



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2025 – 02:00 pm BST

PDB ID : 9QWK / pdb_00009qwk
Title : Crystal structure of S2c-a5b6 TCR in complex with CD1c
Authors : Karuppiah, V.; Rangel, V.L.
Deposited on : 2025-04-14
Resolution : 2.27 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

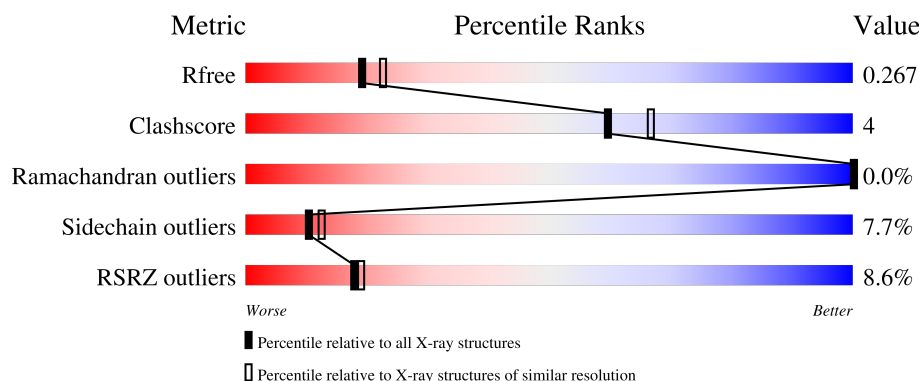
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	442	<div> <div>8%</div> <div>50%</div> <div>8%</div> <div>39%</div> </div>
1	B	442	<div> <div>%</div> <div>20%</div> <div>76%</div> </div>
1	G	442	<div> <div>6%</div> <div>49%</div> <div>10%</div> <div>39%</div> </div>
1	J	442	<div> <div>%</div> <div>20%</div> <div>76%</div> </div>
1	L	442	<div> <div>9%</div> <div>49%</div> <div>8%</div> <div>41%</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	442	
1	Q	442	
1	T	442	
2	D	200	
2	H	200	
2	M	200	
2	R	200	
3	E	246	
3	F	246	
3	K	246	
3	P	246	
4	C	2	
4	N	2	
5	I	2	
6	S	4	
7	U	3	
7	V	3	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26177 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 Beta-2-microglobulin,T-cell surface glycoprotein CD1c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2156	1381	370	397	8			
1	B	104	Total	C	N	O	S	0	0	0
			850	540	145	163	2			
1	G	271	Total	C	N	O	S	0	0	0
			2166	1389	370	399	8			
1	J	104	Total	C	N	O	S	0	0	0
			850	540	145	163	2			
1	L	261	Total	C	N	O	S	0	0	0
			2098	1349	359	382	8			
1	O	104	Total	C	N	O	S	0	0	0
			850	540	145	163	2			
1	Q	268	Total	C	N	O	S	0	0	0
			2141	1374	367	392	8			
1	T	104	Total	C	N	O	S	0	0	0
			850	540	145	163	2			

There are 560 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-128	MET	-	initiating methionine	UNP P61769
A	-127	TYR	-	expression tag	UNP P61769
A	-126	ARG	-	expression tag	UNP P61769
A	-125	MET	-	expression tag	UNP P61769
A	-124	GLN	-	expression tag	UNP P61769
A	-123	LEU	-	expression tag	UNP P61769
A	-122	LEU	-	expression tag	UNP P61769
A	-121	SER	-	expression tag	UNP P61769
A	-120	CYS	-	expression tag	UNP P61769
A	-119	ILE	-	expression tag	UNP P61769
A	-118	ALA	-	expression tag	UNP P61769
A	-117	LEU	-	expression tag	UNP P61769
A	-116	SER	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-115	LEU	-	expression tag	UNP P61769
A	-114	ALA	-	expression tag	UNP P61769
A	-113	LEU	-	expression tag	UNP P61769
A	-112	VAL	-	expression tag	UNP P61769
A	-111	THR	-	expression tag	UNP P61769
A	-110	ASN	-	expression tag	UNP P61769
A	-109	SER	-	expression tag	UNP P61769
A	-10	ILE	-	linker	UNP P61769
A	-9	GLY	-	linker	UNP P61769
A	-8	GLY	-	linker	UNP P61769
A	-7	GLY	-	linker	UNP P61769
A	-6	GLY	-	linker	UNP P61769
A	-5	SER	-	linker	UNP P61769
A	-4	GLY	-	linker	UNP P61769
A	-3	GLY	-	linker	UNP P61769
A	-2	GLY	-	linker	UNP P61769
A	-1	GLY	-	linker	UNP P61769
A	0	SER	-	linker	UNP P61769
A	1	GLY	-	linker	UNP P61769
A	2	GLY	-	linker	UNP P61769
A	3	GLY	-	linker	UNP P61769
A	4	GLY	-	linker	UNP P61769
A	5	SER	-	linker	UNP P61769
A	280	SER	-	expression tag	UNP P29017
A	281	LEU	-	expression tag	UNP P29017
A	282	SER	-	expression tag	UNP P29017
A	283	THR	-	expression tag	UNP P29017
A	284	PRO	-	expression tag	UNP P29017
A	285	PRO	-	expression tag	UNP P29017
A	286	THR	-	expression tag	UNP P29017
A	287	PRO	-	expression tag	UNP P29017
A	288	SER	-	expression tag	UNP P29017
A	289	THR	-	expression tag	UNP P29017
A	290	PRO	-	expression tag	UNP P29017
A	291	PRO	-	expression tag	UNP P29017
A	292	THR	-	expression tag	UNP P29017
A	293	GLY	-	expression tag	UNP P29017
A	294	LEU	-	expression tag	UNP P29017
A	295	ASN	-	expression tag	UNP P29017
A	296	ASP	-	expression tag	UNP P29017
A	297	ILE	-	expression tag	UNP P29017
A	298	PHE	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLU	-	expression tag	UNP P29017
A	300	ALA	-	expression tag	UNP P29017
A	301	GLN	-	expression tag	UNP P29017
A	302	LYS	-	expression tag	UNP P29017
A	303	ILE	-	expression tag	UNP P29017
A	304	GLU	-	expression tag	UNP P29017
A	305	TRP	-	expression tag	UNP P29017
A	306	HIS	-	expression tag	UNP P29017
A	307	GLU	-	expression tag	UNP P29017
A	308	HIS	-	expression tag	UNP P29017
A	309	HIS	-	expression tag	UNP P29017
A	310	HIS	-	expression tag	UNP P29017
A	311	HIS	-	expression tag	UNP P29017
A	312	HIS	-	expression tag	UNP P29017
A	313	HIS	-	expression tag	UNP P29017
B	-19	MET	-	initiating methionine	UNP P61769
B	-18	TYR	-	expression tag	UNP P61769
B	-17	ARG	-	expression tag	UNP P61769
B	-16	MET	-	expression tag	UNP P61769
B	-15	GLN	-	expression tag	UNP P61769
B	-14	LEU	-	expression tag	UNP P61769
B	-13	LEU	-	expression tag	UNP P61769
B	-12	SER	-	expression tag	UNP P61769
B	-11	CYS	-	expression tag	UNP P61769
B	-10	ILE	-	expression tag	UNP P61769
B	-9	ALA	-	expression tag	UNP P61769
B	-8	LEU	-	expression tag	UNP P61769
B	-7	SER	-	expression tag	UNP P61769
B	-6	LEU	-	expression tag	UNP P61769
B	-5	ALA	-	expression tag	UNP P61769
B	-4	LEU	-	expression tag	UNP P61769
B	-3	VAL	-	expression tag	UNP P61769
B	-2	THR	-	expression tag	UNP P61769
B	-1	ASN	-	expression tag	UNP P61769
B	0	SER	-	expression tag	UNP P61769
B	99	ILE	-	linker	UNP P61769
B	100	GLY	-	linker	UNP P61769
B	101	GLY	-	linker	UNP P61769
B	102	GLY	-	linker	UNP P61769
B	103	GLY	-	linker	UNP P61769
B	104	SER	-	linker	UNP P61769
B	105	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	106	GLY	-	linker	UNP P61769
B	107	GLY	-	linker	UNP P61769
B	108	GLY	-	linker	UNP P61769
B	109	SER	-	linker	UNP P61769
B	110	GLY	-	linker	UNP P61769
B	111	GLY	-	linker	UNP P61769
B	112	GLY	-	linker	UNP P61769
B	113	GLY	-	linker	UNP P61769
B	114	SER	-	linker	UNP P61769
B	389	SER	-	expression tag	UNP P29017
B	390	LEU	-	expression tag	UNP P29017
B	391	SER	-	expression tag	UNP P29017
B	392	THR	-	expression tag	UNP P29017
B	393	PRO	-	expression tag	UNP P29017
B	394	PRO	-	expression tag	UNP P29017
B	395	THR	-	expression tag	UNP P29017
B	396	PRO	-	expression tag	UNP P29017
B	397	SER	-	expression tag	UNP P29017
B	398	THR	-	expression tag	UNP P29017
B	399	PRO	-	expression tag	UNP P29017
B	400	PRO	-	expression tag	UNP P29017
B	401	THR	-	expression tag	UNP P29017
B	402	GLY	-	expression tag	UNP P29017
B	403	LEU	-	expression tag	UNP P29017
B	404	ASN	-	expression tag	UNP P29017
B	405	ASP	-	expression tag	UNP P29017
B	406	ILE	-	expression tag	UNP P29017
B	407	PHE	-	expression tag	UNP P29017
B	408	GLU	-	expression tag	UNP P29017
B	409	ALA	-	expression tag	UNP P29017
B	410	GLN	-	expression tag	UNP P29017
B	411	LYS	-	expression tag	UNP P29017
B	412	ILE	-	expression tag	UNP P29017
B	413	GLU	-	expression tag	UNP P29017
B	414	TRP	-	expression tag	UNP P29017
B	415	HIS	-	expression tag	UNP P29017
B	416	GLU	-	expression tag	UNP P29017
B	417	HIS	-	expression tag	UNP P29017
B	418	HIS	-	expression tag	UNP P29017
B	419	HIS	-	expression tag	UNP P29017
B	420	HIS	-	expression tag	UNP P29017
B	421	HIS	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	expression tag	UNP P29017
G	-128	MET	-	initiating methionine	UNP P61769
G	-127	TYR	-	expression tag	UNP P61769
G	-126	ARG	-	expression tag	UNP P61769
G	-125	MET	-	expression tag	UNP P61769
G	-124	GLN	-	expression tag	UNP P61769
G	-123	LEU	-	expression tag	UNP P61769
G	-122	LEU	-	expression tag	UNP P61769
G	-121	SER	-	expression tag	UNP P61769
G	-120	CYS	-	expression tag	UNP P61769
G	-119	ILE	-	expression tag	UNP P61769
G	-118	ALA	-	expression tag	UNP P61769
G	-117	LEU	-	expression tag	UNP P61769
G	-116	SER	-	expression tag	UNP P61769
G	-115	LEU	-	expression tag	UNP P61769
G	-114	ALA	-	expression tag	UNP P61769
G	-113	LEU	-	expression tag	UNP P61769
G	-112	VAL	-	expression tag	UNP P61769
G	-111	THR	-	expression tag	UNP P61769
G	-110	ASN	-	expression tag	UNP P61769
G	-109	SER	-	expression tag	UNP P61769
G	-10	ILE	-	linker	UNP P61769
G	-9	GLY	-	linker	UNP P61769
G	-8	GLY	-	linker	UNP P61769
G	-7	GLY	-	linker	UNP P61769
G	-6	GLY	-	linker	UNP P61769
G	-5	SER	-	linker	UNP P61769
G	-4	GLY	-	linker	UNP P61769
G	-3	GLY	-	linker	UNP P61769
G	-2	GLY	-	linker	UNP P61769
G	-1	GLY	-	linker	UNP P61769
G	0	SER	-	linker	UNP P61769
G	1	GLY	-	linker	UNP P61769
G	2	GLY	-	linker	UNP P61769
G	3	GLY	-	linker	UNP P61769
G	4	GLY	-	linker	UNP P61769
G	5	SER	-	linker	UNP P61769
G	280	SER	-	expression tag	UNP P29017
G	281	LEU	-	expression tag	UNP P29017
G	282	SER	-	expression tag	UNP P29017
G	283	THR	-	expression tag	UNP P29017
G	284	PRO	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
G	285	PRO	-	expression tag	UNP P29017
G	286	THR	-	expression tag	UNP P29017
G	287	PRO	-	expression tag	UNP P29017
G	288	SER	-	expression tag	UNP P29017
G	289	THR	-	expression tag	UNP P29017
G	290	PRO	-	expression tag	UNP P29017
G	291	PRO	-	expression tag	UNP P29017
G	292	THR	-	expression tag	UNP P29017
G	293	GLY	-	expression tag	UNP P29017
G	294	LEU	-	expression tag	UNP P29017
G	295	ASN	-	expression tag	UNP P29017
G	296	ASP	-	expression tag	UNP P29017
G	297	ILE	-	expression tag	UNP P29017
G	298	PHE	-	expression tag	UNP P29017
G	299	GLU	-	expression tag	UNP P29017
G	300	ALA	-	expression tag	UNP P29017
G	301	GLN	-	expression tag	UNP P29017
G	302	LYS	-	expression tag	UNP P29017
G	303	ILE	-	expression tag	UNP P29017
G	304	GLU	-	expression tag	UNP P29017
G	305	TRP	-	expression tag	UNP P29017
G	306	HIS	-	expression tag	UNP P29017
G	307	GLU	-	expression tag	UNP P29017
G	308	HIS	-	expression tag	UNP P29017
G	309	HIS	-	expression tag	UNP P29017
G	310	HIS	-	expression tag	UNP P29017
G	311	HIS	-	expression tag	UNP P29017
G	312	HIS	-	expression tag	UNP P29017
G	313	HIS	-	expression tag	UNP P29017
J	-19	MET	-	initiating methionine	UNP P61769
J	-18	TYR	-	expression tag	UNP P61769
J	-17	ARG	-	expression tag	UNP P61769
J	-16	MET	-	expression tag	UNP P61769
J	-15	GLN	-	expression tag	UNP P61769
J	-14	LEU	-	expression tag	UNP P61769
J	-13	LEU	-	expression tag	UNP P61769
J	-12	SER	-	expression tag	UNP P61769
J	-11	CYS	-	expression tag	UNP P61769
J	-10	ILE	-	expression tag	UNP P61769
J	-9	ALA	-	expression tag	UNP P61769
J	-8	LEU	-	expression tag	UNP P61769
J	-7	SER	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	LEU	-	expression tag	UNP P61769
J	-5	ALA	-	expression tag	UNP P61769
J	-4	LEU	-	expression tag	UNP P61769
J	-3	VAL	-	expression tag	UNP P61769
J	-2	THR	-	expression tag	UNP P61769
J	-1	ASN	-	expression tag	UNP P61769
J	0	SER	-	expression tag	UNP P61769
J	99	ILE	-	linker	UNP P61769
J	100	GLY	-	linker	UNP P61769
J	101	GLY	-	linker	UNP P61769
J	102	GLY	-	linker	UNP P61769
J	103	GLY	-	linker	UNP P61769
J	104	SER	-	linker	UNP P61769
J	105	GLY	-	linker	UNP P61769
J	106	GLY	-	linker	UNP P61769
J	107	GLY	-	linker	UNP P61769
J	108	GLY	-	linker	UNP P61769
J	109	SER	-	linker	UNP P61769
J	110	GLY	-	linker	UNP P61769
J	111	GLY	-	linker	UNP P61769
J	112	GLY	-	linker	UNP P61769
J	113	GLY	-	linker	UNP P61769
J	114	SER	-	linker	UNP P61769
J	389	SER	-	expression tag	UNP P29017
J	390	LEU	-	expression tag	UNP P29017
J	391	SER	-	expression tag	UNP P29017
J	392	THR	-	expression tag	UNP P29017
J	393	PRO	-	expression tag	UNP P29017
J	394	PRO	-	expression tag	UNP P29017
J	395	THR	-	expression tag	UNP P29017
J	396	PRO	-	expression tag	UNP P29017
J	397	SER	-	expression tag	UNP P29017
J	398	THR	-	expression tag	UNP P29017
J	399	PRO	-	expression tag	UNP P29017
J	400	PRO	-	expression tag	UNP P29017
J	401	THR	-	expression tag	UNP P29017
J	402	GLY	-	expression tag	UNP P29017
J	403	LEU	-	expression tag	UNP P29017
J	404	ASN	-	expression tag	UNP P29017
J	405	ASP	-	expression tag	UNP P29017
J	406	ILE	-	expression tag	UNP P29017
J	407	PHE	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
J	408	GLU	-	expression tag	UNP P29017
J	409	ALA	-	expression tag	UNP P29017
J	410	GLN	-	expression tag	UNP P29017
J	411	LYS	-	expression tag	UNP P29017
J	412	ILE	-	expression tag	UNP P29017
J	413	GLU	-	expression tag	UNP P29017
J	414	TRP	-	expression tag	UNP P29017
J	415	HIS	-	expression tag	UNP P29017
J	416	GLU	-	expression tag	UNP P29017
J	417	HIS	-	expression tag	UNP P29017
J	418	HIS	-	expression tag	UNP P29017
J	419	HIS	-	expression tag	UNP P29017
J	420	HIS	-	expression tag	UNP P29017
J	421	HIS	-	expression tag	UNP P29017
J	422	HIS	-	expression tag	UNP P29017
L	-128	MET	-	initiating methionine	UNP P61769
L	-127	TYR	-	expression tag	UNP P61769
L	-126	ARG	-	expression tag	UNP P61769
L	-125	MET	-	expression tag	UNP P61769
L	-124	GLN	-	expression tag	UNP P61769
L	-123	LEU	-	expression tag	UNP P61769
L	-122	LEU	-	expression tag	UNP P61769
L	-121	SER	-	expression tag	UNP P61769
L	-120	CYS	-	expression tag	UNP P61769
L	-119	ILE	-	expression tag	UNP P61769
L	-118	ALA	-	expression tag	UNP P61769
L	-117	LEU	-	expression tag	UNP P61769
L	-116	SER	-	expression tag	UNP P61769
L	-115	LEU	-	expression tag	UNP P61769
L	-114	ALA	-	expression tag	UNP P61769
L	-113	LEU	-	expression tag	UNP P61769
L	-112	VAL	-	expression tag	UNP P61769
L	-111	THR	-	expression tag	UNP P61769
L	-110	ASN	-	expression tag	UNP P61769
L	-109	SER	-	expression tag	UNP P61769
L	-10	ILE	-	linker	UNP P61769
L	-9	GLY	-	linker	UNP P61769
L	-8	GLY	-	linker	UNP P61769
L	-7	GLY	-	linker	UNP P61769
L	-6	GLY	-	linker	UNP P61769
L	-5	SER	-	linker	UNP P61769
L	-4	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	linker	UNP P61769
L	-2	GLY	-	linker	UNP P61769
L	-1	GLY	-	linker	UNP P61769
L	0	SER	-	linker	UNP P61769
L	1	GLY	-	linker	UNP P61769
L	2	GLY	-	linker	UNP P61769
L	3	GLY	-	linker	UNP P61769
L	4	GLY	-	linker	UNP P61769
L	5	SER	-	linker	UNP P61769
L	280	SER	-	expression tag	UNP P29017
L	281	LEU	-	expression tag	UNP P29017
L	282	SER	-	expression tag	UNP P29017
L	283	THR	-	expression tag	UNP P29017
L	284	PRO	-	expression tag	UNP P29017
L	285	PRO	-	expression tag	UNP P29017
L	286	THR	-	expression tag	UNP P29017
L	287	PRO	-	expression tag	UNP P29017
L	288	SER	-	expression tag	UNP P29017
L	289	THR	-	expression tag	UNP P29017
L	290	PRO	-	expression tag	UNP P29017
L	291	PRO	-	expression tag	UNP P29017
L	292	THR	-	expression tag	UNP P29017
L	293	GLY	-	expression tag	UNP P29017
L	294	LEU	-	expression tag	UNP P29017
L	295	ASN	-	expression tag	UNP P29017
L	296	ASP	-	expression tag	UNP P29017
L	297	ILE	-	expression tag	UNP P29017
L	298	PHE	-	expression tag	UNP P29017
L	299	GLU	-	expression tag	UNP P29017
L	300	ALA	-	expression tag	UNP P29017
L	301	GLN	-	expression tag	UNP P29017
L	302	LYS	-	expression tag	UNP P29017
L	303	ILE	-	expression tag	UNP P29017
L	304	GLU	-	expression tag	UNP P29017
L	305	TRP	-	expression tag	UNP P29017
L	306	HIS	-	expression tag	UNP P29017
L	307	GLU	-	expression tag	UNP P29017
L	308	HIS	-	expression tag	UNP P29017
L	309	HIS	-	expression tag	UNP P29017
L	310	HIS	-	expression tag	UNP P29017
L	311	HIS	-	expression tag	UNP P29017
L	312	HIS	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
L	313	HIS	-	expression tag	UNP P29017
O	-19	MET	-	initiating methionine	UNP P61769
O	-18	TYR	-	expression tag	UNP P61769
O	-17	ARG	-	expression tag	UNP P61769
O	-16	MET	-	expression tag	UNP P61769
O	-15	GLN	-	expression tag	UNP P61769
O	-14	LEU	-	expression tag	UNP P61769
O	-13	LEU	-	expression tag	UNP P61769
O	-12	SER	-	expression tag	UNP P61769
O	-11	CYS	-	expression tag	UNP P61769
O	-10	ILE	-	expression tag	UNP P61769
O	-9	ALA	-	expression tag	UNP P61769
O	-8	LEU	-	expression tag	UNP P61769
O	-7	SER	-	expression tag	UNP P61769
O	-6	LEU	-	expression tag	UNP P61769
O	-5	ALA	-	expression tag	UNP P61769
O	-4	LEU	-	expression tag	UNP P61769
O	-3	VAL	-	expression tag	UNP P61769
O	-2	THR	-	expression tag	UNP P61769
O	-1	ASN	-	expression tag	UNP P61769
O	0	SER	-	expression tag	UNP P61769
O	99	ILE	-	linker	UNP P61769
O	100	GLY	-	linker	UNP P61769
O	101	GLY	-	linker	UNP P61769
O	102	GLY	-	linker	UNP P61769
O	103	GLY	-	linker	UNP P61769
O	104	SER	-	linker	UNP P61769
O	105	GLY	-	linker	UNP P61769
O	106	GLY	-	linker	UNP P61769
O	107	GLY	-	linker	UNP P61769
O	108	GLY	-	linker	UNP P61769
O	109	SER	-	linker	UNP P61769
O	110	GLY	-	linker	UNP P61769
O	111	GLY	-	linker	UNP P61769
O	112	GLY	-	linker	UNP P61769
O	113	GLY	-	linker	UNP P61769
O	114	SER	-	linker	UNP P61769
O	389	SER	-	expression tag	UNP P29017
O	390	LEU	-	expression tag	UNP P29017
O	391	SER	-	expression tag	UNP P29017
O	392	THR	-	expression tag	UNP P29017
O	393	PRO	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
O	394	PRO	-	expression tag	UNP P29017
O	395	THR	-	expression tag	UNP P29017
O	396	PRO	-	expression tag	UNP P29017
O	397	SER	-	expression tag	UNP P29017
O	398	THR	-	expression tag	UNP P29017
O	399	PRO	-	expression tag	UNP P29017
O	400	PRO	-	expression tag	UNP P29017
O	401	THR	-	expression tag	UNP P29017
O	402	GLY	-	expression tag	UNP P29017
O	403	LEU	-	expression tag	UNP P29017
O	404	ASN	-	expression tag	UNP P29017
O	405	ASP	-	expression tag	UNP P29017
O	406	ILE	-	expression tag	UNP P29017
O	407	PHE	-	expression tag	UNP P29017
O	408	GLU	-	expression tag	UNP P29017
O	409	ALA	-	expression tag	UNP P29017
O	410	GLN	-	expression tag	UNP P29017
O	411	LYS	-	expression tag	UNP P29017
O	412	ILE	-	expression tag	UNP P29017
O	413	GLU	-	expression tag	UNP P29017
O	414	TRP	-	expression tag	UNP P29017
O	415	HIS	-	expression tag	UNP P29017
O	416	GLU	-	expression tag	UNP P29017
O	417	HIS	-	expression tag	UNP P29017
O	418	HIS	-	expression tag	UNP P29017
O	419	HIS	-	expression tag	UNP P29017
O	420	HIS	-	expression tag	UNP P29017
O	421	HIS	-	expression tag	UNP P29017
O	422	HIS	-	expression tag	UNP P29017
Q	-128	MET	-	initiating methionine	UNP P61769
Q	-127	TYR	-	expression tag	UNP P61769
Q	-126	ARG	-	expression tag	UNP P61769
Q	-125	MET	-	expression tag	UNP P61769
Q	-124	GLN	-	expression tag	UNP P61769
Q	-123	LEU	-	expression tag	UNP P61769
Q	-122	LEU	-	expression tag	UNP P61769
Q	-121	SER	-	expression tag	UNP P61769
Q	-120	CYS	-	expression tag	UNP P61769
Q	-119	ILE	-	expression tag	UNP P61769
Q	-118	ALA	-	expression tag	UNP P61769
Q	-117	LEU	-	expression tag	UNP P61769
Q	-116	SER	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-115	LEU	-	expression tag	UNP P61769
Q	-114	ALA	-	expression tag	UNP P61769
Q	-113	LEU	-	expression tag	UNP P61769
Q	-112	VAL	-	expression tag	UNP P61769
Q	-111	THR	-	expression tag	UNP P61769
Q	-110	ASN	-	expression tag	UNP P61769
Q	-109	SER	-	expression tag	UNP P61769
Q	-10	ILE	-	linker	UNP P61769
Q	-9	GLY	-	linker	UNP P61769
Q	-8	GLY	-	linker	UNP P61769
Q	-7	GLY	-	linker	UNP P61769
Q	-6	GLY	-	linker	UNP P61769
Q	-5	SER	-	linker	UNP P61769
Q	-4	GLY	-	linker	UNP P61769
Q	-3	GLY	-	linker	UNP P61769
Q	-2	GLY	-	linker	UNP P61769
Q	-1	GLY	-	linker	UNP P61769
Q	0	SER	-	linker	UNP P61769
Q	1	GLY	-	linker	UNP P61769
Q	2	GLY	-	linker	UNP P61769
Q	3	GLY	-	linker	UNP P61769
Q	4	GLY	-	linker	UNP P61769
Q	5	SER	-	linker	UNP P61769
Q	280	SER	-	expression tag	UNP P29017
Q	281	LEU	-	expression tag	UNP P29017
Q	282	SER	-	expression tag	UNP P29017
Q	283	THR	-	expression tag	UNP P29017
Q	284	PRO	-	expression tag	UNP P29017
Q	285	PRO	-	expression tag	UNP P29017
Q	286	THR	-	expression tag	UNP P29017
Q	287	PRO	-	expression tag	UNP P29017
Q	288	SER	-	expression tag	UNP P29017
Q	289	THR	-	expression tag	UNP P29017
Q	290	PRO	-	expression tag	UNP P29017
Q	291	PRO	-	expression tag	UNP P29017
Q	292	THR	-	expression tag	UNP P29017
Q	293	GLY	-	expression tag	UNP P29017
Q	294	LEU	-	expression tag	UNP P29017
Q	295	ASN	-	expression tag	UNP P29017
Q	296	ASP	-	expression tag	UNP P29017
Q	297	ILE	-	expression tag	UNP P29017
Q	298	PHE	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	299	GLU	-	expression tag	UNP P29017
Q	300	ALA	-	expression tag	UNP P29017
Q	301	GLN	-	expression tag	UNP P29017
Q	302	LYS	-	expression tag	UNP P29017
Q	303	ILE	-	expression tag	UNP P29017
Q	304	GLU	-	expression tag	UNP P29017
Q	305	TRP	-	expression tag	UNP P29017
Q	306	HIS	-	expression tag	UNP P29017
Q	307	GLU	-	expression tag	UNP P29017
Q	308	HIS	-	expression tag	UNP P29017
Q	309	HIS	-	expression tag	UNP P29017
Q	310	HIS	-	expression tag	UNP P29017
Q	311	HIS	-	expression tag	UNP P29017
Q	312	HIS	-	expression tag	UNP P29017
Q	313	HIS	-	expression tag	UNP P29017
T	-19	MET	-	initiating methionine	UNP P61769
T	-18	TYR	-	expression tag	UNP P61769
T	-17	ARG	-	expression tag	UNP P61769
T	-16	MET	-	expression tag	UNP P61769
T	-15	GLN	-	expression tag	UNP P61769
T	-14	LEU	-	expression tag	UNP P61769
T	-13	LEU	-	expression tag	UNP P61769
T	-12	SER	-	expression tag	UNP P61769
T	-11	CYS	-	expression tag	UNP P61769
T	-10	ILE	-	expression tag	UNP P61769
T	-9	ALA	-	expression tag	UNP P61769
T	-8	LEU	-	expression tag	UNP P61769
T	-7	SER	-	expression tag	UNP P61769
T	-6	LEU	-	expression tag	UNP P61769
T	-5	ALA	-	expression tag	UNP P61769
T	-4	LEU	-	expression tag	UNP P61769
T	-3	VAL	-	expression tag	UNP P61769
T	-2	THR	-	expression tag	UNP P61769
T	-1	ASN	-	expression tag	UNP P61769
T	0	SER	-	expression tag	UNP P61769
T	99	ILE	-	linker	UNP P61769
T	100	GLY	-	linker	UNP P61769
T	101	GLY	-	linker	UNP P61769
T	102	GLY	-	linker	UNP P61769
T	103	GLY	-	linker	UNP P61769
T	104	SER	-	linker	UNP P61769
T	105	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
T	106	GLY	-	linker	UNP P61769
T	107	GLY	-	linker	UNP P61769
T	108	GLY	-	linker	UNP P61769
T	109	SER	-	linker	UNP P61769
T	110	GLY	-	linker	UNP P61769
T	111	GLY	-	linker	UNP P61769
T	112	GLY	-	linker	UNP P61769
T	113	GLY	-	linker	UNP P61769
T	114	SER	-	linker	UNP P61769
T	389	SER	-	expression tag	UNP P29017
T	390	LEU	-	expression tag	UNP P29017
T	391	SER	-	expression tag	UNP P29017
T	392	THR	-	expression tag	UNP P29017
T	393	PRO	-	expression tag	UNP P29017
T	394	PRO	-	expression tag	UNP P29017
T	395	THR	-	expression tag	UNP P29017
T	396	PRO	-	expression tag	UNP P29017
T	397	SER	-	expression tag	UNP P29017
T	398	THR	-	expression tag	UNP P29017
T	399	PRO	-	expression tag	UNP P29017
T	400	PRO	-	expression tag	UNP P29017
T	401	THR	-	expression tag	UNP P29017
T	402	GLY	-	expression tag	UNP P29017
T	403	LEU	-	expression tag	UNP P29017
T	404	ASN	-	expression tag	UNP P29017
T	405	ASP	-	expression tag	UNP P29017
T	406	ILE	-	expression tag	UNP P29017
T	407	PHE	-	expression tag	UNP P29017
T	408	GLU	-	expression tag	UNP P29017
T	409	ALA	-	expression tag	UNP P29017
T	410	GLN	-	expression tag	UNP P29017
T	411	LYS	-	expression tag	UNP P29017
T	412	ILE	-	expression tag	UNP P29017
T	413	GLU	-	expression tag	UNP P29017
T	414	TRP	-	expression tag	UNP P29017
T	415	HIS	-	expression tag	UNP P29017
T	416	GLU	-	expression tag	UNP P29017
T	417	HIS	-	expression tag	UNP P29017
T	418	HIS	-	expression tag	UNP P29017
T	419	HIS	-	expression tag	UNP P29017
T	420	HIS	-	expression tag	UNP P29017
T	421	HIS	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
T	422	HIS	-	expression tag	UNP P29017

