202	THR	C-N-CA	5.18	128.21	120.90
2	B	183	SER	CA-C-N	5.16	127.91	120.38
2	B	183	SER	C-N-CA	5.16	127.91	120.38
1	C	5	THR	CB-CA-C	5.15	118.39	110.14
3	T	178	ASN	OD1-CG-ND2	5.15	127.75	122.60
3	Q	182	ALA	CA-C-N	5.15	131.37	121.54
3	Q	182	ALA	C-N-CA	5.15	131.37	121.54
3	T	148	PHE	CA-CB-CG	5.14	118.94	113.80
3	S	200	PHE	CA-C-N	5.13	127.93	120.79
3	S	200	PHE	C-N-CA	5.13	127.93	120.79
3	T	141	SER	CA-C-N	5.13	128.51	120.82
3	T	141	SER	C-N-CA	5.13	128.51	120.82
2	F	202	THR	CA-C-N	5.11	127.96	120.71
2	F	202	THR	C-N-CA	5.11	127.96	120.71
3	R	196	MET	CA-C-N	5.10	127.62	120.28
3	R	196	MET	C-N-CA	5.10	127.62	120.28
3	Q	224	SER	CA-C-N	5.08	129.32	120.68
3	Q	224	SER	C-N-CA	5.08	129.32	120.68
1	C	36	ASP	CA-C-N	5.07	128.53	121.24
1	C	36	ASP	C-N-CA	5.07	128.53	121.24
3	Q	184	ASP	CA-C-N	5.07	130.60	122.14
3	Q	184	ASP	C-N-CA	5.07	130.60	122.14
3	S	123	ASP	CA-CB-CG	-5.05	107.55	112.60
3	S	226	PHE	CA-C-N	5.05	127.99	120.31
3	S	226	PHE	C-N-CA	5.05	127.99	120.31
3	T	203	PHE	CA-C-N	5.05	130.11	122.99
3	T	203	PHE	C-N-CA	5.05	130.11	122.99
2	H	68	PHE	CA-CB-CG	5.04	118.84	113.80
3	S	186	ARG	N-CA-C	-5.03	105.51	111.69
2	D	219	ASP	CA-CB-CG	5.02	117.62	112.60
2	D	183	SER	CA-C-N	5.02	127.71	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	183	SER	C-N-CA	5.02	127.71	120.38
3	S	211	LYS	CA-C-N	5.02	128.02	120.69
3	S	211	LYS	C-N-CA	5.02	128.02	120.69
2	D	202	THR	CA-C-N	5.01	127.97	120.90
2	D	202	THR	C-N-CA	5.01	127.97	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1650	24	0
1	C	1711	0	1655	28	0
1	E	1708	0	1650	24	0
1	G	1695	0	1641	18	0
2	B	1658	0	1619	31	0
2	D	1670	0	1629	34	0
2	F	1658	0	1619	36	0
2	H	1667	0	1629	25	0
3	Q	1209	0	1150	39	0
3	R	1218	0	1158	21	0
3	S	1209	0	1150	45	0
3	T	1194	0	1134	32	0
4	I	28	0	24	4	0
4	J	28	0	25	4	0
5	K	39	0	34	4	0
6	Q	11	0	10	1	0
7	T	14	0	13	0	0
All	All	18425	0	17790	323	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 9.

All (323) 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)
3:Q:175:ILE:HG23	3:Q:217:ILE:HG23	1.39	1.04
3:T:99:TYR:HH	3:T:203:PHE:HD1	1.07	1.01
3:Q:162:MET:HG2	3:Q:177:PHE:CE1	1.99	0.98
1:A:8:PRO:O	1:A:110:THR:HG22	1.62	0.97
3:R:99:TYR:HH	3:R:203:PHE:HD1	0.99	0.96
3:S:99:TYR:HH	3:S:203:PHE:HD1	0.99	0.95
1:C:13:VAL:HG23	1:C:86:LEU:HD22	1.50	0.92
2:F:64:VAL:CG2	2:F:68:PHE:CG	2.52	0.91
1:C:8:PRO:O	1:C:110:THR:HG22	1.71	0.89
2:D:105:SER:HB2	3:T:119:MET:HE3	1.55	0.88
2:F:60:TYR:HE2	2:F:70:VAL:HG22	1.37	0.88
2:F:64:VAL:HG23	2:F:68:PHE:CG	2.11	0.85
2:F:64:VAL:HG23	2:F:68:PHE:CD1	2.13	0.84
2:D:91:THR:HG22	2:D:122:VAL:H	1.44	0.83
3:S:110:ILE:CG2	3:S:215:LEU:HD11	2.09	0.81
3:Q:162:MET:HG2	3:Q:177:PHE:HE1	1.47	0.80
3:Q:175:ILE:CG2	3:Q:217:ILE:HG23	2.11	0.80
3:T:99:TYR:OH	3:T:203:PHE:HD1	1.65	0.78
2:F:105:SER:HB2	3:Q:119:MET:HE2	1.66	0.78
3:Q:175:ILE:HG23	3:Q:217:ILE:CG2	2.13	0.78
3:S:120:LYS:HD3	5:K:1:NAG:H83	1.66	0.78
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.66	0.77
1:A:13:VAL:HG23	1:A:86:LEU:HD22	1.67	0.75
1:E:13:VAL:HG23	1:E:86:LEU:HD22	1.67	0.74
1:G:13:VAL:HG23	1:G:86:LEU:HD22	1.70	0.74
2:F:81:LEU:HD12	2:F:83:MET:HG3	1.69	0.73
2:D:91:THR:CG2	2:D:122:VAL:H	2.00	0.73
1:G:8:PRO:O	1:G:110:THR:HG22	1.87	0.73
2:F:64:VAL:HG21	2:F:68:PHE:CD2	2.24	0.73
3:S:110:ILE:HG22	3:S:215:LEU:HD11	1.71	0.72
2:F:60:TYR:CE2	2:F:70:VAL:HG22	2.24	0.72
2:B:91:THR:HG22	2:B:122:VAL:H	1.53	0.70
3:Q:179:ILE:HG12	3:Q:215:LEU:HG	1.71	0.70
3:T:172:GLY:HA3	3:T:224:SER:HB3	1.74	0.70
2:D:105:SER:HB2	3:T:119:MET:CE	2.22	0.69
2:H:106:TYR:HD2	3:S:165:ARG:HE	1.40	0.69
2:F:91:THR:HG22	2:F:122:VAL:H	1.55	0.69
2:F:64:VAL:CG2	2:F:68:PHE:HB2	2.23	0.69
2:F:81:LEU:CD1	2:F:83:MET:HG3	2.22	0.69
3:Q:197:ARG:NH2	3:Q:205:ASP:H	1.90	0.69
3:S:126:ILE:HD11	3:S:135:CYS:SG	2.34	0.68
2:B:91:THR:CG2	2:B:122:VAL:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HG	1:C:189:LEU:CD1	2.23	0.68
1:C:187:LEU:HG	1:C:189:LEU:HD11	1.76	0.68
3:Q:197:ARG:HH22	3:Q:205:ASP:H	1.40	0.67
3:S:126:ILE:HD13	3:S:132:LEU:HD23	1.76	0.67
2:F:64:VAL:HG22	2:F:68:PHE:HB2	1.77	0.66
1:E:187:LEU:HG	1:E:189:LEU:CD1	2.26	0.65
2:F:64:VAL:HG21	2:F:68:PHE:CG	2.29	0.65
1:E:129:SER:OG	2:F:133:PHE:HB3	1.97	0.65
2:B:127:THR:HB	3:S:88:LEU:HD11	1.79	0.64
3:Q:99:TYR:HB2	3:Q:110:ILE:HB	1.80	0.64
2:B:106:TYR:HE1	3:R:117:VAL:HB	1.62	0.64
1:E:21:ILE:HG12	1:E:110:THR:HG21	1.80	0.63
1:C:129:SER:OG	2:D:133:PHE:HB3	1.97	0.63
2:F:91:THR:CG2	2:F:122:VAL:H	2.11	0.63
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.81	0.63
1:E:187:LEU:HG	1:E:189:LEU:HD11	1.80	0.63
2:H:181:LEU:HG	2:H:181:LEU:O	1.99	0.62
3:Q:165:ARG:HH11	3:Q:165:ARG:CG	2.14	0.60
3:S:155:ASP:HB3	3:S:159:ASP:H	1.67	0.60
3:S:119:MET:HE1	5:K:1:NAG:H81	1.84	0.60
3:T:148:PHE:HD2	3:T:148:PHE:O	1.83	0.60
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.84	0.60
2:D:106:TYR:CE1	3:T:117:VAL:HB	2.38	0.59
1:E:172:THR:HG22	1:E:182:SER:H	1.66	0.59
3:T:136:LEU:HD13	3:T:141:SER:HB3	1.85	0.59
1:C:41:LEU:HD22	1:C:79:PHE:CG	2.37	0.58
3:T:165:ARG:NH2	3:T:171:GLU:HB2	2.18	0.58
3:S:126:ILE:HG21	3:S:132:LEU:CD2	2.34	0.58
2:F:64:VAL:CG2	2:F:68:PHE:CB	2.81	0.58
3:Q:212:VAL:HG12	4:I:1:NAG:H82	1.86	0.58
2:F:64:VAL:CG2	2:F:68:PHE:CD2	2.86	0.57
3:T:126:ILE:HD13	3:T:132:LEU:HD23	1.85	0.57
2:B:207:CYS:O	2:B:219:ASP:HA	2.04	0.57
1:G:129:SER:OG	2:H:133:PHE:HB3	2.04	0.57
3:Q:190:LYS:HD2	3:Q:193:ARG:NH1	2.20	0.57
1:E:195:GLU:HA	1:E:219:ARG:HD3	1.86	0.57
1:A:34:ARG:HG3	3:R:127:TYR:OH	2.05	0.57
3:T:126:ILE:HD11	3:T:135:CYS:SG	2.45	0.57
3:S:91:LEU:HB3	3:S:200:PHE:CE1	2.40	0.56
2:D:159:GLU:HG2	2:D:160:PRO:HA	1.88	0.56
1:C:101:SER:HB2	3:T:168:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG12	2:H:13:HIS:O	2.06	0.55
1:A:102:SER:HB2	3:R:170:LYS:H	1.72	0.55
3:Q:228:TYR:HA	3:Q:233:HIS:CD2	2.42	0.55
3:T:172:GLY:HA2	3:T:223:PRO:HD2	1.87	0.55
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.89	0.55
3:R:93:MET:HE1	3:R:202:GLY:O	2.07	0.55
3:S:136:LEU:HD13	3:S:141:SER:HB2	1.87	0.55
2:B:36:TRP:NE1	2:B:79:LEU:CD1	2.70	0.54
1:E:34:ARG:HA	3:Q:127:TYR:CE2	2.41	0.54
1:C:45:GLN:HB2	1:C:55:LEU:HD11	1.89	0.54
2:D:12:VAL:HG13	2:D:16:ARG:HB2	1.90	0.54
3:Q:116:SER:HB3	3:Q:214:TYR:CE2	2.43	0.54
3:Q:190:LYS:HD2	3:Q:193:ARG:HH12	1.72	0.54
3:T:179:ILE:HG21	3:T:192:ILE:HB	1.89	0.54
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.90	0.54
3:T:172:GLY:HA3	3:T:224:SER:CB	2.37	0.54
2:H:5:VAL:HG13	2:H:23:ALA:HB3	1.89	0.54
3:R:96:ASN:HB3	3:R:204:HIS:CE1	2.43	0.54
3:S:101:MET:HE3	3:S:144:ALA:HB1	1.90	0.54
3:Q:165:ARG:HH11	3:Q:165:ARG:HG3	1.71	0.54
3:S:126:ILE:HG21	3:S:132:LEU:HD21	1.90	0.54
2:B:106:TYR:CE1	3:R:117:VAL:HB	2.43	0.53
2:F:5:VAL:HG13	2:F:23:ALA:HB3	1.90	0.53
2:F:48:VAL:HG13	2:F:64:VAL:HG11	1.89	0.53
1:G:45:GLN:HB2	1:G:55:LEU:HD11	1.91	0.53
3:S:118:LEU:HD21	3:S:165:ARG:HB2	1.90	0.53
3:T:177:PHE:HB2	3:T:215:LEU:HB2	1.91	0.53
3:T:181:LYS:HE3	3:T:207:CYS:HB2	1.90	0.53
1:A:129:SER:OG	2:B:133:PHE:HB3	2.09	0.52