- Molecule 2 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	191	Total	C	N	O	S	0	0	0
			1486	937	239	302	8			
2	H	192	Total	C	N	O	S	0	0	0
			1492	940	240	304	8			
2	M	192	Total	C	N	O	S	0	0	0
			1492	940	240	304	8			
2	R	192	Total	C	N	O	S	0	0	0
			1492	940	240	304	8			

- Molecule 3 is a protein called TCR beta.

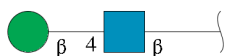
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	245	Total	C	N	O	S	0	0	0
			1972	1235	354	376	7			
3	F	243	Total	C	N	O	S	0	0	0
			1956	1227	352	370	7			
3	K	243	Total	C	N	O	S	0	0	0
			1956	1227	352	370	7			
3	P	243	Total	C	N	O	S	0	0	0
			1956	1227	352	370	7			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



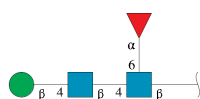
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	N	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



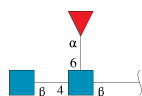
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



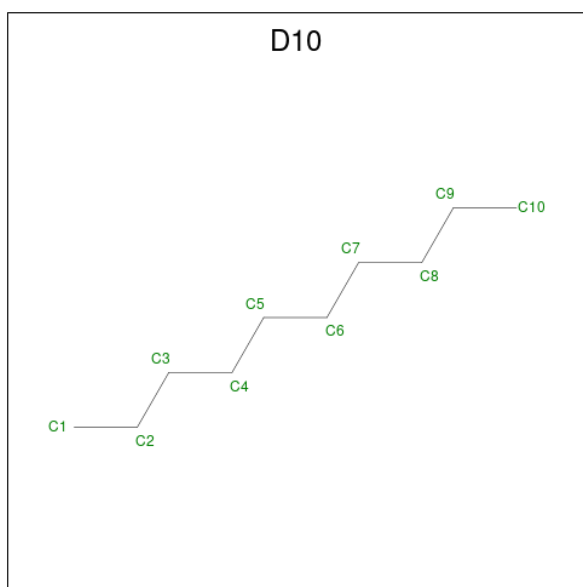
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	S	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	U	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	V	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂) (labeled as "Ligand of Interest" by depositor).



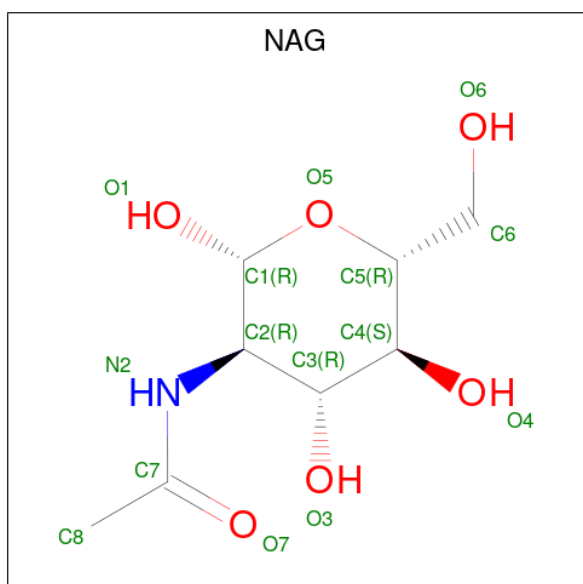
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 10 10	0	0
8	A	1	Total C 10 10	0	0
8	G	1	Total C 10 10	0	0
8	G	1	Total C 10 10	0	0
8	L	1	Total C 10 10	0	0
8	L	1	Total C 10 10	0	0
8	Q	1	Total C 10 10	0	0
8	Q	1	Total C 10 10	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



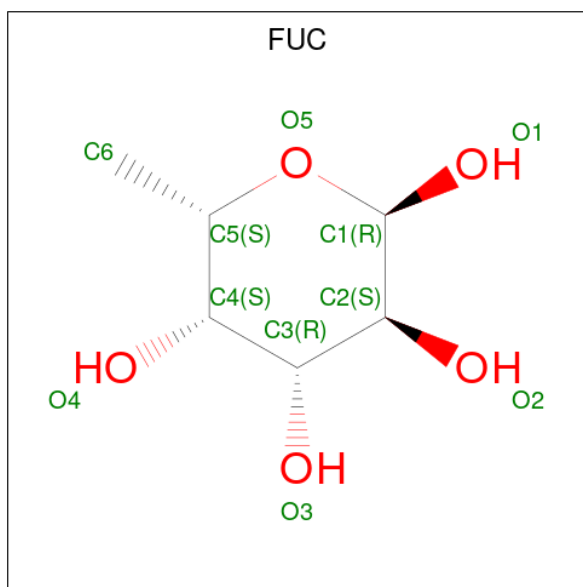
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			4	2	2		
9	H	1	Total	C	O	0	0
			4	2	2		
9	M	1	Total	C	O	0	0
			4	2	2		
9	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			14	8	1	5		
10	Q	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	O	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is water.

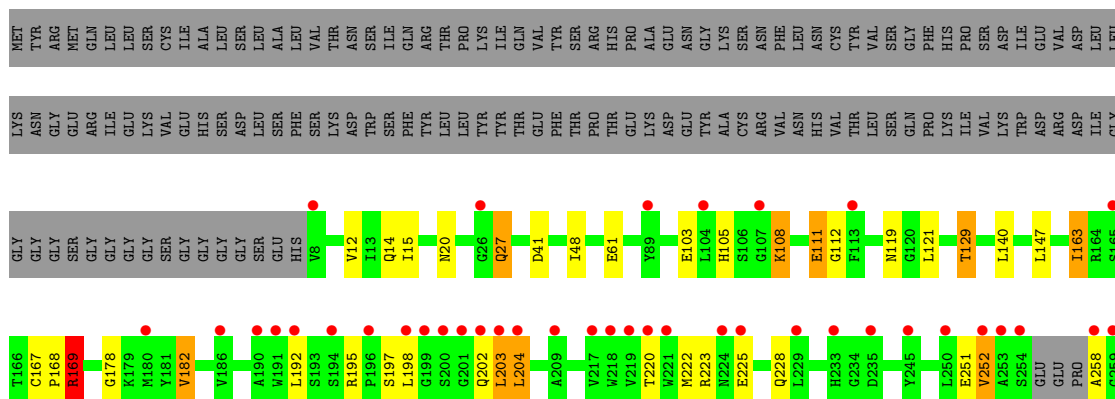
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	13	Total	O	0	0
			13	13		
12	D	8	Total	O	0	0
			8	8		
12	E	22	Total	O	0	0
			22	22		
12	F	4	Total	O	0	0
			4	4		
12	G	6	Total	O	0	0
			6	6		
12	J	7	Total	O	0	0
			7	7		
12	K	10	Total	O	0	0
			10	10		

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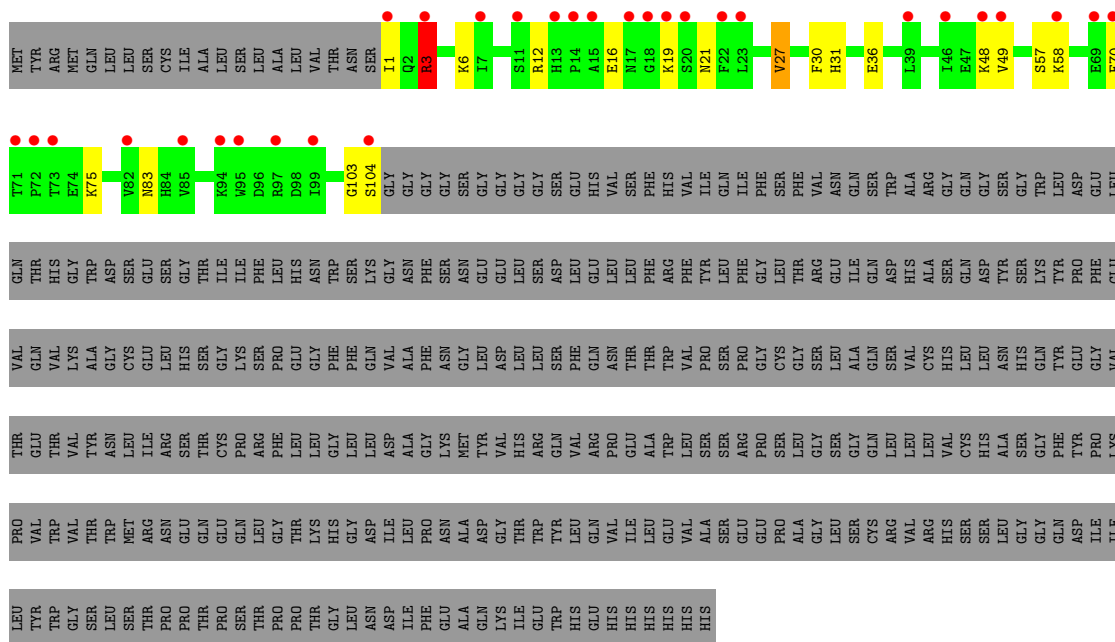
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	2	Total 2	O 2	0	0
12	M	7	Total 7	O 7	0	0
12	P	2	Total 2	O 2	0	0
12	R	1	Total 1	O 1	0	0

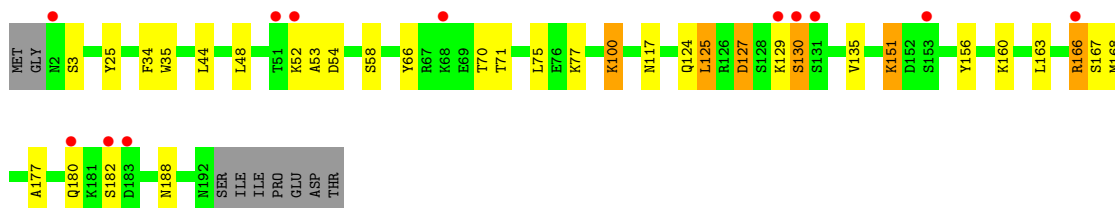
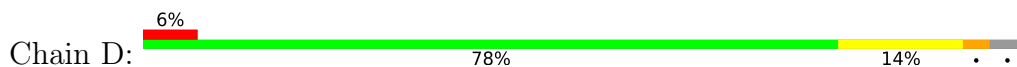
[illegible]



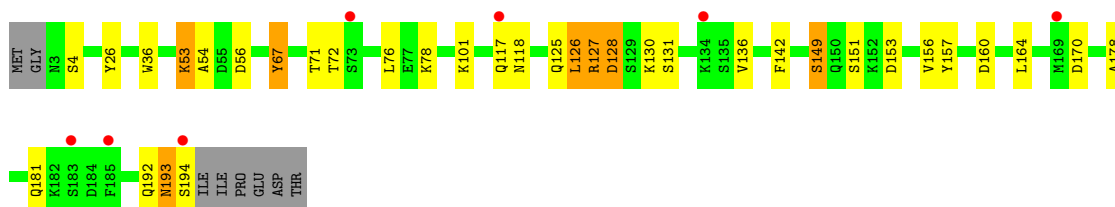
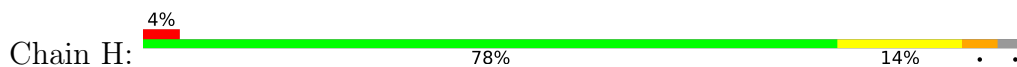
- Molecule 1: Beta-2-microglobulin,T-cell surface glycoprotein CD1c



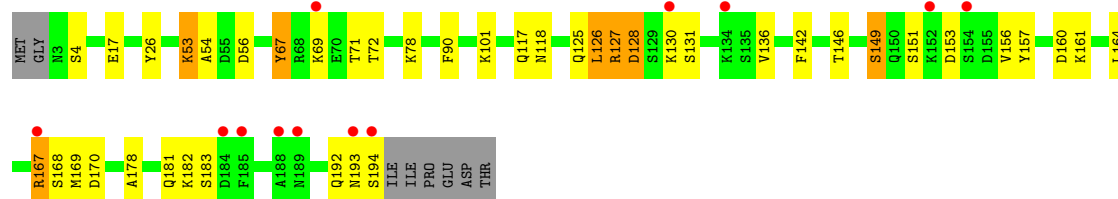
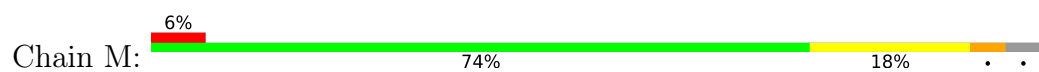
- Molecule 2: TCR alpha



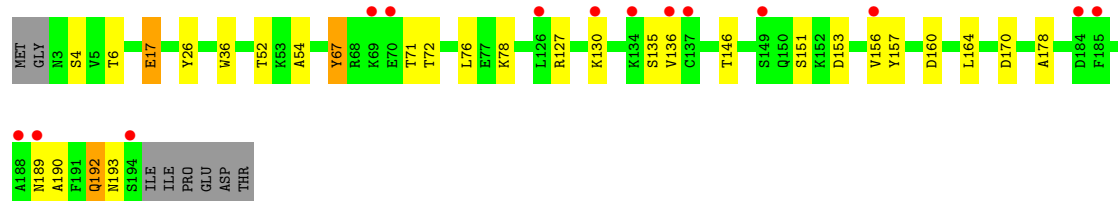
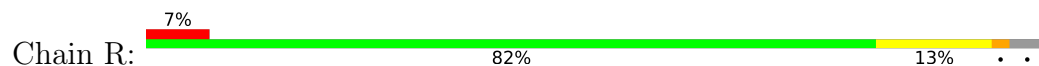
- Molecule 2: TCR alpha



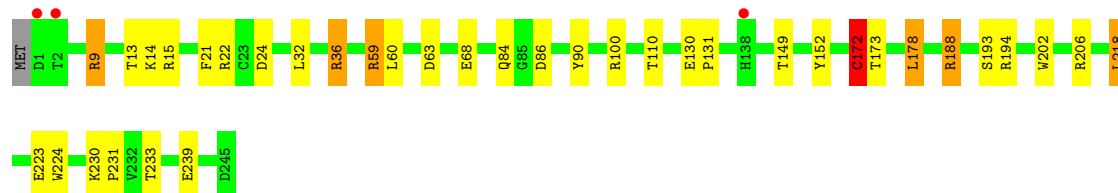
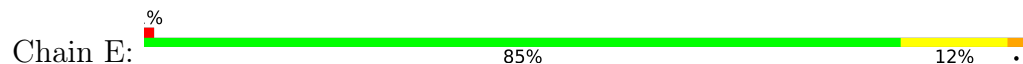
- Molecule 2: TCR alpha



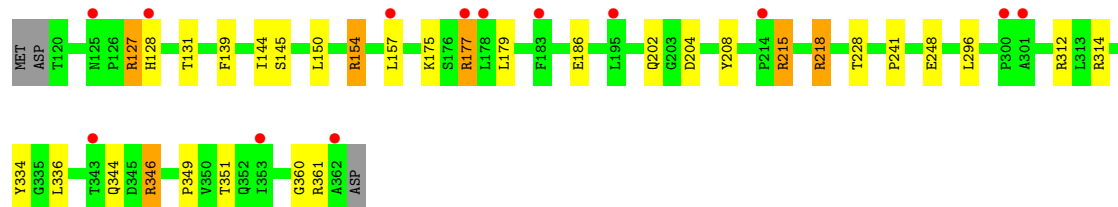
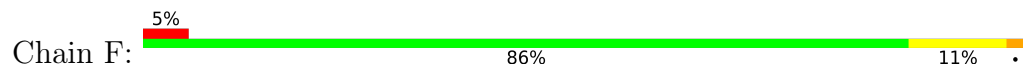
• Molecule 2: TCR alpha



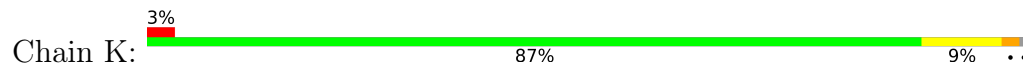
• Molecule 3: TCR beta



• Molecule 3: TCR beta



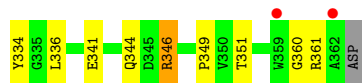
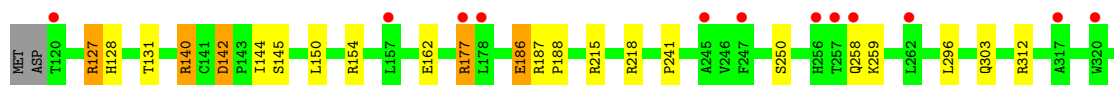
• Molecule 3: TCR beta





- Molecule 3: TCR beta

Chain P: 6% 86% 11% ..



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 50% 50%



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

Chain I: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 75% 25%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 33% 33%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.23Å 83.65Å 180.13Å 91.85° 95.99° 115.61°	Depositor
Resolution (Å)	89.24 – 2.27 89.24 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.5 (89.24-2.27) 98.5 (89.24-2.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.226 , 0.253 0.239 , 0.267	Depositor DCC
R_{free} test set	2022 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26177	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, EDO, FUC, D10

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	0.76	0/2220	1.10	1/3016 (0.0%)
1	B	0.62	0/873	1.03	2/1181 (0.2%)
1	G	0.73	0/2231	1.11	5/3034 (0.2%)
1	J	0.62	0/873	1.00	1/1181 (0.1%)
1	L	0.69	0/2160	1.07	2/2934 (0.1%)
1	O	0.61	0/873	0.97	2/1181 (0.2%)
1	Q	0.68	0/2204	1.08	2/2995 (0.1%)
1	T	0.65	0/873	1.05	2/1181 (0.2%)
2	D	0.75	0/1518	1.19	4/2057 (0.2%)
2	H	0.65	0/1524	1.17	4/2065 (0.2%)
2	M	0.70	0/1524	1.21	7/2065 (0.3%)
2	R	0.69	0/1524	1.16	6/2065 (0.3%)
3	E	0.79	0/2023	1.15	5/2745 (0.2%)
3	F	0.64	0/2007	1.03	3/2723 (0.1%)
3	K	0.72	0/2007	1.16	5/2723 (0.2%)
3	P	0.66	0/2007	1.09	3/2723 (0.1%)
All	All	0.70	0/26441	1.11	54/35869 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	G	0	5
1	J	0	1
1	L	0	5
1	O	0	1
1	Q	0	2
1	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	M	0	1
2	R	0	1
3	E	0	8
3	F	0	5
3	K	0	7
3	P	0	6
All	All	0	48

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	20	ASN	CA-CB-CG	7.10	119.70	112.60
2	M	160	ASP	CA-CB-CG	7.01	119.61	112.60
1	Q	129	THR	CA-CB-OG1	-6.85	99.32	109.60
1	A	34	GLU	CB-CG-CD	6.85	124.25	112.60
2	R	170	ASP	CA-CB-CG	6.75	119.34	112.60
2	D	127	ASP	CA-CB-CG	6.59	119.19	112.60
2	H	170	ASP	CA-CB-CG	6.57	119.17	112.60
2	M	128	ASP	CA-CB-CG	6.40	119.00	112.60
2	R	17	GLU	CB-CA-C	6.38	116.15	109.83
2	R	146	THR	CA-CB-OG1	-6.38	100.03	109.60
2	M	17	GLU	CB-CG-CD	6.35	123.39	112.60
1	G	129	THR	CA-CB-OG1	-6.18	100.33	109.60
3	E	13	THR	CA-CB-OG1	-6.14	100.39	109.60
3	E	233	THR	CA-CB-OG1	-6.09	100.47	109.60
3	K	341	GLU	CB-CG-CD	5.96	122.74	112.60
2	R	6	THR	CA-CB-OG1	-5.90	100.75	109.60
1	G	21	GLN	N-CA-C	-5.84	106.14	113.20
2	H	128	ASP	CA-CB-CG	5.82	118.42	112.60
2	M	117	GLN	N-CA-CB	5.73	118.92	110.33
1	O	71	THR	CA-CB-OG1	-5.71	101.03	109.60
2	M	146	THR	CA-CB-OG1	-5.68	101.07	109.60
3	F	131	THR	CA-CB-OG1	-5.67	101.10	109.60
3	F	208	TYR	CB-CA-C	5.65	119.83	110.78
1	O	56	PHE	CA-CB-CG	5.61	119.41	113.80
2	H	142	PHE	CA-CB-CG	5.60	119.40	113.80
3	K	142	ASP	CB-CA-C	5.59	115.71	110.17
1	G	189	GLU	N-CA-C	-5.59	100.13	109.24
3	K	159	GLN	CA-C-N	-5.57	113.13	121.87
3	K	159	GLN	C-N-CA	-5.57	113.13	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	277	TYR	CA-C-O	-5.55	113.11	119.60
1	L	21	GLN	N-CA-C	-5.51	106.51	113.18
3	P	351	THR	CA-CB-OG1	-5.51	101.33	109.60
3	P	131	THR	CA-CB-OG1	-5.47	101.39	109.60
2	M	142	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	71	THR	CA-CB-OG1	-5.42	101.47	109.60
3	F	351	THR	CA-CB-OG1	-5.42	101.47	109.60
3	E	172	CYS	CB-CA-C	5.39	118.11	110.24
2	M	17	GLU	CB-CA-C	5.32	115.10	109.83
1	B	19	LYS	CB-CG-CD	5.29	123.46	111.30
3	K	131	THR	CA-CB-OG1	-5.25	101.73	109.60
3	E	149	THR	CA-CB-OG1	-5.23	101.76	109.60
1	T	12	ARG	CB-CG-CD	5.22	123.30	111.30
3	E	90	TYR	CB-CA-C	5.20	119.10	110.78
2	D	34	PHE	CA-CB-CG	5.18	118.98	113.80
1	J	71	THR	CA-CB-OG1	-5.17	101.84	109.60
1	L	57	ASN	CA-CB-CG	5.17	117.77	112.60
2	D	100	LYS	CB-CG-CD	5.16	123.16	111.30
2	D	151	LYS	N-CA-C	-5.15	106.24	112.88
2	R	192	GLN	N-CA-C	-5.14	107.17	112.93
1	G	57	ASN	CA-CB-CG	5.11	117.71	112.60
2	R	52	THR	N-CA-C	-5.10	107.19	113.41
1	T	12	ARG	N-CA-CB	5.06	117.66	110.16
2	H	117	GLN	N-CA-CB	5.01	117.85	110.33
3	P	142	ASP	CB-CA-C	5.00	115.72	110.17

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	71	ARG	Sidechain
2	D	166	ARG	Sidechain
3	E	100	ARG	Sidechain
3	E	15	ARG	Sidechain
3	E	188	ARG	Sidechain
3	E	194	ARG	Sidechain
3	E	206	ARG	Sidechain
3	E	22	ARG	Sidechain
3	E	36	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	E	59	ARG	Sidechain
3	F	154	ARG	Sidechain
3	F	218	ARG	Sidechain
3	F	312	ARG	Sidechain
3	F	314	ARG	Sidechain
3	F	346	ARG	Sidechain
1	G	169	ARG	Sidechain
1	G	187	ARG	Sidechain
1	G	223	ARG	Sidechain
1	G	263	ARG	Sidechain
1	G	71	ARG	Sidechain
1	J	12	ARG	Sidechain
3	K	127	ARG	Sidechain
3	K	140	ARG	Sidechain
3	K	154	ARG	Sidechain
3	K	187	ARG	Sidechain
3	K	215	ARG	Sidechain
3	K	218	ARG	Sidechain
3	K	312	ARG	Sidechain
1	L	169	ARG	Sidechain
1	L	187	ARG	Sidechain
1	L	223	ARG	Sidechain
1	L	263	ARG	Sidechain
1	L	71	ARG	Sidechain
2	M	167	ARG	Sidechain
1	O	3	ARG	Sidechain
3	P	140	ARG	Sidechain
3	P	154	ARG	Sidechain
3	P	187	ARG	Sidechain
3	P	218	ARG	Sidechain
3	P	312	ARG	Sidechain
3	P	346	ARG	Sidechain
1	Q	169	ARG	Sidechain
1	Q	263	ARG	Sidechain
2	R	127	ARG	Sidechain
1	T	3	ARG	Sidechain