3:R:182:ALA:HB2	4:J:2:NAG:H83	1.90	0.52
1:A:157:LYS:HE2	2:D:43:LYS:NZ	2.25	0.52
2:B:60:TYR:HE2	2:B:70:VAL:HG12	1.74	0.52
2:D:12:VAL:HG12	2:D:13:HIS:O	2.08	0.52
1:A:8:PRO:HB3	1:C:212:PRO:HB2	1.89	0.52
1:C:31:TYR:CE2	1:C:33:SER:HB3	2.45	0.52
1:A:45:GLN:HB2	1:A:55:LEU:HD11	1.90	0.52
3:R:184:ASP:HB2	4:J:1:NAG:O6	2.09	0.52
2:H:30:GLY:O	2:H:53:HIS:HB2	2.10	0.52
3:R:118:LEU:HD21	3:R:165:ARG:HB2	1.92	0.52
2:F:81:LEU:HD12	2:F:83:MET:CG	2.38	0.52
3:T:165:ARG:HH22	3:T:171:GLU:HB2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:91:LEU:HB3	3:R:200:PHE:CE1	2.45	0.51
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.93	0.51
1:C:21:ILE:HG23	1:C:110:THR:HG21	1.91	0.51
2:D:36:TRP:NE1	2:D:79:LEU:CD1	2.74	0.51
2:F:30:GLY:O	2:F:53:HIS:HB2	2.10	0.51
2:F:108:TRP:HA	3:Q:122:TYR:CZ	2.46	0.51
2:F:130:PRO:HD2	2:F:216:THR:HG21	1.93	0.51
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.92	0.51
2:F:209:VAL:O	2:F:217:LYS:HA	2.11	0.51
2:D:5:VAL:HG13	2:D:23:ALA:HB3	1.92	0.51
3:Q:165:ARG:HD3	3:Q:171:GLU:HB2	1.93	0.50
3:Q:228:TYR:HA	3:Q:233:HIS:HD2	1.74	0.50
3:S:175:ILE:HD12	3:S:217:ILE:HB	1.92	0.50
3:S:155:ASP:C	3:S:157:LEU:H	2.19	0.50
2:B:126:SER:HB3	3:S:88:LEU:HG	1.93	0.50
2:F:91:THR:HG22	2:F:121:THR:HA	1.93	0.50
1:G:12:ALA:HA	1:G:113:GLU:O	2.11	0.50
1:G:31:TYR:HE2	3:S:166:ASN:ND2	2.09	0.50
2:F:87:ARG:O	2:F:122:VAL:HG11	2.12	0.50
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.94	0.49
1:E:41:LEU:HD22	1:E:79:PHE:CG	2.47	0.49
2:B:91:THR:HG22	2:B:121:THR:HA	1.94	0.49
3:T:148:PHE:O	3:T:148:PHE:CD2	2.66	0.49
2:D:195:VAL:HG11	2:D:205:TYR:CZ	2.48	0.49
3:R:138:LYS:HB2	3:R:141:SER:OG	2.12	0.49
2:D:30:GLY:O	2:D:53:HIS:HB2	2.12	0.49
1:G:152:ALA:HB2	1:G:206:HIS:HD2	1.77	0.49
1:E:2:ILE:HG22	1:E:4:MET:CE	2.43	0.49
2:H:195:VAL:HG11	2:H:205:TYR:CZ	2.48	0.49
2:B:30:GLY:O	2:B:53:HIS:HB2	2.12	0.49
1:C:155:GLN:HG2	1:C:162:LEU:HD11	1.94	0.49
3:Q:181:LYS:HE3	3:Q:207:CYS:HB2	1.94	0.49
3:T:91:LEU:HB3	3:T:200:PHE:CE1	2.48	0.48
2:B:195:VAL:HG11	2:B:205:TYR:CZ	2.48	0.48
2:D:14:PRO:HD3	2:D:124:GLY:N	2.27	0.48
3:S:148:PHE:CE2	3:S:152:LEU:HD11	2.47	0.48
2:D:204:THR:HG22	2:D:221:ARG:HH21	1.78	0.48
2:H:221:ARG:NH1	2:H:223:GLU:HG3	2.28	0.48
2:B:5:VAL:HG13	2:B:23:ALA:HB3	1.95	0.48
1:E:102:SER:HB2	3:Q:169:LYS:HA	1.95	0.48
2:H:60:TYR:HE2	2:H:70:VAL:HG12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:155:ASP:OD1	3:S:157:LEU:HB2	2.13	0.48
1:A:36:ASP:OD2	3:Q:88:LEU:HD11	2.14	0.48
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.96	0.48
3:R:169:LYS:HB3	3:R:171:GLU:OE1	2.14	0.48
2:H:195:VAL:HG13	2:H:196:PRO:HD2	1.96	0.47
2:B:204:THR:HG22	2:B:221:ARG:HH21	1.79	0.47
3:T:120:LYS:HG3	3:T:163:LEU:HD11	1.96	0.47
1:E:152:ALA:HB2	1:E:206:HIS:HD2	1.77	0.47
2:D:137:PRO:HD3	2:D:149:LEU:HD23	1.97	0.47
2:D:91:THR:HG22	2:D:121:THR:HA	1.97	0.47
2:F:195:VAL:HG11	2:F:205:TYR:CZ	2.50	0.47
2:H:137:PRO:HD3	2:H:149:LEU:HD23	1.95	0.47
3:S:124:VAL:CG2	3:S:166:ASN:HB3	2.45	0.47
3:T:118:LEU:HD12	3:T:176:GLN:HB2	1.97	0.47
1:A:128:PRO:HB3	1:A:139:SER:H	1.80	0.47
3:S:120:LYS:CD	5:K:1:NAG:H83	2.42	0.47
1:G:102:SER:HB2	3:S:169:LYS:HA	1.96	0.46
1:G:153:LYS:HE2	1:G:155:GLN:HE21	1.80	0.46
2:H:204:THR:HG22	2:H:221:ARG:HH21	1.80	0.46
3:S:126:ILE:O	3:S:161:PRO:HB3	2.15	0.46
1:G:40:TYR:HB2	1:G:100:TYR:HB2	1.98	0.46
3:Q:148:PHE:CE2	3:Q:152:LEU:HD11	2.51	0.46
1:C:40:TYR:HB2	1:C:100:TYR:HB2	1.97	0.46
2:D:33:ILE:HG21	2:D:107:ALA:HB2	1.96	0.46
1:E:40:TYR:HB2	1:E:100:TYR:HB2	1.97	0.46
1:E:153:LYS:HE2	1:E:155:GLN:HE21	1.80	0.46
2:D:60:TYR:HE2	2:D:70:VAL:HG12	1.80	0.46
3:Q:197:ARG:HH22	3:Q:205:ASP:HB2	1.80	0.46
3:R:112:VAL:HG11	3:R:206:PRO:HG2	1.98	0.46
1:E:41:LEU:HD22	1:E:79:PHE:CD1	2.51	0.46
3:S:174:ASN:ND2	3:S:218:ASN:HD21	2.14	0.46
3:T:98:PHE:HE2	3:T:228:TYR:HB3	1.81	0.46
1:G:6:GLN:HE21	1:G:110:THR:HG23	1.79	0.45
2:D:91:THR:HG22	2:D:122:VAL:N	2.23	0.45
2:D:211:HIS:CD2	2:D:213:PRO:HD2	2.51	0.45
1:G:11:LEU:HD11	1:G:13:VAL:HG13	1.97	0.45
3:Q:196:MET:HB3	3:Q:203:PHE:CE1	2.51	0.45
3:S:154:HIS:NE2	3:S:162:MET:HE1	2.31	0.45
2:B:137:PRO:HD3	2:B:149:LEU:HD23	1.99	0.45
1:C:99:TYR:CZ	2:D:110:ILE:HD11	2.51	0.45
2:D:73:ASP:OD2	2:D:76:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:182:GLN:OE1	2:F:188:SER:HB2	2.15	0.45
2:F:68:PHE:CD2	2:F:81:LEU:HD11	2.52	0.45
1:C:152:ALA:HB2	1:C:206:HIS:HD2	1.81	0.45
1:G:9:GLU:HG3	2:H:43:LYS:NZ	2.32	0.45
2:F:204:THR:HG22	2:F:221:ARG:HH21	1.81	0.44
2:H:108:TRP:HA	3:S:122:TYR:CZ	2.51	0.44
3:Q:177:PHE:HB2	3:Q:215:LEU:HB2	1.98	0.44
3:Q:179:ILE:HG22	3:Q:189:GLY:HA2	1.98	0.44
3:S:182:ALA:HB3	5:K:1:NAG:H62	2.00	0.44
1:A:40:TYR:HB2	1:A:100:TYR:HB2	1.99	0.44
2:B:48:VAL:HG13	2:B:64:VAL:HG21	1.99	0.44
2:B:218:VAL:HG12	2:B:219:ASP:N	2.33	0.44
1:C:41:LEU:HD22	1:C:79:PHE:CD1	2.52	0.44
3:Q:214:TYR:CZ	4:I:1:NAG:H83	2.52	0.44
1:A:142:CYS:HB2	1:A:156:TRP:CZ2	2.53	0.44
2:D:48:VAL:HG13	2:D:64:VAL:HG21	1.98	0.44
1:G:128:PRO:HB3	1:G:139:SER:H	1.83	0.44
3:Q:165:ARG:HH11	3:Q:165:ARG:CB	2.30	0.44