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	2156	0	2044	22	0
1	B	850	0	813	7	0
1	G	2166	0	2061	19	0
1	J	850	0	813	7	0
1	L	2098	0	1996	25	0
1	O	850	0	813	8	0
1	Q	2141	0	2040	19	0
1	T	850	0	813	9	0
2	D	1486	0	1407	13	0
2	H	1492	0	1412	17	0
2	M	1492	0	1412	24	0
2	R	1492	0	1412	10	0
3	E	1972	0	1882	15	0
3	F	1956	0	1871	15	0
3	K	1956	0	1871	13	0
3	P	1956	0	1871	9	0
4	C	24	0	21	0	0
4	N	24	0	22	0	0
5	I	25	0	22	0	0
6	S	49	0	43	1	0
7	U	38	0	34	4	0
7	V	38	0	34	1	0
8	A	20	0	44	0	0
8	G	20	0	44	0	0
8	L	20	0	44	2	0
8	Q	20	0	44	0	0
9	D	4	0	6	0	0
9	H	4	0	6	0	0
9	M	4	0	6	0	0
9	R	4	0	6	0	0
10	L	14	0	13	1	0
10	Q	14	0	13	0	0
11	O	10	0	10	0	0
12	A	13	0	0	0	0
12	D	8	0	0	0	0
12	E	22	0	0	0	0
12	F	4	0	0	0	0
12	G	6	0	0	0	0
12	J	7	0	0	0	0
12	K	10	0	0	0	0
12	L	2	0	0	0	0
12	M	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	P	2	0	0	0	0
12	R	1	0	0	0	0
All	All	26177	0	24943	213	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 (213) 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:L:223:ARG:HA	1:L:260:LEU:HA	1.31	1.10
1:L:222:MET:HA	1:L:227:GLU:HA	1.66	0.78
2:D:70:THR:O	2:D:71:THR:HG22	1.88	0.74
2:H:71:THR:O	2:H:72:THR:HG22	1.88	0.73
3:P:177:ARG:HH11	3:P:177:ARG:HB2	1.52	0.73
2:R:71:THR:O	2:R:72:THR:HG22	1.89	0.72
2:M:71:THR:O	2:M:72:THR:HG22	1.89	0.72
1:G:112:GLY:HA3	1:G:163:ILE:HG23	1.72	0.72
3:K:248:GLU:O	2:M:126:LEU:HB3	1.90	0.71
1:A:192:LEU:HD23	1:A:278:TRP:HB2	1.74	0.70
1:L:223:ARG:HA	1:L:260:LEU:CA	2.16	0.69
3:F:248:GLU:O	2:H:126:LEU:HB3	1.92	0.68
1:Q:112:GLY:HA3	1:Q:163:ILE:HG23	1.75	0.68
2:H:127:ARG:HG2	2:H:127:ARG:HH21	1.57	0.68
1:A:277:TYR:O	1:A:278:TRP:HB3	1.94	0.67
3:K:177:ARG:HH11	3:K:177:ARG:HB2	1.60	0.67
2:D:125:LEU:HB3	3:E:130:GLU:O	1.95	0.67
2:M:193:ASN:O	2:M:194:SER:C	2.37	0.66
1:A:41:ASP:HB2	1:A:48:ILE:HD11	1.77	0.66
2:H:193:ASN:O	2:H:194:SER:C	2.39	0.66
1:A:264:VAL:HB	1:A:274:ILE:HB	1.80	0.64
2:M:127:ARG:HG2	2:M:127:ARG:HH21	1.62	0.63
1:T:36:GLU:OE1	1:T:83:ASN:HB3	1.99	0.62
1:L:12:VAL:HG12	1:L:14:GLN:HE21	1.65	0.62
1:T:3:ARG:HD2	1:T:31:HIS:HB2	1.80	0.62
1:G:12:VAL:HG12	1:G:14:GLN:HE21	1.65	0.62
3:F:177:ARG:HB2	3:F:177:ARG:HH11	1.65	0.61
1:Q:12:VAL:HG12	1:Q:14:GLN:HE21	1.66	0.60
1:Q:41:ASP:HB2	1:Q:48:ILE:HD11	1.83	0.60
1:G:41:ASP:HB2	1:G:48:ILE:HD11	1.84	0.59
1:Q:105:HIS:CE1	1:Q:111:GLU:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:153:ASP:HB3	2:R:156:VAL:HG12	1.83	0.59
1:L:41:ASP:HB2	1:L:48:ILE:HD11	1.84	0.59
1:A:220:THR:HG23	1:A:263:ARG:HD3	1.85	0.58
1:L:277:TYR:O	1:L:278:TRP:HB3	2.03	0.58
1:Q:197:SER:HB2	1:Q:204:LEU:HD13	1.87	0.57
1:A:34:GLU:HG3	1:A:244:TRP:CZ2	2.39	0.56
2:M:153:ASP:HB3	2:M:156:VAL:HG12	1.86	0.56
1:G:197:SER:HB2	1:G:204:LEU:HD13	1.88	0.56
3:E:9:ARG:NH1	3:E:9:ARG:HG2	2.19	0.56
1:A:117:ALA:HB2	1:B:60:TRP:CE2	2.41	0.56
3:K:296:LEU:C	3:K:296:LEU:HD12	2.31	0.56
1:T:103:GLY:O	1:T:104:SER:C	2.50	0.55
1:L:12:VAL:HG12	1:L:14:GLN:NE2	2.21	0.55
3:P:186:GLU:HG2	3:P:188:PRO:HD3	1.88	0.55
1:O:103:GLY:O	1:O:104:SER:C	2.50	0.55
2:D:129:LYS:NZ	3:E:239:GLU:H	2.05	0.55
3:F:177:ARG:HB2	3:F:177:ARG:NH1	2.22	0.54
1:G:12:VAL:HG12	1:G:14:GLN:NE2	2.22	0.54
3:E:178:LEU:C	3:E:178:LEU:HD12	2.33	0.54
2:M:151:SER:OG	2:M:156:VAL:HG13	2.08	0.54
3:E:224:TRP:HB2	3:E:230:LYS:HD2	1.90	0.54
1:A:223:ARG:NH1	1:A:228:GLN:OE1	2.40	0.54
1:Q:121:LEU:HD11	1:T:1:ILE:HG23	1.90	0.53
1:L:121:LEU:HD11	1:O:1:ILE:HG23	1.90	0.53
2:H:153:ASP:HB3	2:H:156:VAL:HG12	1.90	0.53
1:A:218:TRP:HB2	1:A:265:ARG:HB3	1.90	0.53
1:Q:277:TYR:O	1:Q:278:TRP:C	2.51	0.53
1:L:167:CYS:HB3	1:L:168:PRO:HD3	1.91	0.52
3:P:336:LEU:HD22	3:P:349:PRO:HG2	1.91	0.52
1:A:222:MET:N	1:A:261:SER:O	2.43	0.52
1:G:117:ALA:HB2	1:J:60:TRP:CE2	2.45	0.52
1:G:137:CYS:HB3	1:G:141:ALA:HB2	1.91	0.52
1:L:80:GLU:HG2	8:L:403:D10:H62	1.91	0.52
1:O:27:VAL:HG23	1:O:30:PHE:CE1	2.45	0.52
3:F:154:ARG:HH12	3:F:204:ASP:HA	1.75	0.51
3:F:175:LYS:HE2	3:F:179:LEU:HD23	1.92	0.51
3:F:215:ARG:HH12	1:G:80:GLU:CD	2.18	0.51
1:L:222:MET:HG2	1:L:263:ARG:HG2	1.92	0.51
3:E:131:PRO:HD2	3:E:202:TRP:CE2	2.45	0.51
1:L:169:ARG:HD2	7:U:1:NAG:H83	1.92	0.51
3:K:336:LEU:HD22	3:K:349:PRO:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:192:GLN:OE1	2:M:192:GLN:HA	2.11	0.51
3:F:336:LEU:HD22	3:F:349:PRO:HG2	1.93	0.50
1:G:201:GLY:O	1:G:202:GLN:HB2	2.10	0.50
1:L:223:ARG:O	1:L:225:GLU:N	2.44	0.50
1:G:15:ILE:C	1:G:15:ILE:HD12	2.36	0.50
1:T:16:GLU:HB3	1:T:19:LYS:HG3	1.94	0.50
1:Q:169:ARG:HH21	7:V:1:NAG:H81	1.75	0.49
1:Q:261:SER:HB3	1:Q:277:TYR:CD1	2.47	0.49
1:J:27:VAL:HG23	1:J:30:PHE:CE1	2.48	0.49
2:R:151:SER:OG	2:R:156:VAL:HG13	2.13	0.49
2:R:189:ASN:O	2:R:190:ALA:C	2.56	0.49
3:K:216:MET:HE3	3:K:216:MET:HA	1.93	0.49
2:M:125:GLN:C	2:M:126:LEU:HD23	2.38	0.49
2:D:129:LYS:HZ3	3:E:239:GLU:H	1.61	0.49
1:L:23:TRP:CG	10:L:401:NAG:H62	2.48	0.49
2:M:157:TYR:O	2:M:178:ALA:HA	2.13	0.49
1:Q:167:CYS:HB3	1:Q:168:PRO:HD3	1.94	0.49
2:M:149:SER:OG	2:M:192:GLN:HB2	2.12	0.48
1:T:27:VAL:HG23	1:T:30:PHE:CE1	2.48	0.48
2:H:157:TYR:O	2:H:178:ALA:HA	2.13	0.48
1:G:167:CYS:HB3	1:G:168:PRO:HD3	1.95	0.48
2:M:127:ARG:HG2	2:M:127:ARG:NH2	2.28	0.48
1:T:6:LYS:O	1:T:27:VAL:HA	2.13	0.48
2:H:4:SER:O	2:H:26:TYR:HA	2.14	0.48
2:D:70:THR:O	2:D:71:THR:CG2	2.61	0.48
2:D:156:TYR:O	2:D:177:ALA:HA	2.14	0.48
3:E:218:LEU:HD22	3:E:231:PRO:HG2	1.95	0.48
2:R:4:SER:O	2:R:26:TYR:HA	2.14	0.48
1:J:6:LYS:O	1:J:27:VAL:HA	2.14	0.47
1:L:15:ILE:C	1:L:15:ILE:HD12	2.39	0.47
1:A:10:PHE:HB2	1:A:171:LEU:HD13	1.96	0.47
1:O:6:LYS:O	1:O:27:VAL:HA	2.15	0.47
1:A:88:ASP:C	1:A:90:SER:H	2.22	0.47
1:A:222:MET:O	1:A:261:SER:N	2.48	0.47
1:B:27:VAL:HG23	1:B:30:PHE:CE1	2.50	0.47
2:D:124:GLN:C	2:D:125:LEU:HD23	2.40	0.47
3:E:152:TYR:HB2	3:E:188:ARG:HG3	1.96	0.47
3:F:241:PRO:HD3	3:F:349:PRO:HB3	1.97	0.47
2:H:125:GLN:C	2:H:126:LEU:HD23	2.40	0.47
2:H:151:SER:OG	2:H:156:VAL:HG13	2.15	0.47
1:A:117:ALA:HB2	1:B:60:TRP:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:SER:HB2	1:A:204:LEU:HD13	1.97	0.47
1:G:169:ARG:HH21	6:S:1:NAG:H81	1.80	0.47
3:F:127:ARG:NH1	3:F:127:ARG:HG2	2.30	0.47
1:B:6:LYS:O	1:B:27:VAL:HA	2.15	0.46
3:F:128:HIS:CG	3:F:334:TYR:HB3	2.50	0.46
3:F:215:ARG:NH1	1:G:80:GLU:OE1	2.39	0.46
2:M:169:MET:O	2:M:170:ASP:C	2.58	0.46
2:M:54:ALA:HA	2:M:67:TYR:CD1	2.49	0.46
1:G:253:ALA:O	1:G:254:SER:C	2.57	0.46
3:F:139:PHE:CD1	3:F:228:THR:HG21	2.51	0.46
1:Q:108:LYS:HB2	1:Q:108:LYS:HE2	1.63	0.46
1:L:277:TYR:O	1:L:278:TRP:CB	2.63	0.46
3:P:128:HIS:CG	3:P:334:TYR:HB3	2.50	0.46
1:G:85:ALA:O	1:G:86:SER:C	2.59	0.46
2:R:54:ALA:HA	2:R:67:TYR:CD1	2.51	0.46
1:A:34:GLU:HG3	1:A:244:TRP:HZ2	1.79	0.46
2:H:54:ALA:HA	2:H:67:TYR:CD1	2.51	0.46
2:D:127:ASP:HB3	2:D:130:SER:O	2.16	0.45
3:E:36:ARG:HH12	3:E:86:ASP:HA	1.81	0.45
1:Q:15:ILE:HB	1:Q:27:GLN:HG3	1.98	0.45
1:L:169:ARG:HH21	7:U:1:NAG:H81	1.82	0.45
2:M:71:THR:O	2:M:72:THR:CG2	2.62	0.45
3:P:127:ARG:NH1	3:P:127:ARG:HG2	2.30	0.45
3:P:241:PRO:HD3	3:P:349:PRO:HB3	1.99	0.45
1:A:15:ILE:C	1:A:15:ILE:HD12	2.42	0.45
2:D:163:LEU:HB3	3:E:172:CYS:HB3	1.99	0.44
2:M:53:LYS:O	2:M:56:ASP:HB2	2.16	0.44
1:A:89:TYR:HD1	1:A:92:TYR:CD2	2.34	0.44
3:E:173:THR:HG23	3:E:193:SER:HB2	1.99	0.44
2:D:125:LEU:HD23	2:D:125:LEU:N	2.32	0.44
3:E:32:LEU:HD23	3:E:32:LEU:C	2.42	0.44
3:K:169:ASN:HD22	1:L:75:PHE:HE1	1.66	0.43
2:M:4:SER:O	2:M:26:TYR:HA	2.16	0.43
2:R:71:THR:O	2:R:72:THR:CG2	2.62	0.43
1:L:178:GLY:O	1:L:182:VAL:HG13	2.19	0.43
1:Q:223:ARG:CD	1:Q:258:ALA:O	2.66	0.43
3:K:128:HIS:CG	3:K:334:TYR:HB3	2.54	0.43
2:H:71:THR:O	2:H:72:THR:CG2	2.61	0.43
2:H:127:ARG:HG2	2:H:127:ARG:NH2	2.26	0.43
1:L:214:PRO:HB2	1:L:216:PRO:HD2	2.01	0.43
3:P:150:LEU:HD23	3:P:150:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:21:ASN:HB3	1:T:70:PHE:CE1	2.54	0.43
1:G:117:ALA:HB2	1:J:60:TRP:CD2	2.54	0.43
2:H:128:ASP:HB3	2:H:131:SER:O	2.18	0.43
3:K:231:THR:HG21	3:K:271:PRO:HB3	2.00	0.43
3:K:216:MET:HE1	8:L:403:D10:H13	2.01	0.42
3:E:9:ARG:HG2	3:E:9:ARG:HH11	1.83	0.42
3:K:150:LEU:C	3:K:150:LEU:HD23	2.44	0.42
7:U:1:NAG:O5	7:U:3:FUC:H5	2.19	0.42
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.85	0.42
1:G:277:TYR:O	1:G:278:TRP:HB3	2.19	0.42
2:H:36:TRP:CE2	2:H:76:LEU:HB2	2.54	0.42
2:M:53:LYS:HE3	2:M:53:LYS:HB3	1.55	0.42
3:F:150:LEU:C	3:F:150:LEU:HD23	2.45	0.42
2:M:69:LYS:HE3	2:M:69:LYS:HB2	1.95	0.42
1:A:88:ASP:C	1:A:90:SER:N	2.77	0.42
3:K:160:GLY:HA2	2:M:90:PHE:CE1	2.55	0.42
2:R:164:LEU:C	2:R:164:LEU:HD12	2.45	0.42
2:M:128:ASP:HB3	2:M:131:SER:O	2.19	0.42
1:L:278:TRP:O	1:L:278:TRP:CE3	2.73	0.42
1:Q:169:ARG:HE	1:Q:169:ARG:HB2	1.58	0.42
1:B:51:HIS:HA	1:B:65:LEU:O	2.20	0.41
2:D:3:SER:O	2:D:25:TYR:HA	2.20	0.41
2:M:126:LEU:HD23	2:M:126:LEU:N	2.35	0.41
1:Q:223:ARG:HD3	1:Q:258:ALA:O	2.19	0.41
2:H:53:LYS:O	2:H:56:ASP:HB2	2.20	0.41
2:H:164:LEU:C	2:H:164:LEU:HD12	2.46	0.41
1:L:117:ALA:HB2	1:O:60:TRP:CE2	2.55	0.41
1:L:188:PRO:HB3	1:L:212:PHE:HB3	2.02	0.41
1:Q:119:ASN:O	1:T:1:ILE:N	2.51	0.41
1:A:263:ARG:NH2	1:A:273:ASP:OD2	2.54	0.41
1:B:95:TRP:CZ2	1:B:97:ARG:HA	2.55	0.41
3:K:247:PHE:HB3	2:M:126:LEU:HB2	2.02	0.41
2:M:164:LEU:C	2:M:164:LEU:HD12	2.45	0.41
1:Q:105:HIS:HE1	1:Q:111:GLU:HB2	1.85	0.41
3:K:174:GLU:OE2	2:M:101:LYS:NZ	2.49	0.41
1:Q:203:LEU:HB3	1:Q:252:VAL:HG23	2.01	0.41
1:L:172:LEU:HD12	7:U:2:NAG:H82	2.01	0.41
3:P:360:GLY:O	3:P:361:ARG:HG3	2.21	0.41
2:H:149:SER:OG	2:H:192:GLN:CG	2.69	0.41
1:O:23:LEU:O	1:O:67:TYR:HA	2.21	0.41
1:J:16:GLU:HB3	1:J:19:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:51:HIS:HA	1:J:65:LEU:O	2.21	0.41
1:O:77:GLU:OE1	1:O:94:LYS:NZ	2.54	0.41
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.86	0.41
1:B:21:ASN:HB3	1:B:70:PHE:CE1	2.56	0.41
3:E:21:PHE:CD1	3:E:110:THR:HG21	2.55	0.41
1:J:95:TRP:CZ2	1:J:97:ARG:HA	2.56	0.41
1:L:87:GLN:HE21	1:L:87:GLN:HB3	1.56	0.41
1:Q:178:GLY:O	1:Q:182:VAL:HG13	2.21	0.41
2:D:53:ALA:O	2:D:54:ASP:HB2	2.20	0.40
3:F:360:GLY:O	3:F:361:ARG:HG3	2.21	0.40
2:R:36:TRP:CE2	2:R:76:LEU:HB2	2.56	0.40
2:D:35:TRP:CE2	2:D:75:LEU:HB2	2.56	0.40
1:O:95:TRP:CZ2	1:O:97:ARG:HA	2.56	0.40
3:P:144:ILE:O	3:P:145:SER:C	2.65	0.40
2:R:157:TYR:O	2:R:178:ALA:HA	2.21	0.40
3:F:144:ILE:O	3:F:145:SER:C	2.65	0.40
1:G:193:SER:OG	1:G:208:HIS:HE1	2.04	0.40
1:G:222:MET:N	1:G:261:SER:O	2.54	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	265/442 (60%)	250 (94%)	15 (6%)	0	100	100
1	B	102/442 (23%)	101 (99%)	1 (1%)	0	100	100
1	G	269/442 (61%)	254 (94%)	15 (6%)	0	100	100
1	J	102/442 (23%)	99 (97%)	3 (3%)	0	100	100
1	L	255/442 (58%)	245 (96%)	9 (4%)	1 (0%)	30	36
1	O	102/442 (23%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	264/442 (60%)	255 (97%)	9 (3%)	0	100	100
1	T	102/442 (23%)	101 (99%)	1 (1%)	0	100	100
2	D	189/200 (94%)	180 (95%)	9 (5%)	0	100	100
2	H	190/200 (95%)	183 (96%)	7 (4%)	0	100	100
2	M	190/200 (95%)	182 (96%)	8 (4%)	0	100	100
2	R	190/200 (95%)	181 (95%)	9 (5%)	0	100	100
3	E	243/246 (99%)	236 (97%)	7 (3%)	0	100	100
3	F	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
3	K	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
3	P	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
All	All	3186/5320 (60%)	3074 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	224	ASN

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	234/384 (61%)	210 (90%)	24 (10%)	6	6
1	B	95/384 (25%)	90 (95%)	5 (5%)	19	25
1	G	235/384 (61%)	209 (89%)	26 (11%)	5	5
1	J	95/384 (25%)	89 (94%)	6 (6%)	15	19
1	L	228/384 (59%)	208 (91%)	20 (9%)	8	9
1	O	95/384 (25%)	91 (96%)	4 (4%)	25	35
1	Q	232/384 (60%)	209 (90%)	23 (10%)	6	7
1	T	95/384 (25%)	88 (93%)	7 (7%)	11	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	165/173 (95%)	146 (88%)	19 (12%)	4	4
2	H	166/173 (96%)	153 (92%)	13 (8%)	10	12
2	M	166/173 (96%)	151 (91%)	15 (9%)	8	8
2	R	166/173 (96%)	157 (95%)	9 (5%)	18	24
3	E	214/215 (100%)	202 (94%)	12 (6%)	17	23
3	F	212/215 (99%)	202 (95%)	10 (5%)	22	30
3	K	212/215 (99%)	203 (96%)	9 (4%)	25	35
3	P	212/215 (99%)	197 (93%)	15 (7%)	12	15
All	All	2822/4624 (61%)	2605 (92%)	217 (8%)	10	12

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	GLN
1	A	32	LEU
1	A	61	GLU
1	A	137	CYS
1	A	140	LEU
1	A	142	GLN
1	A	147	LEU
1	A	163	ILE
1	A	179	LYS
1	A	180	MET
1	A	192	LEU
1	A	195	ARG
1	A	203	LEU
1	A	204	LEU
1	A	220	THR
1	A	222	MET
1	A	225	GLU
1	A	228	GLN
1	A	232	LYS
1	A	251	GLU
1	A	256	GLU
1	A	263	ARG
1	A	275	ILE
1	B	19	LYS
1	B	27	VAL

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Mol	Chain	Res	Type
1	B	58	LYS
1	B	70	PHE
1	B	75	LYS
2	D	44	LEU
2	D	48	LEU
2	D	52	LYS
2	D	58	SER
2	D	66	TYR
2	D	77	LYS
2	D	100	LYS
2	D	117	ASN
2	D	125	LEU
2	D	130	SER
2	D	135	VAL
2	D	151	LYS
2	D	160	LYS
2	D	166	ARG
2	D	167	SER
2	D	168	MET
2	D	180	GLN
2	D	182	SER
2	D	188	ASN
3	E	9	ARG
3	E	14	LYS
3	E	24	ASP
3	E	59	ARG
3	E	60	LEU
3	E	63	ASP
3	E	68	GLU
3	E	84	GLN
3	E	172	CYS
3	E	178	LEU
3	E	218	LEU
3	E	223	GLU
3	F	127	ARG
3	F	157	LEU
3	F	177	ARG
3	F	186	GLU
3	F	202	GLN
3	F	215	ARG
3	F	218	ARG
3	F	296	LEU

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Mol	Chain	Res	Type
3	F	344	GLN
3	F	346	ARG
1	G	15	ILE
1	G	21	GLN
1	G	61	GLU
1	G	87	GLN
1	G	99	LYS
1	G	108	LYS
1	G	111	GLU
1	G	134	SER
1	G	137	CYS
1	G	140	LEU
1	G	163	ILE
1	G	169	ARG
1	G	179	LYS
1	G	180	MET
1	G	192	LEU
1	G	194	SER
1	G	195	ARG
1	G	203	LEU
1	G	204	LEU
1	G	220	THR
1	G	222	MET
1	G	223	ARG
1	G	225	GLU
1	G	232	LYS
1	G	255	GLU
1	G	256	GLU
2	H	53	LYS
2	H	67	TYR
2	H	78	LYS
2	H	101	LYS
2	H	118	ASN
2	H	126	LEU
2	H	127	ARG
2	H	130	LYS
2	H	136	VAL
2	H	149	SER
2	H	160	ASP
2	H	181	GLN
2	H	193	ASN
1	J	20	SER

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Mol	Chain	Res	Type
1	J	27	VAL
1	J	58	LYS
1	J	69	GLU
1	J	70	PHE
1	J	75	LYS
3	K	120	THR
3	K	125	ASN
3	K	127	ARG
3	K	140	ARG
3	K	177	ARG
3	K	189	LYS
3	K	215	ARG
3	K	336	LEU
3	K	341	GLU
1	L	15	ILE
1	L	21	GLN
1	L	61	GLU
1	L	87	GLN
1	L	140	LEU
1	L	147	LEU
1	L	165	SER
1	L	182	VAL
1	L	195	ARG
1	L	197	SER
1	L	203	LEU
1	L	204	LEU
1	L	220	THR
1	L	222	MET
1	L	223	ARG
1	L	225	GLU
1	L	227	GLU
1	L	251	GLU
1	L	252	VAL
1	L	260	LEU
2	M	53	LYS
2	M	67	TYR
2	M	78	LYS
2	M	118	ASN
2	M	126	LEU
2	M	127	ARG
2	M	130	LYS
2	M	136	VAL

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Mol	Chain	Res	Type
2	M	149	SER
2	M	161	LYS
2	M	167	ARG
2	M	168	SER
2	M	181	GLN
2	M	182	LYS
2	M	183	SER
1	O	27	VAL
1	O	57	SER
1	O	70	PHE
1	O	75	LYS
3	P	127	ARG
3	P	140	ARG
3	P	142	ASP
3	P	162	GLU
3	P	177	ARG
3	P	186	GLU
3	P	215	ARG
3	P	250	SER
3	P	258	GLN
3	P	259	LYS
3	P	296	LEU
3	P	303	GLN
3	P	341	GLU
3	P	344	GLN
3	P	346	ARG
1	Q	27	GLN
1	Q	61	GLU
1	Q	103	GLU
1	Q	108	LYS
1	Q	111	GLU
1	Q	129	THR
1	Q	140	LEU
1	Q	147	LEU
1	Q	163	ILE
1	Q	169	ARG
1	Q	182	VAL
1	Q	192	LEU
1	Q	195	ARG
1	Q	198	LEU
1	Q	202	GLN
1	Q	203	LEU

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Mol	Chain	Res	Type
1	Q	204	LEU
1	Q	220	THR
1	Q	222	MET
1	Q	225	GLU
1	Q	228	GLN
1	Q	251	GLU
1	Q	252	VAL
2	R	17	GLU
2	R	67	TYR
2	R	78	LYS
2	R	130	LYS
2	R	135	SER
2	R	136	VAL
2	R	160	ASP
2	R	192	GLN
2	R	193	ASN
1	T	3	ARG
1	T	27	VAL
1	T	48	LYS
1	T	49	VAL
1	T	57	SER
1	T	58	LYS
1	T	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
3	E	176	GLN
3	E	181	GLN
3	E	214	GLN
3	F	159	GLN
3	F	256	HIS
3	F	294	GLN
3	F	299	GLN
3	F	332	GLN
3	F	344	GLN
1	G	20	ASN
1	G	87	GLN
1	G	105	HIS
1	G	115	GLN
1	G	142	GLN

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Mol	Chain	Res	Type
2	H	103	GLN
3	K	125	ASN
3	K	155	GLN
3	K	169	ASN
3	K	299	GLN
3	K	332	GLN
1	L	87	GLN
2	M	39	GLN
2	M	103	GLN
2	M	193	ASN
3	P	169	ASN
3	P	237	ASN
3	P	294	GLN
3	P	299	GLN
3	P	303	GLN
3	P	332	GLN
1	Q	27	GLN
1	Q	105	HIS
1	Q	127	GLN
1	Q	233	HIS
2	R	103	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 ⓘ

16 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	C	1	1,4	14,14,15	0.47	0	17,19,21	1.05	2 (11%)
4	FUC	C	2	4	10,10,11	0.25	0	14,14,16	0.76	1 (7%)
5	NAG	I	1	5	14,14,15	0.65	0	17,19,21	1.56	4 (23%)
5	BMA	I	2	5	11,11,12	0.51	0	15,15,17	1.91	2 (13%)
4	NAG	N	1	4	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
4	FUC	N	2	4	10,10,11	0.28	0	14,14,16	0.43	0
6	NAG	S	1	1,6	14,14,15	0.50	0	17,19,21	1.75	4 (23%)
6	NAG	S	2	6	14,14,15	0.41	0	17,19,21	0.70	1 (5%)
6	BMA	S	3	6	11,11,12	0.54	0	15,15,17	1.07	2 (13%)
6	FUC	S	4	6	10,10,11	0.43	0	14,14,16	1.26	2 (14%)
7	NAG	U	1	1,7	14,14,15	0.61	0	17,19,21	2.30	5 (29%)
7	NAG	U	2	7	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
7	FUC	U	3	7	10,10,11	0.59	0	14,14,16	1.77	2 (14%)
7	NAG	V	1	1,7	14,14,15	0.44	0	17,19,21	1.42	2 (11%)
7	NAG	V	2	7	14,14,15	0.41	0	17,19,21	0.52	0
7	FUC	V	3	7	10,10,11	0.45	0	14,14,16	1.29	1 (7%)

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	C	1	1,4	-	1/6/23/26	0/1/1/1
4	FUC	C	2	4	-	-	0/1/1/1
5	NAG	I	1	5	-	0/6/23/26	0/1/1/1
5	BMA	I	2	5	-	1/2/19/22	1/1/1/1
4	NAG	N	1	4	-	2/6/23/26	0/1/1/1
4	FUC	N	2	4	-	-	0/1/1/1
6	NAG	S	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	FUC	S	4	6	-	-	0/1/1/1
7	NAG	U	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	FUC	U	3	7	-	-	0/1/1/1
7	NAG	V	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	V	3	7	-	-	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	1	NAG	C2-N2-C7	6.90	132.73	122.90
5	I	2	BMA	C1-O5-C5	6.10	120.45	112.19
7	U	3	FUC	C1-C2-C3	4.81	115.58	109.67
6	S	1	NAG	C2-N2-C7	4.68	129.56	122.90
7	V	1	NAG	C2-N2-C7	3.90	128.46	122.90
4	N	1	NAG	O5-C1-C2	-3.69	105.46	111.29
7	U	3	FUC	O5-C1-C2	3.63	116.38	110.77
6	S	1	NAG	C1-C2-N2	3.63	116.69	110.49
7	U	1	NAG	C1-C2-N2	3.50	116.47	110.49
6	S	4	FUC	C1-C2-C3	3.49	113.95	109.67
7	V	3	FUC	C1-C2-C3	3.46	113.91	109.67
5	I	1	NAG	C1-C2-N2	3.45	116.39	110.49
5	I	2	BMA	C1-C2-C3	3.43	113.88	109.67
7	V	1	NAG	C1-C2-N2	2.88	115.41	110.49
7	U	1	NAG	O5-C1-C2	-2.70	107.02	111.29
7	U	1	NAG	C1-O5-C5	2.65	115.79	112.19
7	U	1	NAG	O6-C6-C5	2.63	120.32	111.29
4	C	2	FUC	C1-C2-C3	2.53	112.77	109.67
5	I	1	NAG	C3-C4-C5	-2.48	105.81	110.24
7	U	2	NAG	O5-C1-C2	-2.40	107.50	111.29
6	S	1	NAG	C1-O5-C5	2.22	115.20	112.19
6	S	3	BMA	C1-C2-C3	-2.22	106.94	109.67
4	C	1	NAG	O4-C4-C5	-2.19	103.85	109.30
6	S	4	FUC	O5-C1-C2	2.16	114.11	110.77
6	S	2	NAG	O5-C1-C2	-2.16	107.88	111.29
4	C	1	NAG	O5-C1-C2	-2.14	107.90	111.29
5	I	1	NAG	O3-C3-C2	-2.14	105.05	109.47
6	S	3	BMA	O5-C1-C2	-2.09	107.55	110.77
6	S	1	NAG	O5-C1-C2	-2.05	108.05	111.29
5	I	1	NAG	O3-C3-C4	2.03	115.04	110.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
6	S	3	BMA	C4-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
7	U	1	NAG	O7-C7-N2-C2
7	V	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C1-C2-N2-C7
7	V	1	NAG	C4-C5-C6-O6
7	V	2	NAG	C8-C7-N2-C2
7	V	1	NAG	O5-C5-C6-O6
7	V	2	NAG	O7-C7-N2-C2
5	I	2	BMA	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
7	U	1	NAG	C1-C2-N2-C7
7	U	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C3-C2-N2-C7
6	S	2	NAG	O5-C5-C6-O6
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

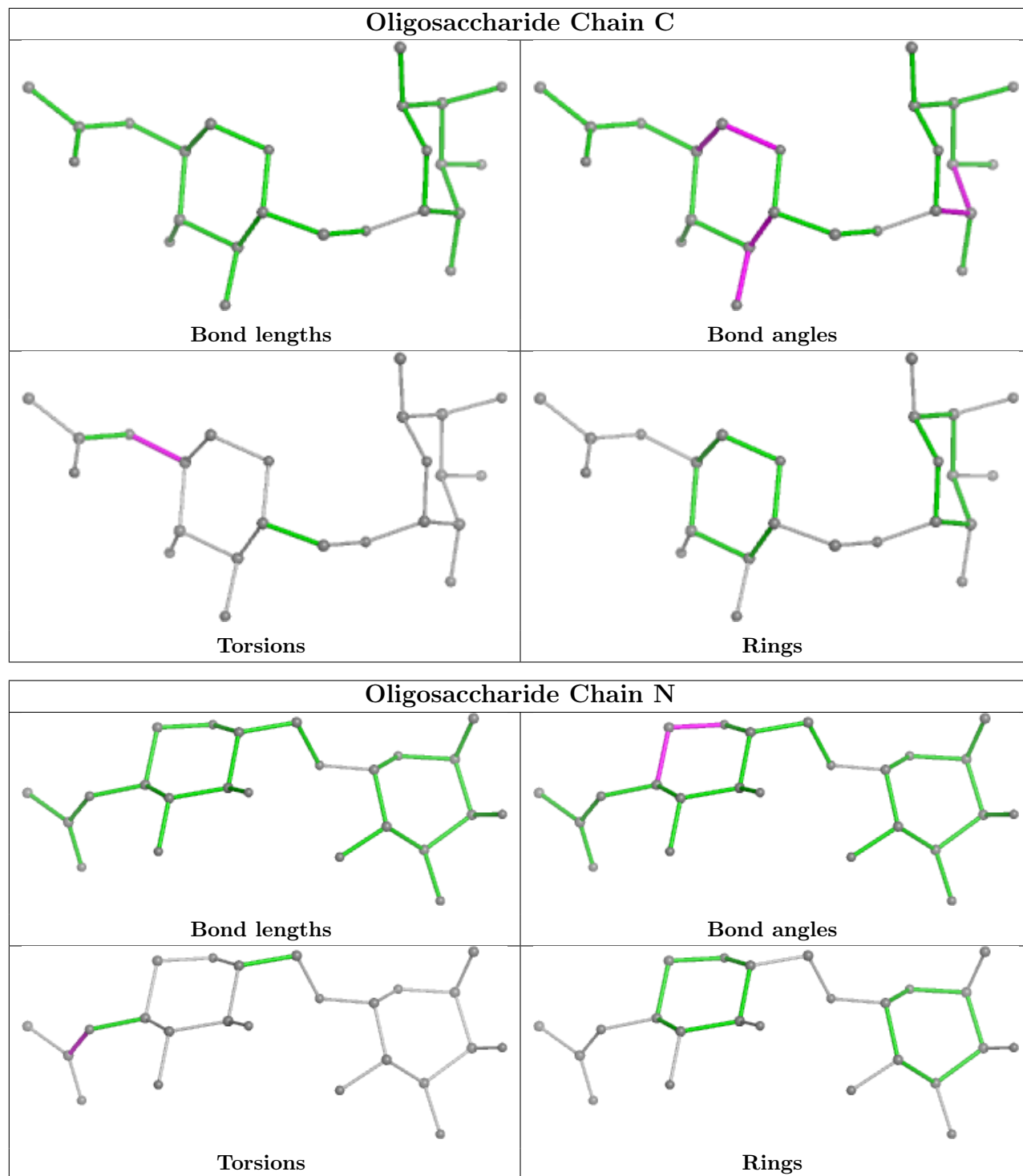
Mol	Chain	Res	Type	Atoms
5	I	2	BMA	C1-C2-C3-C4-C5-O5