3:S:174:ASN:HD22	3:S:218:ASN:HD21	1.65	0.44
3:Q:109:LEU:O	3:Q:217:ILE:HA	2.16	0.44
1:C:13:VAL:HG21	1:C:19:ALA:HB2	2.00	0.44
3:Q:108:PHE:HB3	3:Q:217:ILE:HD11	2.00	0.44
1:A:152:ALA:HB2	1:A:206:HIS:HD2	1.82	0.44
3:S:165:ARG:HD2	3:S:171:GLU:HB2	1.98	0.44
3:Q:212:VAL:HG12	4:I:1:NAG:C8	2.47	0.43
2:B:195:VAL:HG13	2:B:196:PRO:HD2	1.99	0.43
2:D:195:VAL:HG13	2:D:196:PRO:HD2	2.00	0.43
2:D:170:LEU:HD21	2:D:193:VAL:HG11	2.01	0.43
2:F:195:VAL:HG13	2:F:196:PRO:HD2	2.00	0.43
3:T:152:LEU:HD21	3:T:196:MET:HG2	1.99	0.43
3:T:136:LEU:HD13	3:T:141:SER:CB	2.47	0.43
1:C:142:CYS:HB2	1:C:156:TRP:CZ2	2.53	0.43
1:E:128:PRO:HB3	1:E:139:SER:H	1.83	0.43
2:H:48:VAL:HG13	2:H:64:VAL:HG21	2.01	0.43
3:T:181:LYS:HD2	3:T:208:GLU:C	2.44	0.43
1:A:146:ASN:HD21	2:B:175:HIS:CE1	2.37	0.43
2:D:158:PRO:HD2	2:D:213:PRO:CB	2.48	0.43
2:H:206:ILE:HG13	2:H:221:ARG:HG3	2.01	0.43
1:E:159:ASP:HA	1:E:199:VAL:HG12	2.01	0.43
3:S:89:PRO:HG2	3:S:147:TRP:CE3	2.53	0.43
1:A:33:SER:O	1:A:34:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASP:HA	1:A:199:VAL:HG12	2.01	0.42
1:C:155:GLN:HB2	1:C:203:GLU:HG2	2.00	0.42
1:E:45:GLN:HB3	1:E:55:LEU:HD21	2.01	0.42
1:G:6:GLN:NE2	1:G:110:THR:HG23	2.34	0.42
3:S:160:PRO:HA	3:S:161:PRO:HD3	1.97	0.42
3:T:110:ILE:HG13	3:T:217:ILE:HG23	2.00	0.42
2:B:14:PRO:O	3:S:140:ASP:HB2	2.19	0.42
1:G:142:CYS:HB2	1:G:156:TRP:CZ2	2.55	0.42
1:G:159:ASP:HA	1:G:199:VAL:HG12	2.01	0.42
2:H:18:LEU:HD23	2:H:19:ARG:N	2.33	0.42
3:Q:177:PHE:HD2	3:Q:215:LEU:HB2	1.84	0.42
3:S:124:VAL:HG21	3:S:166:ASN:HB3	2.01	0.42
1:E:144:LEU:HB2	1:E:183:LEU:HB3	2.01	0.42
3:R:182:ALA:HB3	4:J:1:NAG:C6	2.49	0.42
1:A:144:LEU:HB2	1:A:183:LEU:HB3	2.01	0.42
2:H:73:ASP:OD2	2:H:76:LYS:HD2	2.20	0.42
3:R:165:ARG:HD3	3:R:171:GLU:OE1	2.19	0.42
3:T:157:LEU:HD23	3:T:158:MET:HE3	2.01	0.42
2:B:18:LEU:HD23	2:B:19:ARG:N	2.35	0.42
1:E:142:CYS:HB2	1:E:156:TRP:CZ2	2.54	0.42
3:S:110:ILE:HG23	3:S:215:LEU:HD11	1.92	0.42
2:H:51:ILE:HD11	2:H:55:GLU:HG2	2.01	0.42
2:H:91:THR:HG23	2:H:121:THR:HA	2.02	0.42
2:B:211:HIS:ND1	2:B:214:SER:HB3	2.35	0.42
1:C:128:PRO:HB3	1:C:139:SER:H	1.85	0.42
1:C:142:CYS:HB2	1:C:156:TRP:CH2	2.55	0.42
3:S:208:GLU:HB2	3:S:211:LYS:HB2	2.02	0.42
1:E:198:LYS:HE3	1:E:218:ASN:HB3	2.02	0.41
1:A:50:GLN:HA	2:B:116:GLN:NE2	2.36	0.41
2:B:73:ASP:OD2	2:B:76:LYS:HD2	2.21	0.41
1:A:4:MET:SD	1:A:98:GLN:HB2	2.61	0.41
2:B:51:ILE:HD11	2:B:55:GLU:HG2	2.01	0.41
3:S:145:ILE:HD12	3:S:217:ILE:HG21	2.01	0.41
1:C:2:ILE:HB	1:C:98:GLN:NE2	2.35	0.41
3:Q:136:LEU:O	3:Q:167:LYS:HD2	2.21	0.41
1:A:3:VAL:HG22	1:A:26:SER:HB3	2.02	0.41
2:B:12:VAL:HG13	2:B:16:ARG:HB2	2.03	0.41
2:F:137:PRO:HD3	2:F:149:LEU:HD23	2.03	0.41
3:Q:99:TYR:OH	3:Q:203:PHE:HD2	2.03	0.41
3:R:99:TYR:HB2	3:R:110:ILE:HB	2.01	0.41
2:B:124:GLY:O	3:S:143:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:182:ALA:HB3	4:J:1:NAG:H62	2.02	0.41
3:T:132:LEU:HD23	3:T:132:LEU:HA	1.95	0.41
3:Q:112:VAL:HG11	3:Q:206:PRO:HG2	2.02	0.41
3:R:204:HIS:O	3:R:206:PRO:HD3	2.21	0.41
1:A:157:LYS:HE2	2:D:43:LYS:HZ1	1.86	0.41
1:A:160:ASN:OD1	1:C:108:GLY:N	2.54	0.41
1:C:102:SER:HB2	3:T:169:LYS:HA	2.03	0.41
2:F:22:CYS:HB3	2:F:79:LEU:HB3	2.03	0.41
3:Q:165:ARG:HG3	3:Q:165:ARG:NH1	2.35	0.41
3:S:136:LEU:HD13	3:S:141:SER:CB	2.51	0.41
3:S:187:VAL:HG23	3:S:188:TYR:H	1.84	0.41
3:T:165:ARG:CZ	3:T:171:GLU:HB2	2.51	0.41
1:C:46:GLN:HG3	1:C:52:PRO:HG3	2.03	0.41
1:C:188:THR:C	1:C:189:LEU:HD12	2.46	0.41
2:D:18:LEU:HD23	2:D:19:ARG:N	2.36	0.41
2:H:161:VAL:HG23	2:H:211:HIS:HB2	2.03	0.41
3:R:176:GLN:HA	3:R:215:LEU:O	2.21	0.41
1:A:91:VAL:HG13	1:A:112:VAL:O	2.22	0.40
1:C:144:LEU:HB2	1:C:183:LEU:HB3	2.02	0.40
6:Q:303:BMA:H2	4:I:2:NAG:O3	2.21	0.40
2:D:36:TRP:NE1	2:D:79:LEU:HD11	2.37	0.40
1:E:46:GLN:HG3	1:E:52:PRO:HG3	2.03	0.40
1:E:188:THR:C	1:E:189:LEU:HD12	2.46	0.40
2:F:18:LEU:HD23	2:F:19:ARG:N	2.36	0.40
3:S:179:ILE:HA	3:S:189:GLY:HA2	2.03	0.40
3:S:190:LYS:HD2	3:S:193:ARG:HH21	1.87	0.40
3:T:126:ILE:HG23	3:T:131:ASP:HB2	2.03	0.40
1:A:132:GLN:O	1:A:135:SER:HB3	2.21	0.40
2:B:161:VAL:HG23	2:B:211:HIS:HB2	2.03	0.40
1:G:144:LEU:HB2	1:G:183:LEU:HB3	2.02	0.40
2:H:162:THR:OG1	2:H:210:ASN:HB3	2.21	0.40
3:S:136:LEU:C	3:S:138:LYS:H	2.29	0.40
1:C:104:PRO:HD3	2:D:109:ASP:OD2	2.21	0.40
1:E:1:ASP:CG	1:E:103:PRO:HD2	2.46	0.40
3:R:114:ASP:O	3:R:212:VAL:HG23	2.22	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	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	6	34
1	C	220/221 (100%)	206 (94%)	11 (5%)	3 (1%)	9	38
1	E	219/221 (99%)	205 (94%)	9 (4%)	5 (2%)	5	30
1	G	217/221 (98%)	206 (95%)	8 (4%)	3 (1%)	9	38
2	B	214/226 (95%)	201 (94%)	11 (5%)	2 (1%)	14	47
2	D	216/226 (96%)	204 (94%)	8 (4%)	4 (2%)	6	33
2	F	214/226 (95%)	201 (94%)	9 (4%)	4 (2%)	6	33
2	H	216/226 (96%)	202 (94%)	12 (6%)	2 (1%)	14	47
3	Q	149/152 (98%)	132 (89%)	15 (10%)	2 (1%)	9	40
3	R	150/152 (99%)	132 (88%)	17 (11%)	1 (1%)	18	53
3	S	149/152 (98%)	128 (86%)	16 (11%)	5 (3%)	3	24
3	T	147/152 (97%)	131 (89%)	15 (10%)	1 (1%)	18	53
All	All	2330/2396 (97%)	2151 (92%)	143 (6%)	36 (2%)	8	37