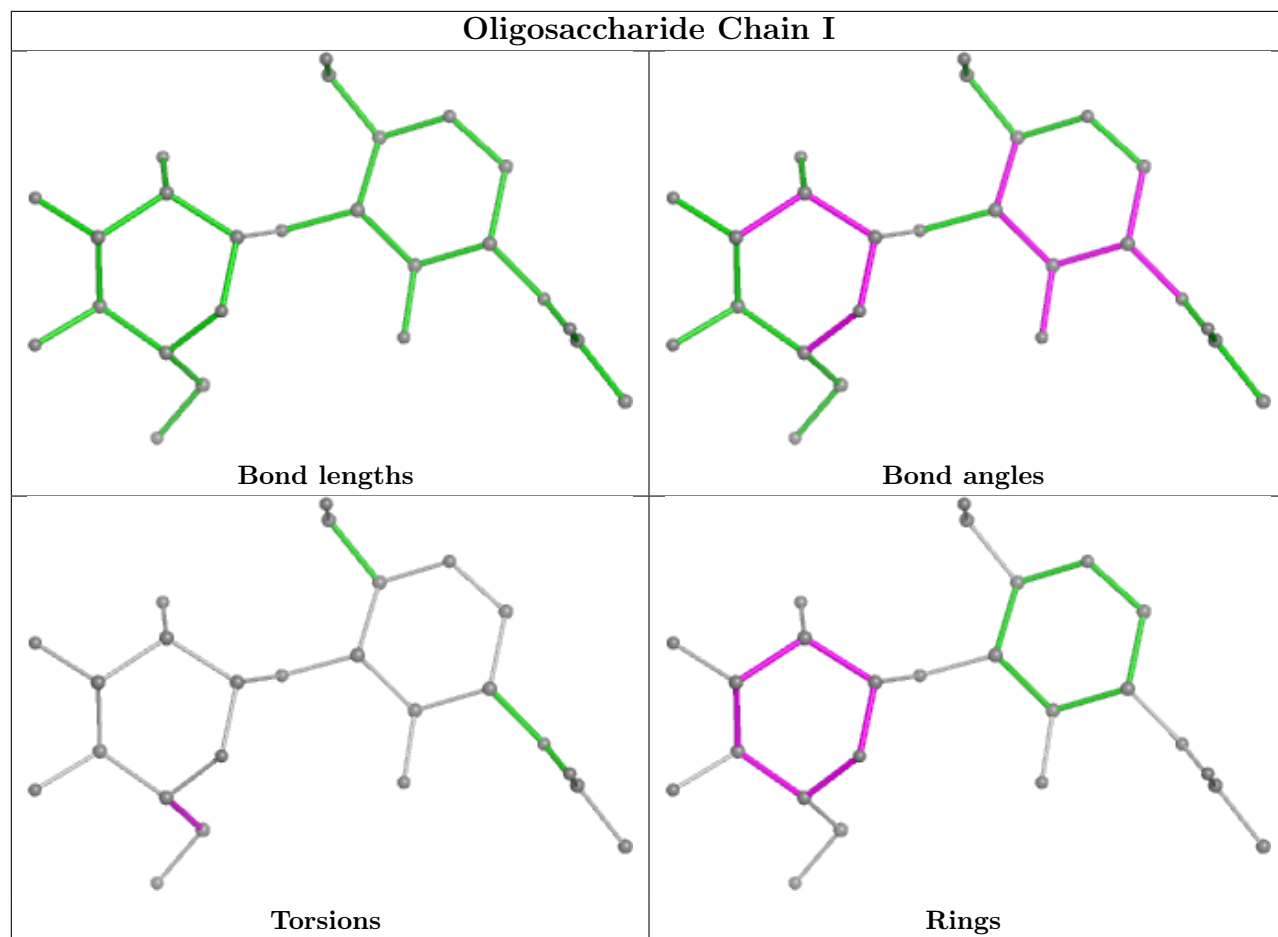
5 monomers are involved in 6 short contacts:

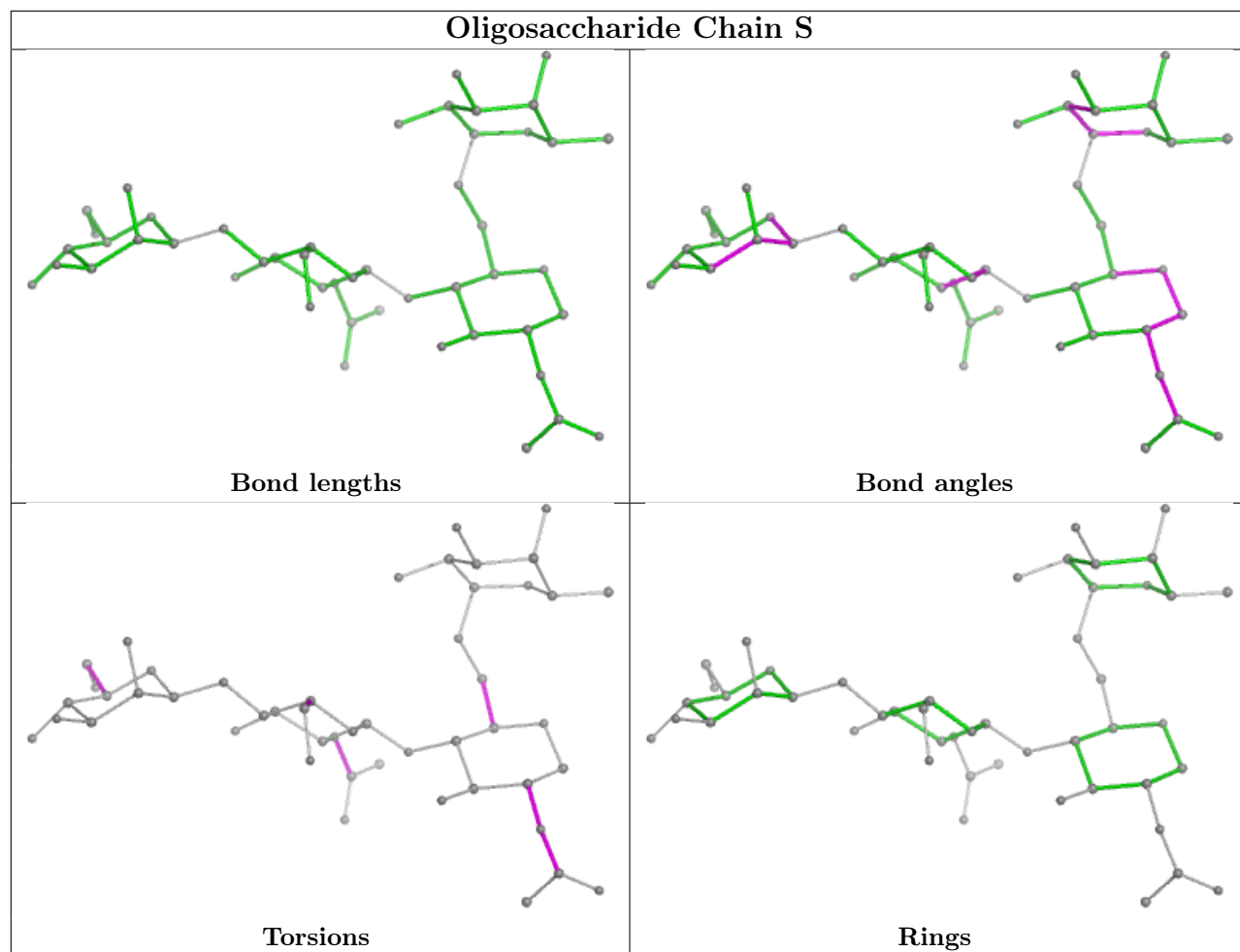
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	3	FUC	1	0
7	V	1	NAG	1	0
6	S	1	NAG	1	0
7	U	2	NAG	1	0
7	U	1	NAG	3	0

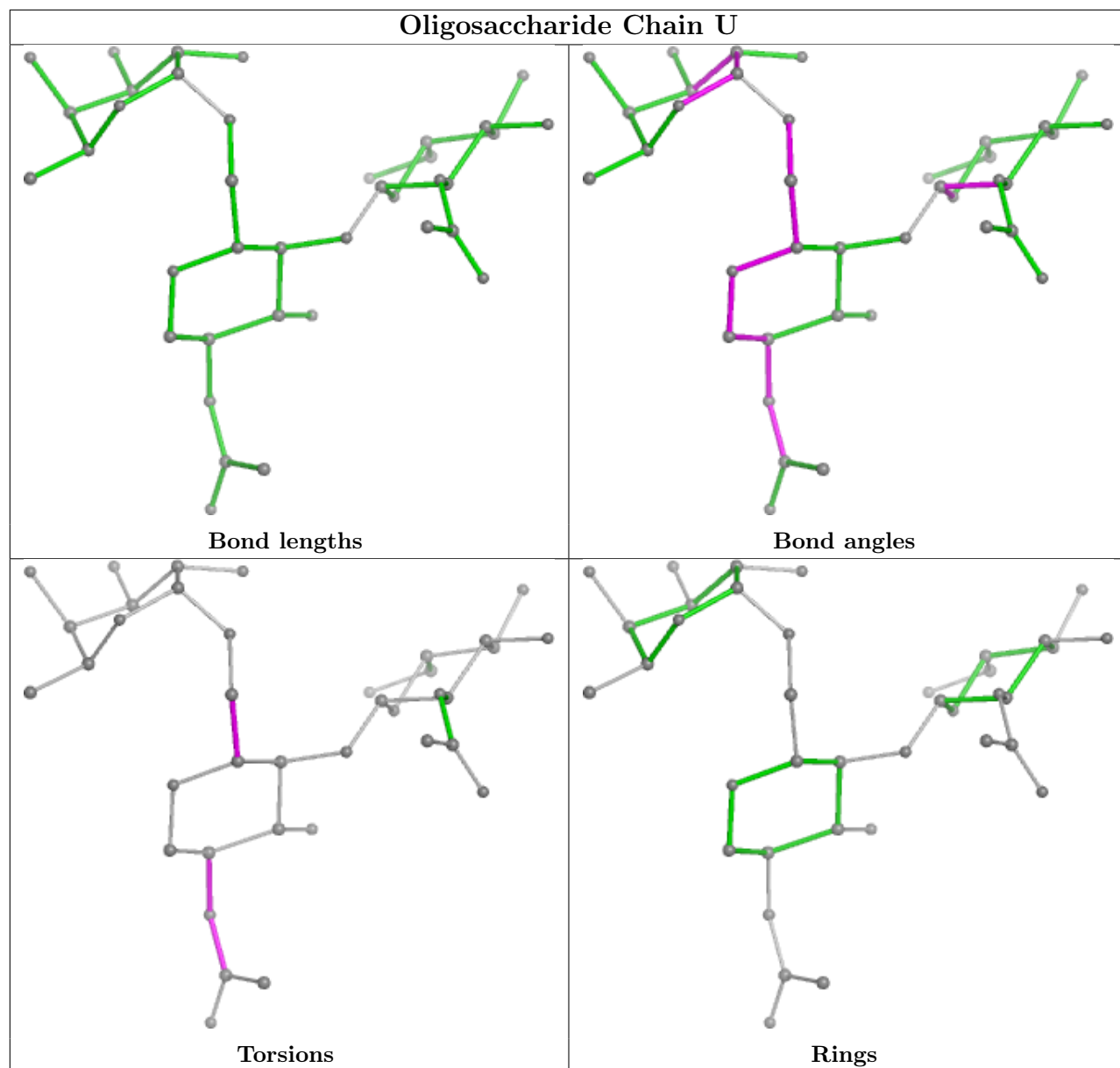
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

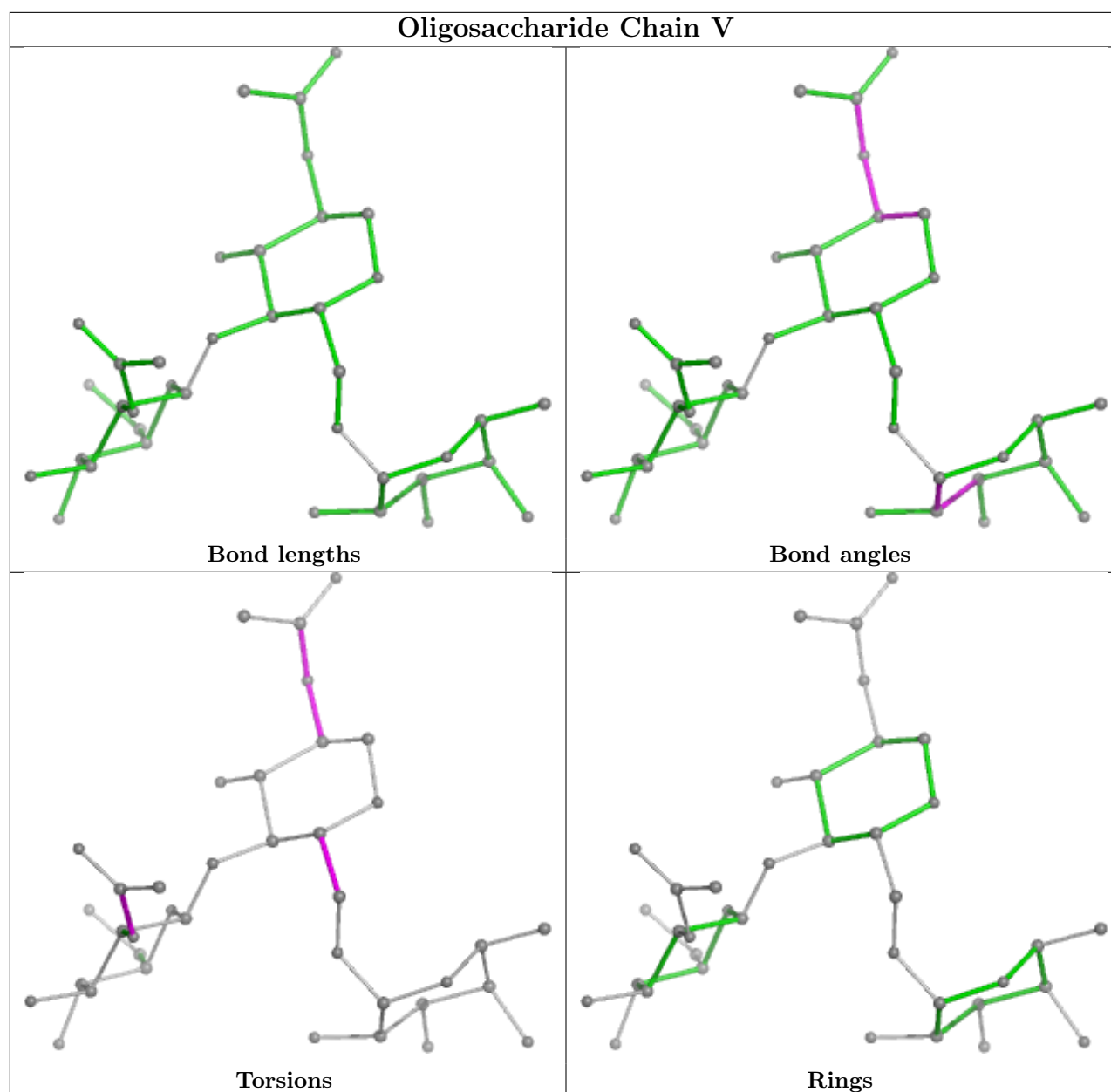
bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

15 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
9	EDO	R	301	-	3,3,3	0.30	0	2,2,2	0.44	0
11	FUC	O	501	-	10,10,11	0.31	0	14,14,16	0.44	0
8	D10	Q	403	-	9,9,9	0.39	0	8,8,8	0.38	0
8	D10	L	402	-	9,9,9	0.37	0	8,8,8	0.38	0
9	EDO	M	301	-	3,3,3	0.40	0	2,2,2	0.35	0
10	NAG	L	401	1	14,14,15	0.41	0	17,19,21	0.90	2 (11%)
8	D10	Q	402	-	9,9,9	0.34	0	8,8,8	0.34	0
10	NAG	Q	401	1	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
9	EDO	D	200	-	3,3,3	0.39	0	2,2,2	0.50	0
8	D10	G	402	-	9,9,9	0.32	0	8,8,8	0.30	0
8	D10	A	402	-	9,9,9	0.11	0	8,8,8	0.10	0
8	D10	G	401	-	9,9,9	0.45	0	8,8,8	0.38	0
8	D10	L	403	-	9,9,9	0.37	0	8,8,8	0.31	0
8	D10	A	401	-	9,9,9	0.11	0	8,8,8	0.09	0
9	EDO	H	301	-	3,3,3	0.37	0	2,2,2	0.24	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
9	EDO	R	301	-	-	0/1/1/1	-
11	FUC	O	501	-	-	-	0/1/1/1
8	D10	Q	403	-	-	6/7/7/7	-
8	D10	L	402	-	-	4/7/7/7	-
9	EDO	M	301	-	-	0/1/1/1	-
10	NAG	L	401	1	-	3/6/23/26	0/1/1/1
8	D10	Q	402	-	-	4/7/7/7	-
10	NAG	Q	401	1	-	4/6/23/26	0/1/1/1
9	EDO	D	200	-	-	1/1/1/1	-
8	D10	G	402	-	-	5/7/7/7	-
8	D10	A	402	-	-	2/7/7/7	-
8	D10	G	401	-	-	4/7/7/7	-
8	D10	L	403	-	-	6/7/7/7	-
8	D10	A	401	-	-	2/7/7/7	-
9	EDO	H	301	-	-	0/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	401	NAG	C1-O5-C5	2.81	116.00	112.19
10	Q	401	NAG	C1-C2-N2	2.80	115.27	110.49
10	Q	401	NAG	O5-C1-C2	-2.18	107.84	111.29
10	L	401	NAG	O5-C1-C2	2.04	114.51	111.29

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	401	NAG	O7-C7-N2-C2
10	Q	401	NAG	C8-C7-N2-C2
10	Q	401	NAG	O7-C7-N2-C2
10	L	401	NAG	C8-C7-N2-C2
10	Q	401	NAG	C4-C5-C6-O6
10	Q	401	NAG	O5-C5-C6-O6
8	A	402	D10	C5-C6-C7-C8
8	Q	403	D10	C6-C7-C8-C9
8	G	402	D10	C6-C7-C8-C9
8	Q	403	D10	C2-C3-C4-C5
8	L	403	D10	C4-C5-C6-C7
8	G	402	D10	C2-C3-C4-C5
8	Q	402	D10	C5-C6-C7-C8
8	Q	402	D10	C2-C3-C4-C5
8	G	402	D10	C3-C4-C5-C6
8	Q	403	D10	C4-C5-C6-C7
8	L	402	D10	C5-C6-C7-C8
8	L	403	D10	C2-C3-C4-C5
8	G	402	D10	C1-C2-C3-C4
8	L	402	D10	C7-C8-C9-C10
8	L	403	D10	C1-C2-C3-C4
8	Q	403	D10	C1-C2-C3-C4
8	G	402	D10	C4-C5-C6-C7
8	G	401	D10	C3-C4-C5-C6
8	Q	402	D10	C6-C7-C8-C9
8	L	402	D10	C6-C7-C8-C9
8	G	401	D10	C2-C3-C4-C5
8	L	402	D10	C4-C5-C6-C7
8	A	401	D10	C7-C8-C9-C10
8	L	403	D10	C6-C7-C8-C9
10	L	401	NAG	C3-C2-N2-C7
8	L	403	D10	C3-C4-C5-C6

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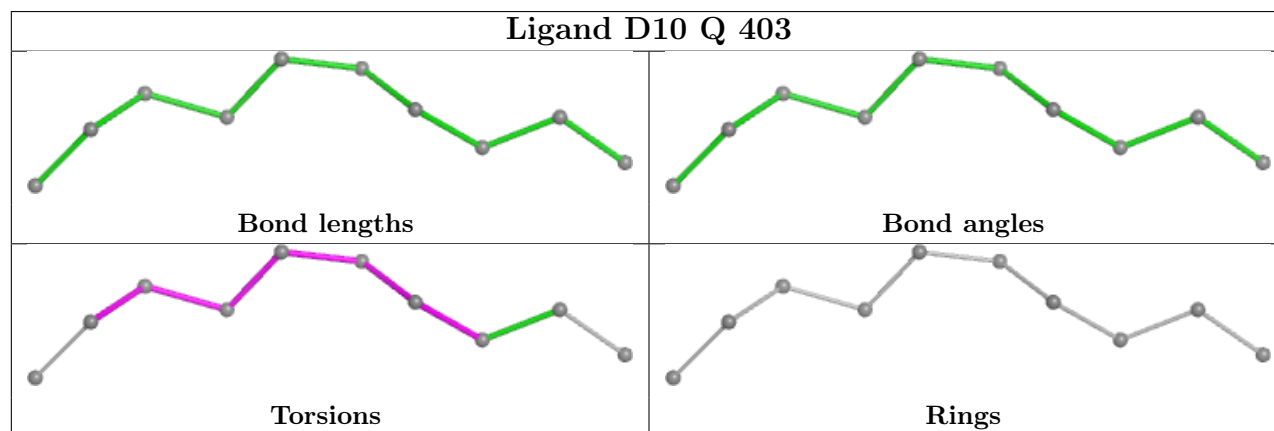
Mol	Chain	Res	Type	Atoms
8	A	401	D10	C2-C3-C4-C5
8	A	402	D10	C3-C4-C5-C6
8	G	401	D10	C7-C8-C9-C10
8	G	401	D10	C6-C7-C8-C9
8	Q	402	D10	C3-C4-C5-C6
8	L	403	D10	C7-C8-C9-C10
9	D	200	EDO	O1-C1-C2-O2
8	Q	403	D10	C5-C6-C7-C8
8	Q	403	D10	C3-C4-C5-C6

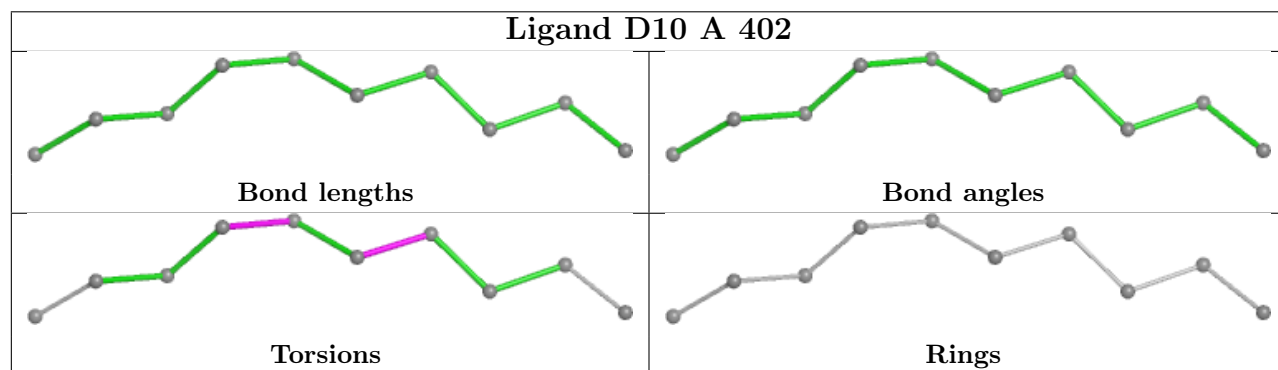
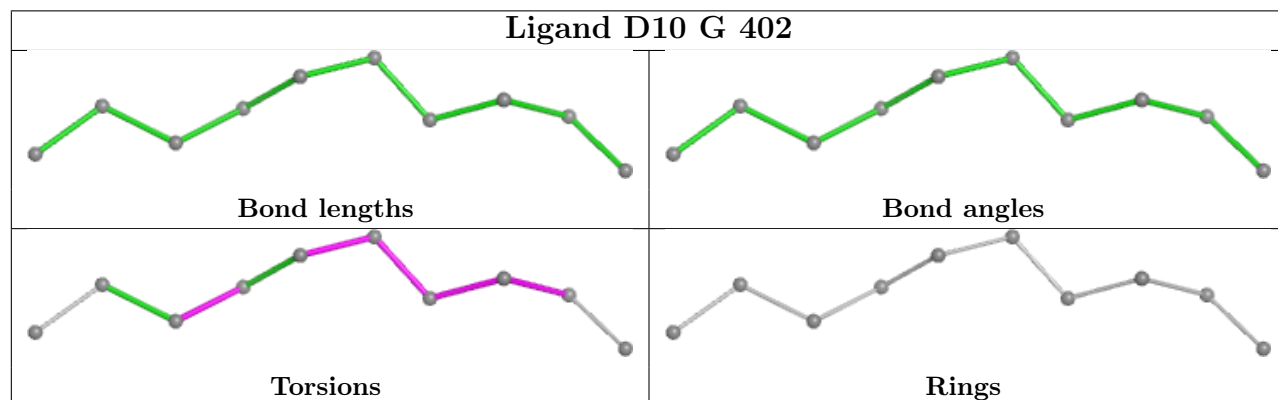
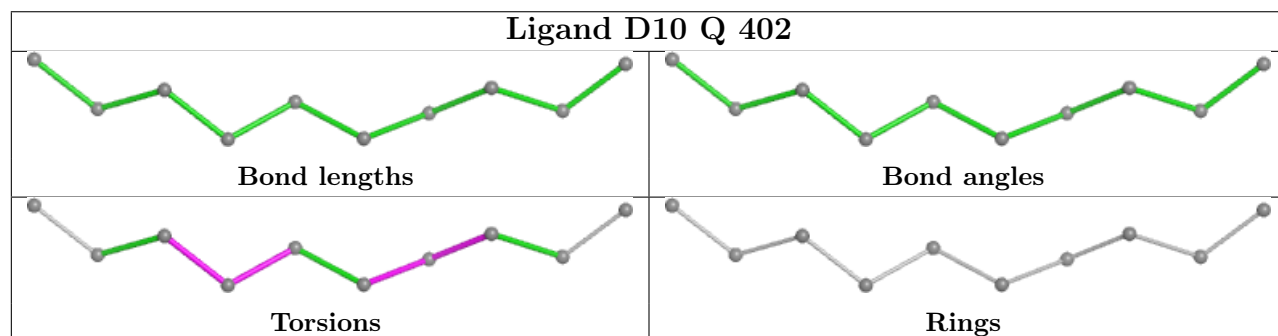
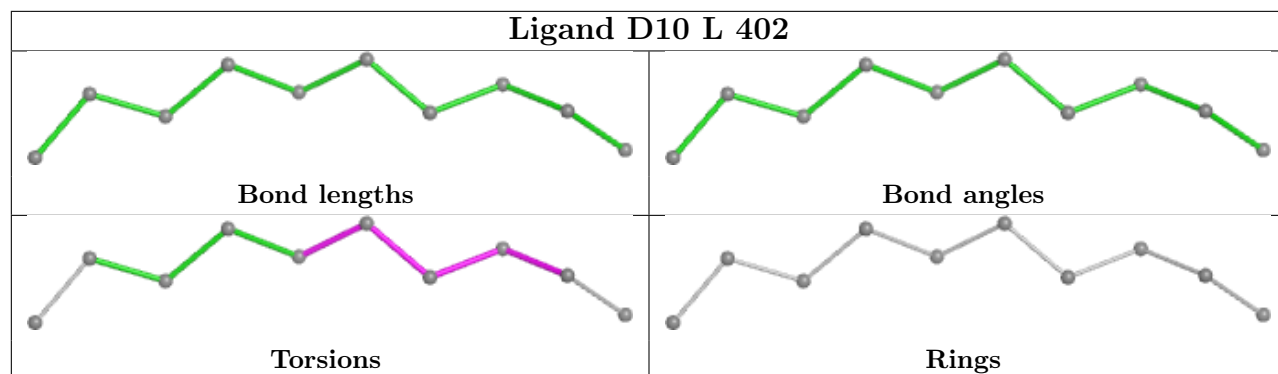
There are no ring outliers.

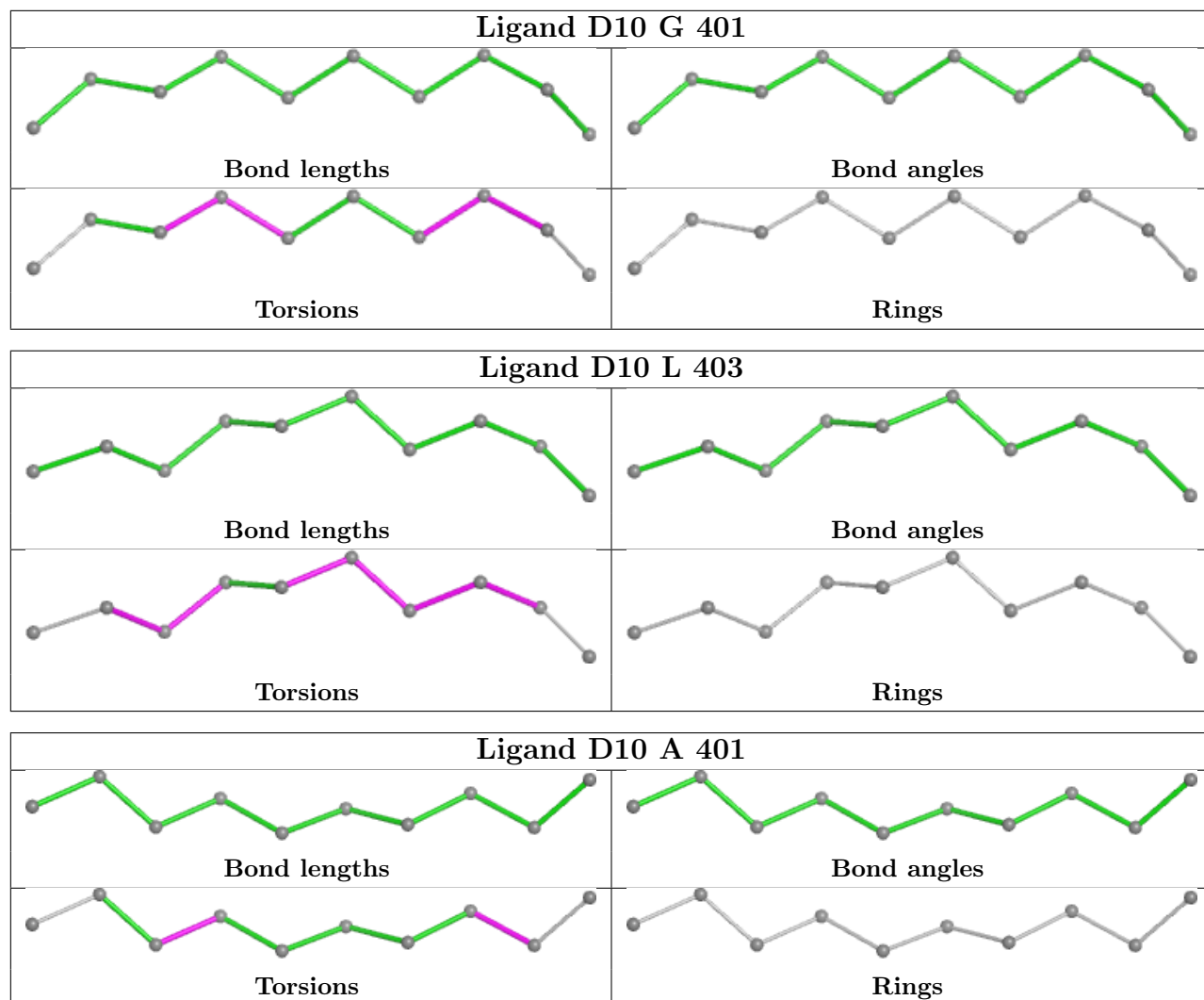
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	401	NAG	1	0
8	L	403	D10	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	269/442 (60%)	0.77	37 (13%) 8 8	33, 56, 172, 214	0
1	B	104/442 (23%)	0.67	4 (3%) 44 46	38, 82, 120, 152	0
1	G	271/442 (61%)	0.78	26 (9%) 15 16	45, 62, 112, 151	0
1	J	104/442 (23%)	0.44	4 (3%) 44 46	45, 64, 100, 107	0
1	L	261/442 (59%)	0.96	39 (14%) 7 7	42, 75, 167, 188	0
1	O	104/442 (23%)	0.88	6 (5%) 30 31	57, 87, 119, 124	0
1	Q	268/442 (60%)	1.18	48 (17%) 4 5	53, 83, 183, 220	0
1	T	104/442 (23%)	1.57	30 (28%) 1 1	60, 92, 127, 140	0
2	D	191/200 (95%)	0.30	12 (6%) 27 28	34, 48, 92, 136	0
2	H	192/200 (96%)	0.55	7 (3%) 46 48	48, 64, 117, 148	0
2	M	192/200 (96%)	0.38	12 (6%) 27 28	37, 53, 111, 133	0
2	R	192/200 (96%)	0.75	14 (7%) 22 23	49, 73, 135, 159	0
3	E	245/246 (99%)	0.04	3 (1%) 76 77	30, 45, 72, 96	0
3	F	243/246 (98%)	0.64	13 (5%) 33 34	53, 71, 108, 122	0
3	K	243/246 (98%)	0.14	7 (2%) 54 55	38, 50, 77, 89	0
3	P	243/246 (98%)	0.66	14 (5%) 30 31	47, 75, 113, 131	0
All	All	3226/5320 (60%)	0.65	276 (8%) 18 19	30, 66, 135, 220	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	6.4
1	T	18	GLY	6.4
1	Q	254	SER	5.8
1	G	8	VAL	5.6
1	L	278	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	T	72	PRO	5.5
1	Q	198	LEU	5.4
1	Q	258	ALA	5.3
1	T	15	ALA	5.3
3	E	1	ASP	5.2
1	L	252	VAL	5.2
3	P	362	ALA	5.0
1	T	71	THR	4.8
1	L	279	GLY	4.7
1	A	278	TRP	4.6
1	G	257	PRO	4.4
1	Q	8	VAL	4.3
1	L	8	VAL	4.3
3	P	258	GLN	4.2
1	A	276	LEU	4.1
1	A	253	ALA	4.1
1	A	256	GLU	4.0
1	A	229	LEU	4.0
1	L	259	GLY	3.9
1	Q	278	TRP	3.9
1	T	70	PHE	3.8
1	Q	264	VAL	3.8
1	Q	202	GLN	3.8
1	A	254	SER	3.8
1	G	258	ALA	3.8
1	Q	253	ALA	3.8
3	P	262	LEU	3.8
1	A	89	TYR	3.7
1	Q	274	ILE	3.7
1	G	253	ALA	3.7
2	R	194	SER	3.6
1	L	196	PRO	3.6
1	Q	196	PRO	3.6
1	L	203	LEU	3.6
1	Q	276	LEU	3.5
1	G	225	GLU	3.5
1	L	275	ILE	3.5
1	L	151	GLN	3.4
2	R	185	PHE	3.4
1	G	90	SER	3.4
1	A	203	LEU	3.4
2	M	193	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	218	TRP	3.4
1	T	49	VAL	3.4
2	R	126	LEU	3.4
2	R	184	ASP	3.3
1	T	73	THR	3.3
1	L	70	PHE	3.3
3	P	247	PHE	3.3
1	A	20	ASN	3.3
1	Q	199	GLY	3.3
1	T	17	ASN	3.3
3	K	120	THR	3.3
2	H	185	PHE	3.3
1	Q	259	GLY	3.3
1	A	275	ILE	3.2
1	G	198	LEU	3.2
3	P	157	LEU	3.2
1	A	218	TRP	3.2
3	K	362	ALA	3.2
1	B	69	GLU	3.2
3	K	157	LEU	3.2
1	Q	26	GLY	3.1
1	A	277	TYR	3.1
1	T	11	SER	3.1
1	G	89	TYR	3.1
1	L	220	THR	3.1
1	L	276	LEU	3.1
1	T	22	PHE	3.0
2	M	188	ALA	3.0
1	T	19	LYS	3.0
1	Q	209	ALA	3.0
1	L	270	GLY	3.0
1	T	69	GLU	3.0
3	P	120	THR	2.9
1	O	1	ILE	2.9
1	A	198	LEU	2.9
1	Q	104	LEU	2.9
1	Q	245	TYR	2.9
1	Q	165	SER	2.9
1	L	153	GLU	2.9
2	M	130	LYS	2.9
1	Q	218	TRP	2.9
3	F	177	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	52	LYS	2.9
1	Q	275	ILE	2.9
1	G	20	ASN	2.9
1	Q	89	TYR	2.9
1	A	137	CYS	2.8
3	K	179	LEU	2.8
1	O	18	GLY	2.8
1	Q	186	VAL	2.8
3	P	320	TRP	2.8
2	D	166	ARG	2.8
1	Q	190	ALA	2.8
1	A	233	HIS	2.8
3	P	256	HIS	2.8
2	D	183	ASP	2.8
1	A	252	VAL	2.8
1	G	137	CYS	2.8
3	E	138	HIS	2.8
1	T	1	ILE	2.7
3	F	353	ILE	2.7
1	G	254	SER	2.7
1	O	58	LYS	2.7
1	L	277	TYR	2.7
1	Q	219	VAL	2.7
1	Q	260	LEU	2.7
1	A	224	ASN	2.7
2	H	169	MET	2.7
1	Q	252	VAL	2.7
1	G	156	THR	2.7
1	L	269	LEU	2.7
1	Q	220	THR	2.7
3	P	178	LEU	2.7
2	D	2	ASN	2.7
1	A	196	PRO	2.7
2	R	136	VAL	2.7
1	Q	203	LEU	2.6
1	Q	250	LEU	2.6
1	L	137	CYS	2.6
1	L	271	GLY	2.6
1	A	23	TRP	2.6
1	T	46	ILE	2.6
1	L	88	ASP	2.6
1	L	190	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	69	GLU	2.6
1	B	104	SER	2.6
2	H	117	GLN	2.6
2	H	134	LYS	2.6
1	Q	180	MET	2.6
1	L	89	TYR	2.6
1	Q	204	LEU	2.6
1	A	255	GLU	2.5
3	F	362	ALA	2.5
1	A	204	LEU	2.5
1	L	129	THR	2.5
1	L	204	LEU	2.5
1	L	205	LEU	2.5
1	L	249	ILE	2.5
1	T	20	SER	2.5
1	Q	270	GLY	2.5
1	Q	229	LEU	2.5
1	Q	277	TYR	2.5
1	G	139	SER	2.5
1	B	70	PHE	2.5
1	T	82	VAL	2.5
3	K	273	HIS	2.5
1	L	194	SER	2.5
1	T	95	TRP	2.5
1	T	94	LYS	2.5
1	G	129	THR	2.5
1	A	200	SER	2.4
2	R	188	ALA	2.4
1	G	70	PHE	2.4
1	L	250	LEU	2.4
3	F	157	LEU	2.4
2	M	167	ARG	2.4
1	T	14	PRO	2.4
1	A	249	ILE	2.4
1	L	274	ILE	2.4
2	H	73	SER	2.4
2	R	134	LYS	2.4
3	K	177	ARG	2.4
1	G	104	LEU	2.4
1	L	104	LEU	2.4
2	R	156	VAL	2.4
1	J	104	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	103	GLY	2.4
1	L	219	VAL	2.4
2	D	129	LYS	2.4
2	M	152	LYS	2.4
2	R	130	LYS	2.4
1	A	274	ILE	2.4
2	D	131	SER	2.4
2	D	153	SER	2.4
2	H	183	SER	2.4
1	A	7	HIS	2.4
1	A	205	LEU	2.4
1	G	278	TRP	2.3
2	M	185	PHE	2.3
3	F	300	PRO	2.3
1	T	104	SER	2.3
1	G	201	GLY	2.3
1	Q	107	GLY	2.3
1	A	250	LEU	2.3
1	T	23	LEU	2.3
3	F	125	ASN	2.3
3	F	301	ALA	2.3
1	G	75	PHE	2.3
1	Q	201	GLY	2.3
1	L	260	LEU	2.3
1	L	91	LYS	2.3
1	T	58	LYS	2.3
1	G	18	PHE	2.3
3	F	343	THR	2.3
1	G	218	TRP	2.3
1	J	49	VAL	2.3
2	D	130	SER	2.3
2	R	149	SER	2.3
1	A	136	GLY	2.3
1	L	229	LEU	2.2
3	E	2	THR	2.2
1	A	183	HIS	2.2
3	F	128	HIS	2.2
1	Q	191	TRP	2.2
1	Q	194	SER	2.2
1	A	230	GLY	2.2
1	A	192	LEU	2.2
1	Q	192	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	265	ARG	2.2
1	L	156	THR	2.2
3	K	128	HIS	2.2
1	O	99	ILE	2.2
1	Q	221	TRP	2.2
1	A	180	MET	2.2
2	M	189	ASN	2.2
2	D	51	THR	2.2
1	Q	200	SER	2.2
2	M	154	SER	2.2
3	P	245	ALA	2.2
3	P	257	THR	2.2
2	D	182	SER	2.1
1	A	221	TRP	2.1
3	F	195	LEU	2.1
1	T	13	HIS	2.1
1	G	180	MET	2.1
1	Q	235	ASP	2.1
1	O	104	SER	2.1
1	T	3	ARG	2.1
1	T	7	ILE	2.1
1	B	95	TRP	2.1
2	D	68	LYS	2.1
1	Q	217	VAL	2.1
3	F	183	PHE	2.1
1	Q	263	ARG	2.1
2	M	184	ASP	2.1
1	G	259	GLY	2.1
1	T	48	LYS	2.1
2	M	134	LYS	2.1
1	A	217	VAL	2.1
1	T	85	VAL	2.1
1	T	97	ARG	2.1
1	T	99	ILE	2.1
1	L	146	HIS	2.1
1	Q	233	HIS	2.1
2	M	69	LYS	2.1
1	Q	224	ASN	2.1
3	P	359	TRP	2.1
1	J	44	GLU	2.0
2	R	70	GLU	2.0
1	L	195	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	75	PHE	2.0
1	Q	113	PHE	2.0
1	A	22	SER	2.0
2	H	194	SER	2.0
2	D	180	GLN	2.0
1	G	175	LEU	2.0
2	R	189	ASN	2.0
1	G	24	ALA	2.0
1	L	111	GLU	2.0
1	Q	225	GLU	2.0
3	P	177	ARG	2.0
3	P	317	ALA	2.0
2	M	194	SER	2.0
2	R	69	LYS	2.0
1	G	140	LEU	2.0
1	T	39	LEU	2.0
3	F	178	LEU	2.0
3	F	214	PRO	2.0
2	R	137	CYS	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.