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	C	32	SER
3	S	183	ASP
1	A	35	SER
1	A	146	ASN
1	C	146	ASN
1	E	146	ASN
2	F	216	THR
1	G	146	ASN
3	Q	183	ASP
3	S	141	SER
1	A	59	ALA

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Mol	Chain	Res	Type
1	E	33	SER
1	E	35	SER
1	G	59	ALA
3	R	191	LYS
2	B	155	ASP
1	C	59	ALA
2	D	155	ASP
1	E	59	ALA
2	F	9	GLY
2	F	155	ASP
1	G	35	SER
2	H	155	ASP
3	S	137	ASN
2	D	9	GLY
2	D	16	ARG
1	E	34	ARG
2	F	43	LYS
2	H	9	GLY
2	D	43	LYS
3	Q	205	ASP
3	T	205	ASP
2	B	9	GLY
3	S	187	VAL
3	S	126	ILE

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	195/195 (100%)	186 (95%)	9 (5%)	24	47
1	C	196/195 (100%)	184 (94%)	12 (6%)	17	42
1	E	195/195 (100%)	185 (95%)	10 (5%)	21	46
1	G	194/195 (100%)	181 (93%)	13 (7%)	15	40
2	B	186/193 (96%)	178 (96%)	8 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	188/193 (97%)	180 (96%)	8 (4%)	26	49
2	F	186/193 (96%)	178 (96%)	8 (4%)	26	49
2	H	188/193 (97%)	177 (94%)	11 (6%)	18	43
3	Q	136/137 (99%)	128 (94%)	8 (6%)	18	43
3	R	137/137 (100%)	125 (91%)	12 (9%)	9	32
3	S	136/137 (99%)	128 (94%)	8 (6%)	18	43
3	T	134/137 (98%)	127 (95%)	7 (5%)	21	45
All	All	2071/2100 (99%)	1957 (94%)	114 (6%)	19	45

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	13	VAL
1	A	41	LEU
1	A	53	LYS
1	A	77	THR
1	A	86	LEU
1	A	102	SER
1	A	184	SER
1	A	199	VAL
2	B	31	THR
2	B	78	THR
2	B	85	SER
2	B	96	CYS
2	B	146	THR
2	B	159	GLU
2	B	190	SER
2	B	219	ASP
1	C	7	SER
1	C	13	VAL
1	C	14	SER
1	C	15	LEU
1	C	53	LYS
1	C	77	THR
1	C	86	LEU
1	C	111	LYS
1	C	184	SER
1	C	196	LYS
1	C	199	VAL

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Mol	Chain	Res	Type
1	C	221	GLU
2	D	5	VAL
2	D	31	THR
2	D	78	THR
2	D	96	CYS
2	D	146	THR
2	D	190	SER
2	D	193	VAL
2	D	226	SER
1	E	15	LEU
1	E	30	LEU
1	E	53	LYS
1	E	55	LEU
1	E	73	SER
1	E	77	THR
1	E	86	LEU
1	E	179	SER
1	E	184	SER
1	E	219	ARG
2	F	12	VAL
2	F	31	THR
2	F	78	THR
2	F	96	CYS
2	F	122	VAL
2	F	146	THR
2	F	159	GLU
2	F	190	SER
1	G	3	VAL
1	G	9	GLU
1	G	11	LEU
1	G	15	LEU
1	G	31	TYR
1	G	41	LEU
1	G	53	LYS
1	G	77	THR
1	G	86	LEU
1	G	122	SER
1	G	130	ASP
1	G	184	SER
1	G	196	LYS
2	H	28	THR
2	H	31	THR

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Mol	Chain	Res	Type
2	H	78	THR
2	H	83	MET
2	H	85	SER
2	H	88	ILE
2	H	96	CYS
2	H	146	THR
2	H	159	GLU
2	H	190	SER
2	H	223	GLU
3	Q	94	LEU
3	Q	95	ASN
3	Q	118	LEU
3	Q	162	MET
3	Q	164	CYS
3	Q	165	ARG
3	Q	191	LYS
3	Q	213	CYS
3	R	87	GLU
3	R	88	LEU
3	R	97	SER
3	R	112	VAL
3	R	113	SER
3	R	149	SER
3	R	162	MET
3	R	164	CYS
3	R	187	VAL
3	R	194	ASN
3	R	213	CYS
3	R	215	LEU
3	S	88	LEU
3	S	94	LEU
3	S	97	SER
3	S	112	VAL
3	S	116	SER
3	S	127	TYR
3	S	162	MET
3	S	165	ARG
3	T	94	LEU
3	T	164	CYS
3	T	165	ARG
3	T	170	LYS
3	T	194	ASN

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Mol	Chain	Res	Type
3	T	204	HIS
3	T	213	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	145	ASN
1	A	146	ASN
1	A	155	GLN
1	C	145	ASN
1	C	168	GLN
1	C	197	HIS
1	E	27	GLN
1	E	37	ASN
1	E	46	GLN
1	E	145	ASN
1	E	146	ASN
1	E	155	GLN
1	E	168	GLN
2	F	39	GLN
2	F	175	HIS
1	G	46	GLN
1	G	146	ASN
1	G	155	GLN
2	H	39	GLN
2	H	175	HIS
2	H	182	GLN
3	Q	233	HIS
3	R	150	ASN
3	R	174	ASN
3	R	238	GLN
3	S	174	ASN
3	T	95	ASN
3	T	96	ASN
3	T	174	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 ⓘ

7 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	$\# Z > 2$
4	NAG	I	1	3,4	14,14,15	0.70	0	17,19,21	1.39	3 (17%)
4	NAG	I	2	4	14,14,15	1.12	1 (7%)	17,19,21	2.88	7 (41%)
4	NAG	J	1	3,4	14,14,15	0.60	0	17,19,21	1.43	2 (11%)
4	NAG	J	2	4	14,14,15	0.65	0	17,19,21	1.27	2 (11%)
5	NAG	K	1	3,5	14,14,15	0.45	0	17,19,21	1.74	3 (17%)
5	NAG	K	2	5	14,14,15	0.56	0	17,19,21	1.00	1 (5%)
5	BMA	K	3	5	11,11,12	0.62	0	15,15,17	1.07	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	O5-C1	2.01	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	O5-C1-C2	8.12	123.85	111.29
5	K	1	NAG	C2-N2-C7	5.14	129.79	122.90
4	I	2	NAG	C1-C2-N2	4.00	116.73	110.43
4	I	2	NAG	O4-C4-C3	3.90	119.58	110.38
4	J	1	NAG	C1-C2-N2	3.58	116.07	110.43
4	I	2	NAG	C1-O5-C5	3.37	116.70	112.19
4	I	2	NAG	O3-C3-C4	3.34	118.24	110.38
4	J	2	NAG	C1-C2-N2	-3.32	105.21	110.43
4	J	1	NAG	O5-C1-C2	3.20	116.25	111.29
4	I	2	NAG	C2-N2-C7	2.97	126.88	122.90
5	K	1	NAG	C1-O5-C5	2.76	115.88	112.19
4	I	1	NAG	C2-N2-C7	2.64	126.44	122.90
4	I	1	NAG	O5-C1-C2	2.63	115.35	111.29
4	I	2	NAG	O5-C5-C4	-2.48	104.79	110.83
5	K	3	BMA	O2-C2-C3	2.41	115.15	110.15
4	J	2	NAG	C1-O5-C5	2.39	115.39	112.19
4	I	1	NAG	O4-C4-C5	-2.35	103.55	109.32
5	K	1	NAG	O3-C3-C4	-2.33	104.87	110.38
5	K	3	BMA	O3-C3-C4	2.26	115.70	110.38
5	K	2	NAG	O3-C3-C4	-2.12	105.37	110.38

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C4-C5-C6-O6

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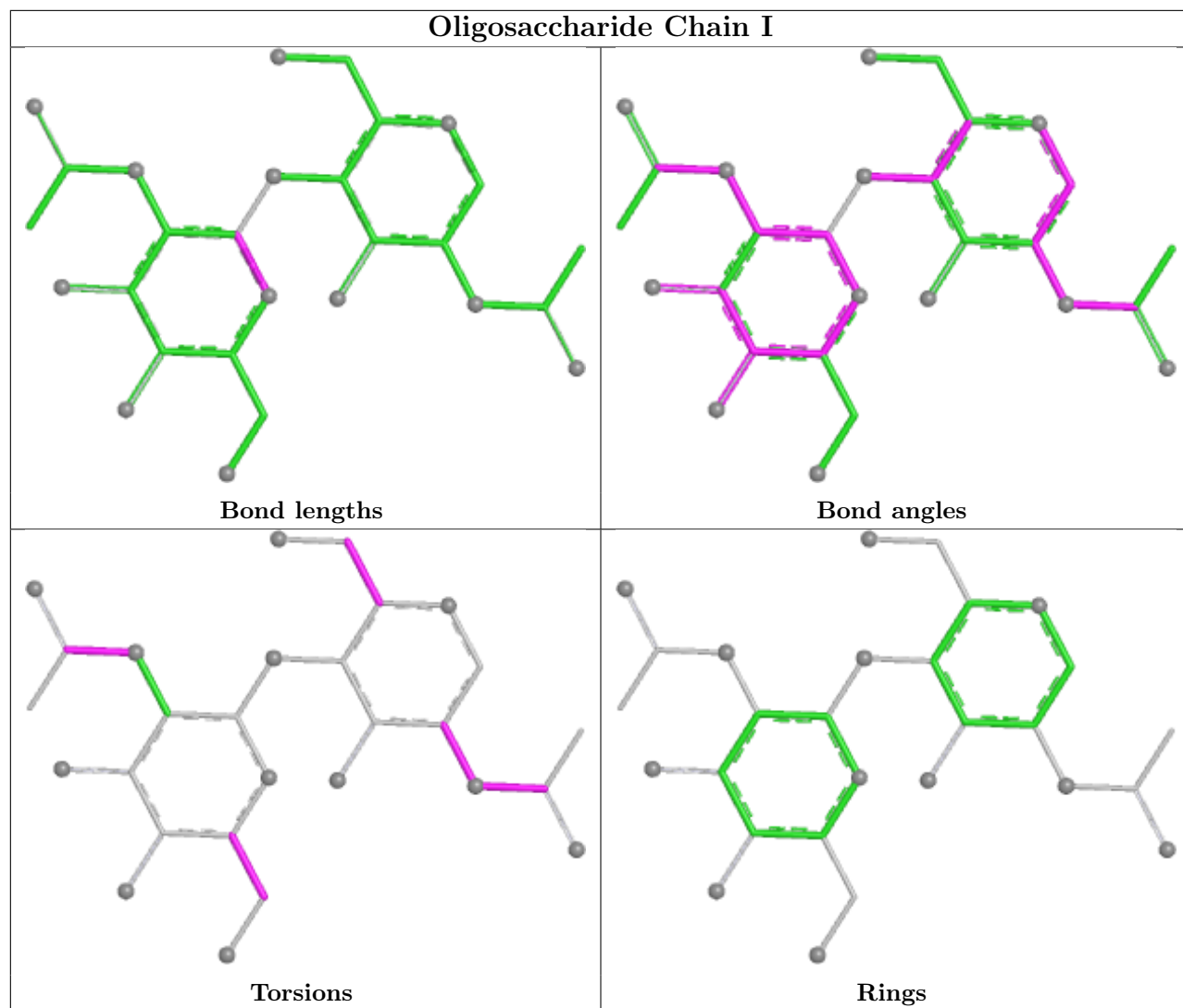
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	J	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6

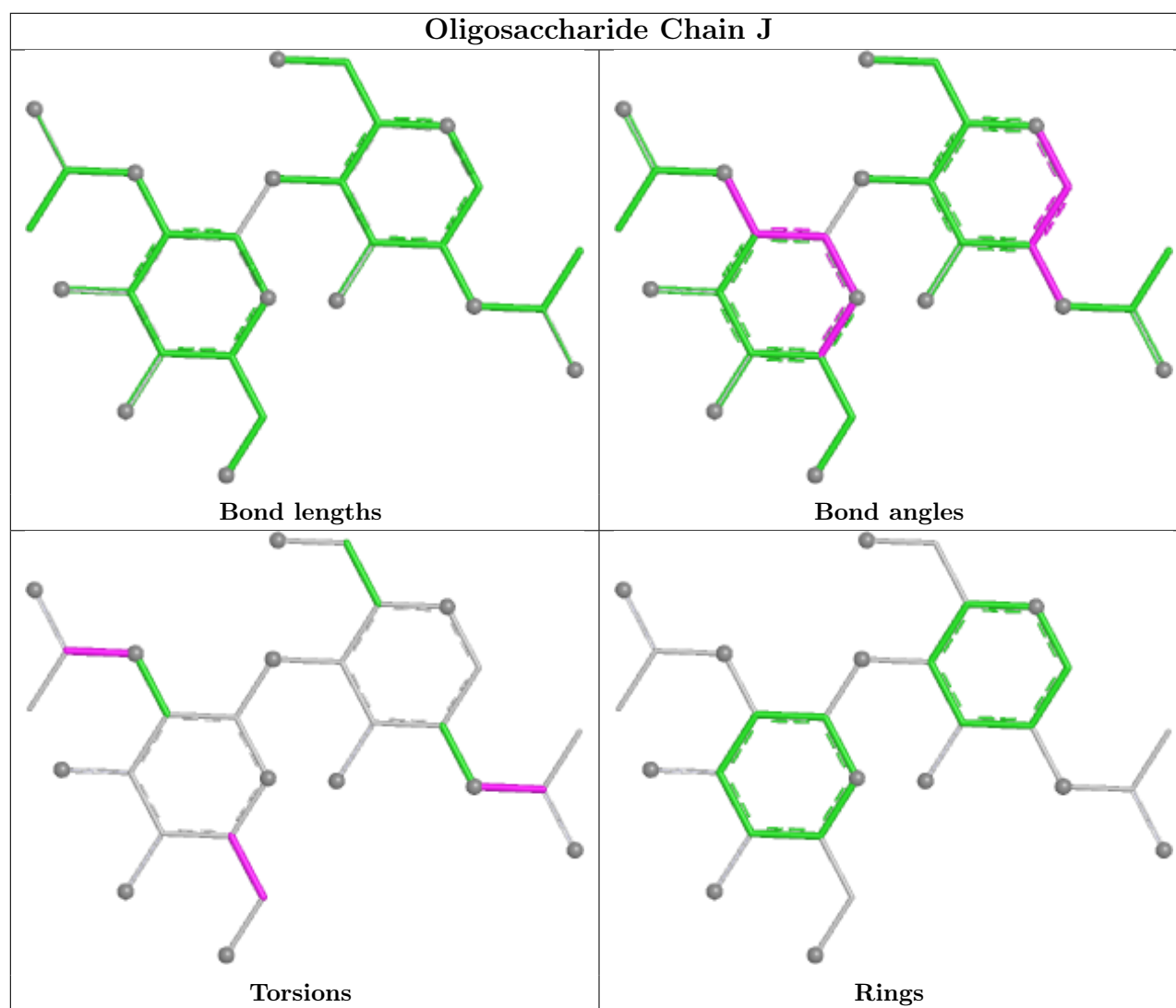
There are no ring outliers.

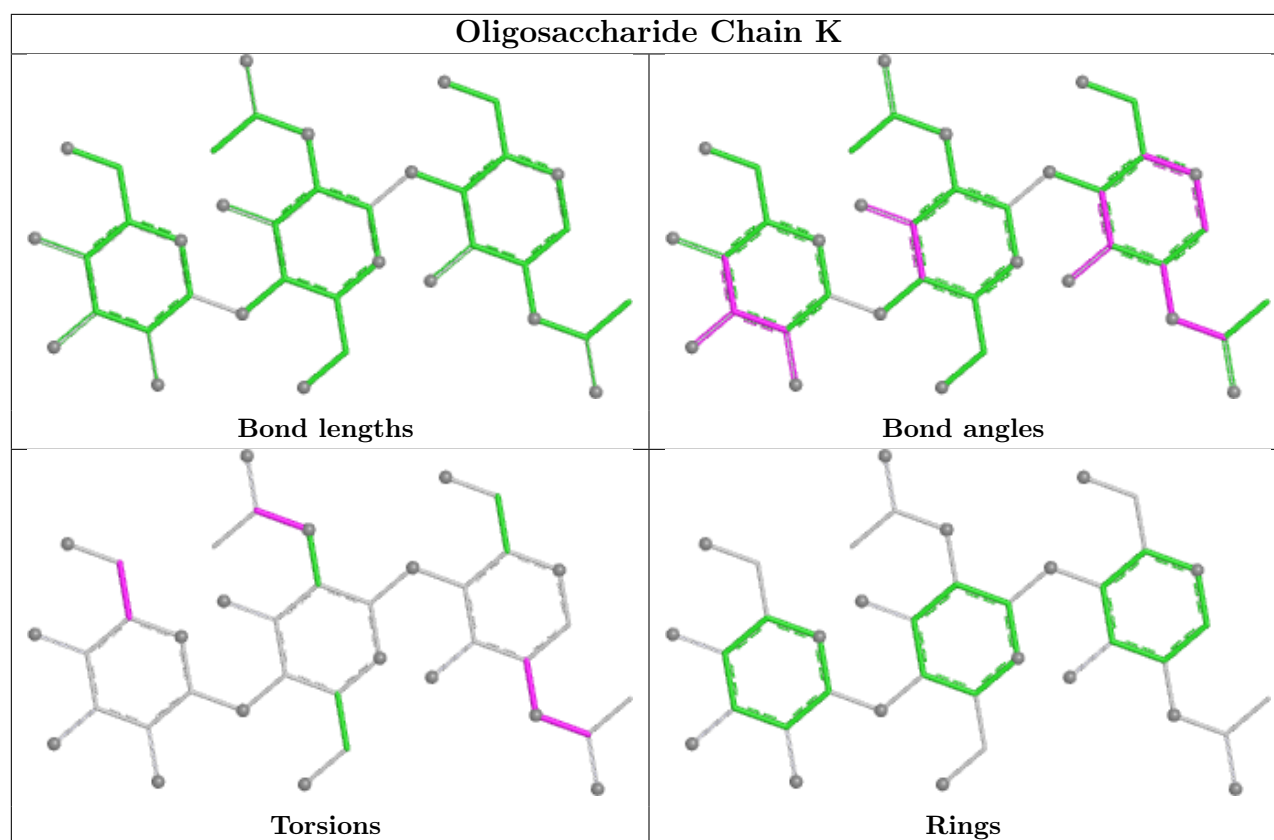
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	3	0
4	I	1	NAG	3	0
4	I	2	NAG	1	0
4	J	2	NAG	1	0
5	K	1	NAG	4	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	$\# Z > 2$
7	NAG	T	301	3	14,14,15	0.57	0	17,19,21	1.53	3 (17%)
6	BMA	Q	303	-	11,11,12	1.58	2 (18%)	15,15,17	2.37	6 (40%)

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
7	NAG	T	301	3	-	4/6/23/26	0/1/1/1
6	BMA	Q	303	-	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	303	BMA	C1-C2	-3.88	1.42	1.52
6	Q	303	BMA	O5-C5	2.45	1.48	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	303	BMA	O2-C2-C3	5.51	121.57	110.15
7	T	301	NAG	C2-N2-C7	3.66	127.81	122.90
6	Q	303	BMA	C1-O5-C5	3.17	116.44	112.19
6	Q	303	BMA	O3-C3-C4	2.99	117.42	110.38
6	Q	303	BMA	C2-C3-C4	2.81	115.80	110.86
6	Q	303	BMA	O5-C1-C2	-2.74	104.24	110.79
7	T	301	NAG	C1-O5-C5	2.66	115.75	112.19
7	T	301	NAG	C1-C2-N2	2.63	114.58	110.43
6	Q	303	BMA	C6-C5-C4	2.63	119.48	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	301	NAG	C3-C2-N2-C7
7	T	301	NAG	C8-C7-N2-C2
7	T	301	NAG	O7-C7-N2-C2
7	T	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	303	BMA	1	0

5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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	221/221 (100%)	-0.46	1 (0%) 87 72	21, 34, 49, 60	0
1	C	221/221 (100%)	-0.50	1 (0%) 87 72	21, 33, 49, 60	1 (0%)
1	E	221/221 (100%)	-0.45	0 100 100	21, 33, 49, 60	0
1	G	219/221 (99%)	-0.48	1 (0%) 87 72	21, 33, 49, 60	0
2	B	218/226 (96%)	-0.40	1 (0%) 87 72	20, 34, 49, 76	0
2	D	220/226 (97%)	-0.45	2 (0%) 81 62	20, 34, 49, 80	0
2	F	218/226 (96%)	-0.48	1 (0%) 87 72	20, 34, 49, 76	0
2	H	219/226 (96%)	-0.54	1 (0%) 87 72	18, 34, 49, 76	1 (0%)
3	Q	151/152 (99%)	-0.41	1 (0%) 84 67	38, 50, 60, 76	0
3	R	152/152 (100%)	-0.44	3 (1%) 65 45	18, 24, 35, 49	0
3	S	151/152 (99%)	-0.52	1 (0%) 84 67	12, 18, 30, 43	0
3	T	149/152 (98%)	-0.50	0 100 100	12, 18, 28, 43	0
All	All	2360/2396 (98%)	-0.47	13 (0%) 85 70	12, 33, 52, 80	2 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	138	SER	3.4
1	C	125	ILE	2.9
3	R	89	PRO	2.9
2	D	68	PHE	2.5
2	H	138	SER	2.5
3	R	87	GLU	2.5
1	G	4	MET	2.3
3	R	103	GLY	2.2
3	S	108	PHE	2.1
2	D	138	SER	2.1
2	B	185	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	190	LYS	2.0
1	A	35	SER	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](#)

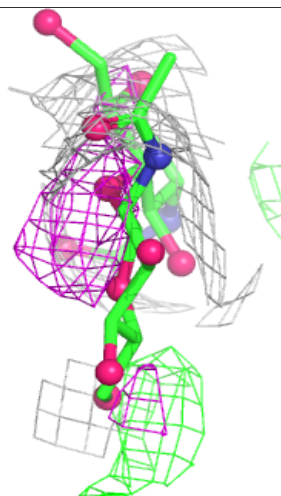
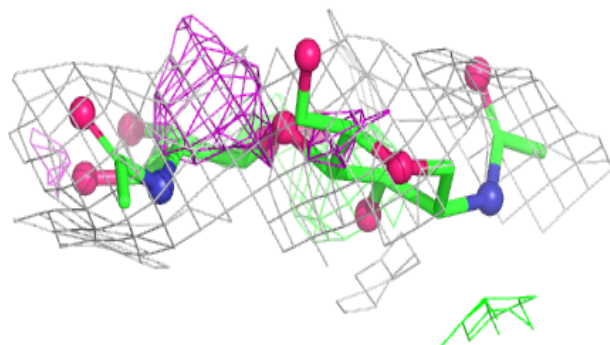
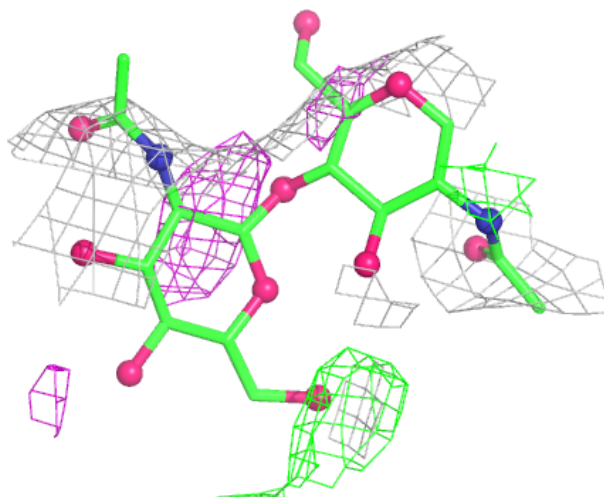
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	-	-	30,30,30,30	0
4	NAG	I	2	14/15	-	-	30,30,30,30	0
4	NAG	J	1	14/15	-	-	30,30,30,30	0
4	NAG	J	2	14/15	-	-	30,30,30,30	0
5	NAG	K	1	14/15	-	-	30,30,30,30	0
5	NAG	K	2	14/15	-	-	30,30,30,30	0
5	BMA	K	3	11/12	-	-	30,30,30,30	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.

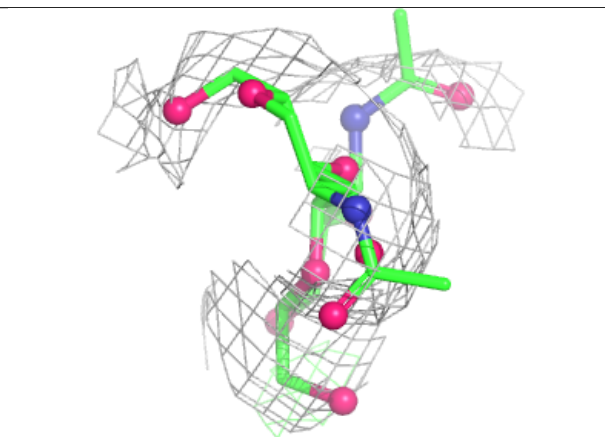
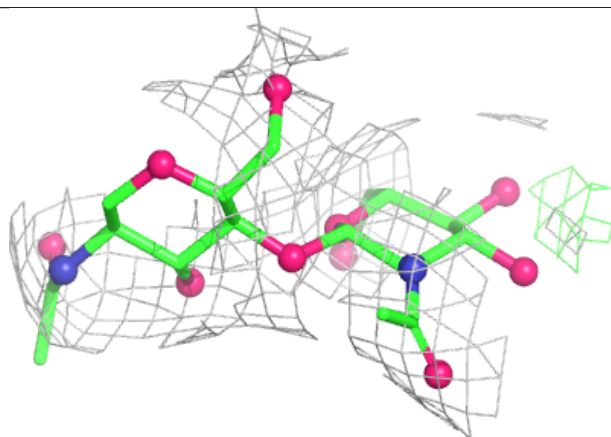
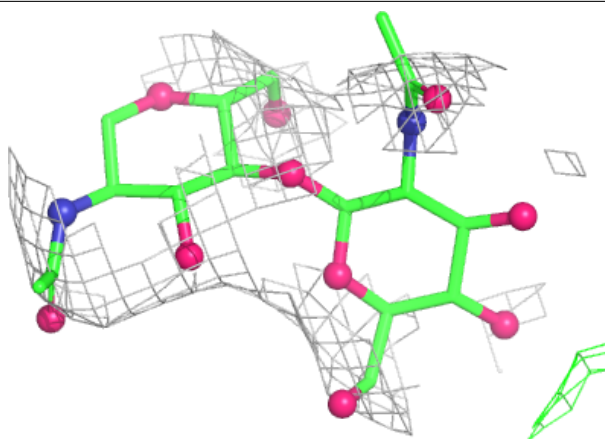
Electron density around Chain I:

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

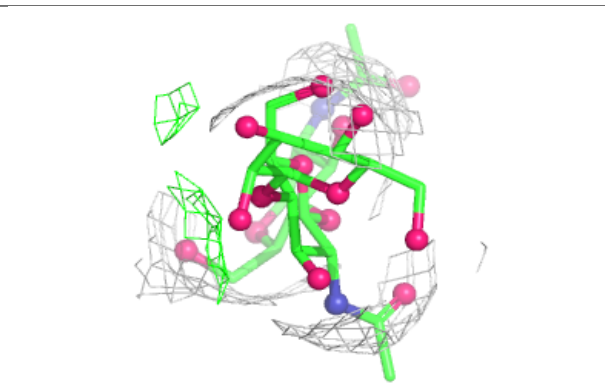
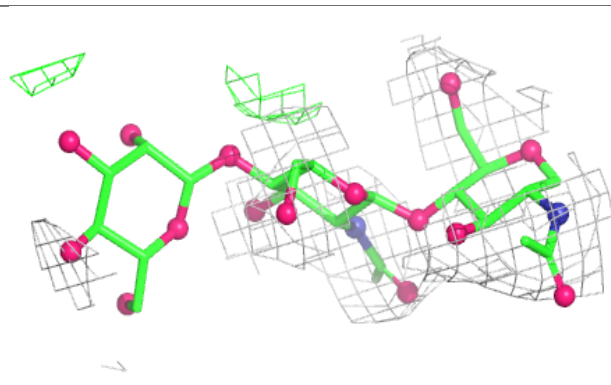
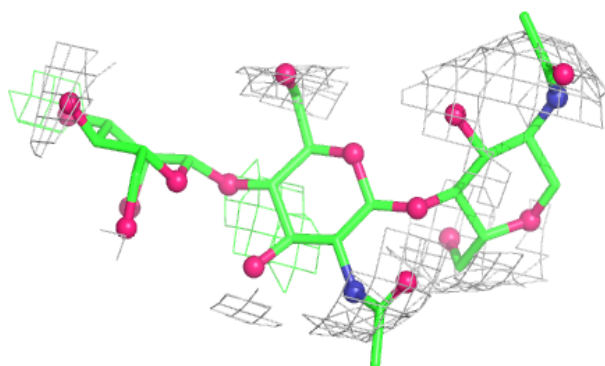


Electron density around Chain J:

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

**Electron density around Chain K:**

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



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
7	NAG	T	301	14/15	0.74	0.13	30,30,30,30	0
6	BMA	Q	303	11/12	0.86	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.