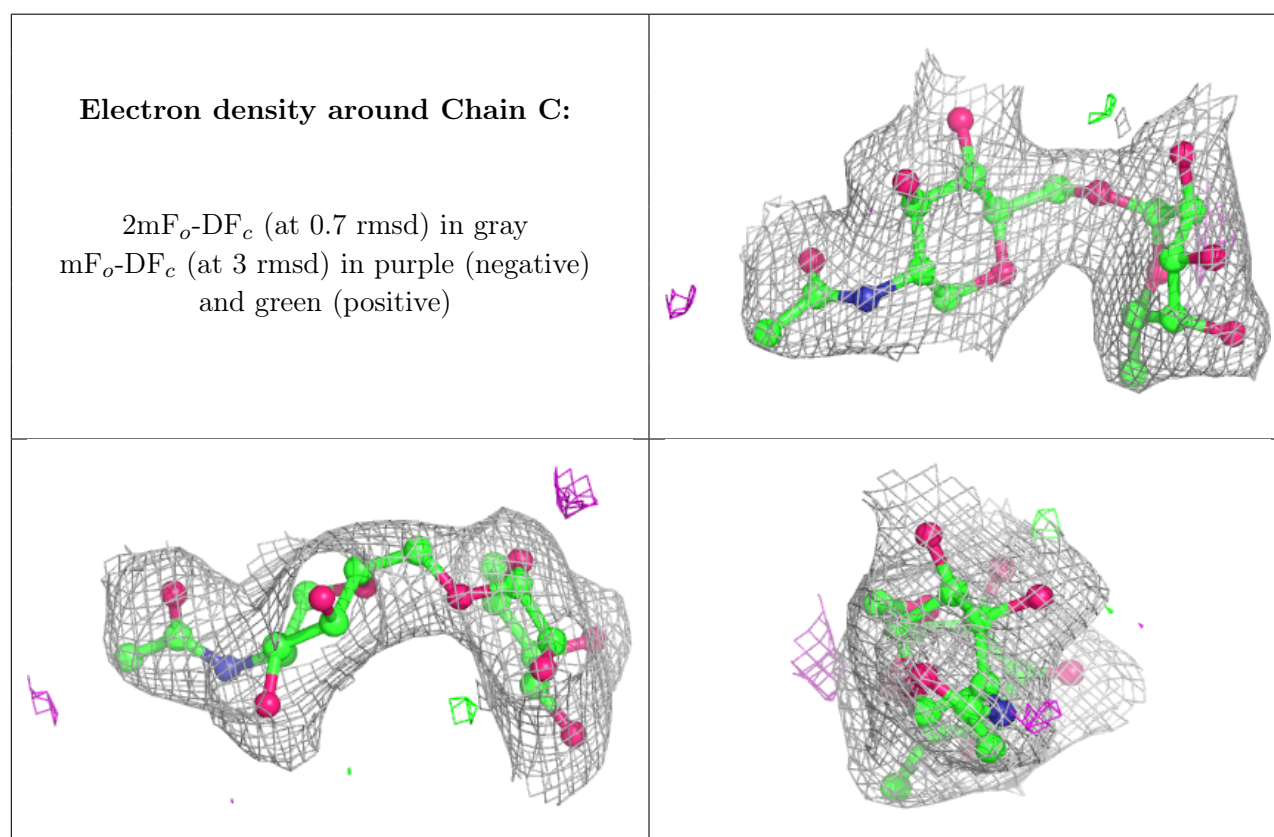
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	1	14/15	-	-	41,44,46,47	0
4	FUC	C	2	10/11	-	-	43,45,49,50	0
4	NAG	N	1	14/15	-	-	20,20,20,20	0
4	FUC	N	2	10/11	-	-	104,110,116,120	0
5	NAG	I	1	14/15	-	-	44,56,58,70	0
5	BMA	I	2	11/12	-	-	84,91,106,111	0
6	NAG	S	1	14/15	0.80	0.29	62,67,72,72	0
6	NAG	S	2	14/15	-	-	76,88,103,118	0
6	BMA	S	3	11/12	-	-	121,128,136,138	0

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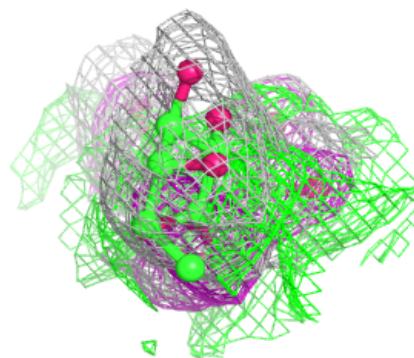
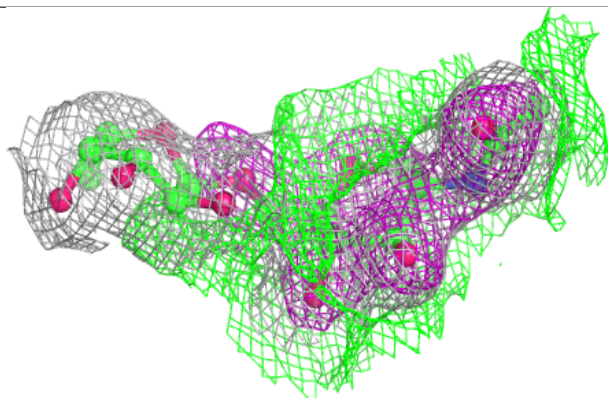
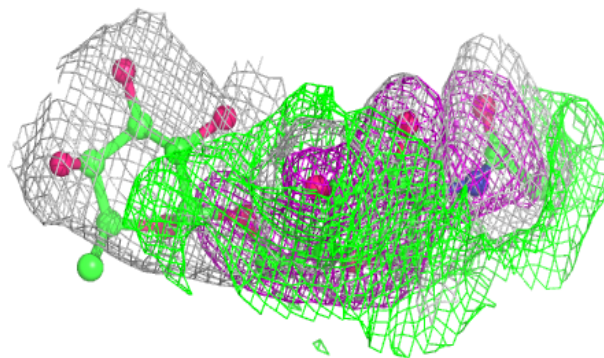
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	FUC	S	4	10/11	-	-	74,78,83,86	0
7	NAG	V	2	14/15	0.81	0.13	76,97,106,110	0
7	NAG	V	1	14/15	0.82	0.13	63,69,75,77	0
7	NAG	U	1	14/15	0.82	0.15	54,62,67,72	0
7	NAG	U	2	14/15	0.88	0.12	64,77,91,93	0
7	FUC	V	3	10/11	0.90	0.09	80,82,84,86	0
7	FUC	U	3	10/11	0.92	0.11	66,67,70,71	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.

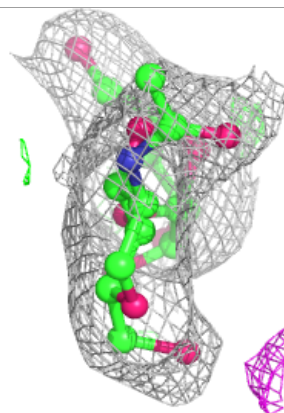
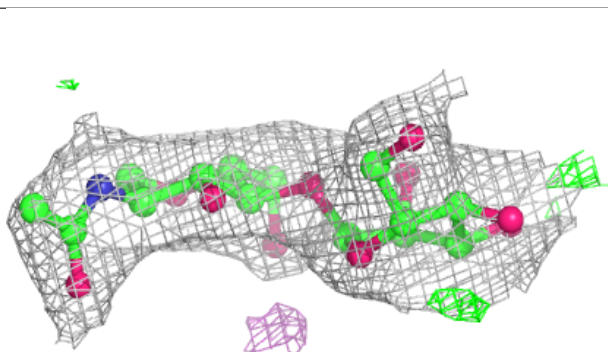
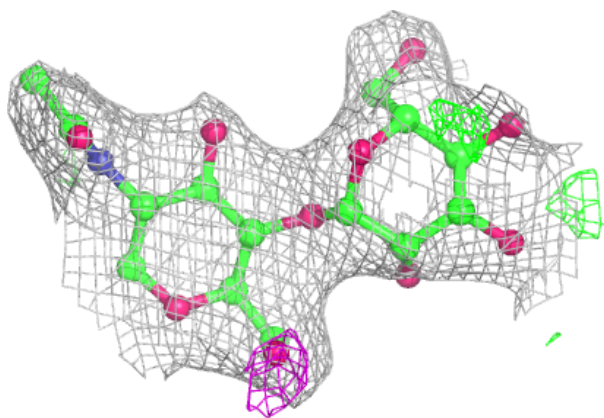


Electron density around Chain N:

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

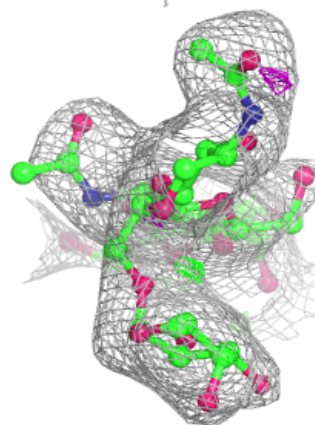
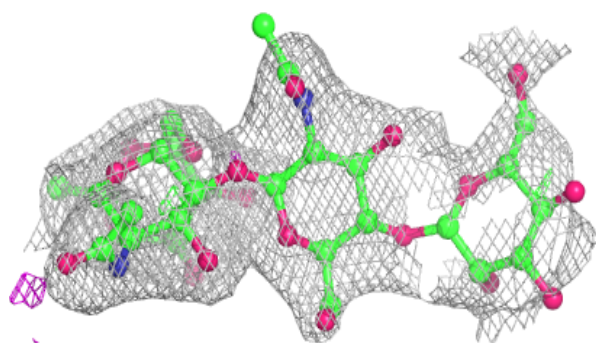
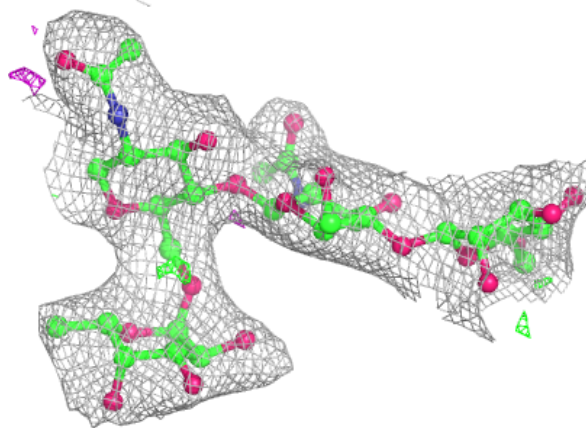
**Electron density around Chain I:**

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



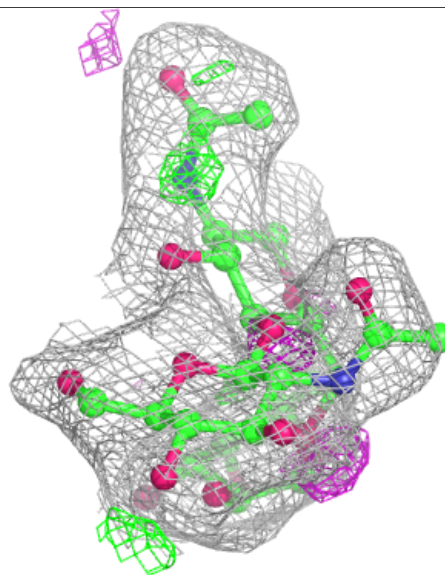
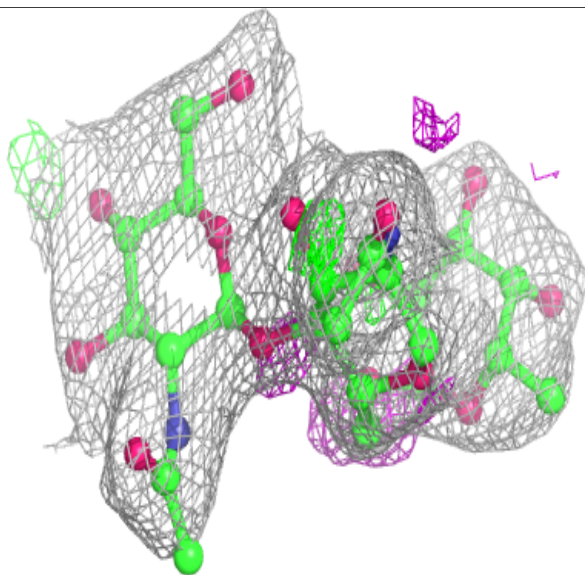
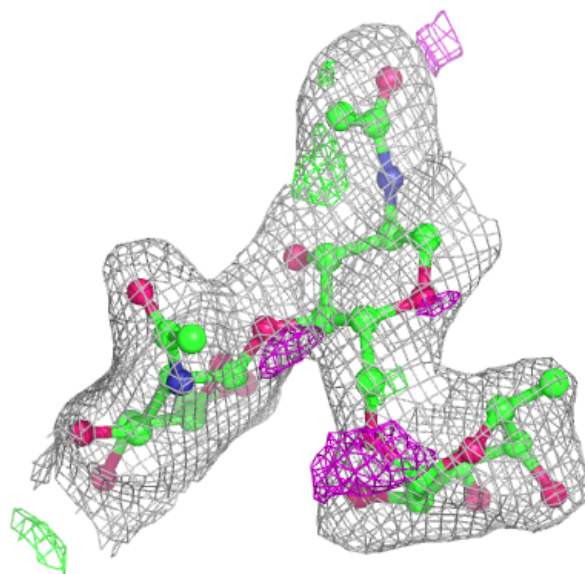
Electron density around Chain S:

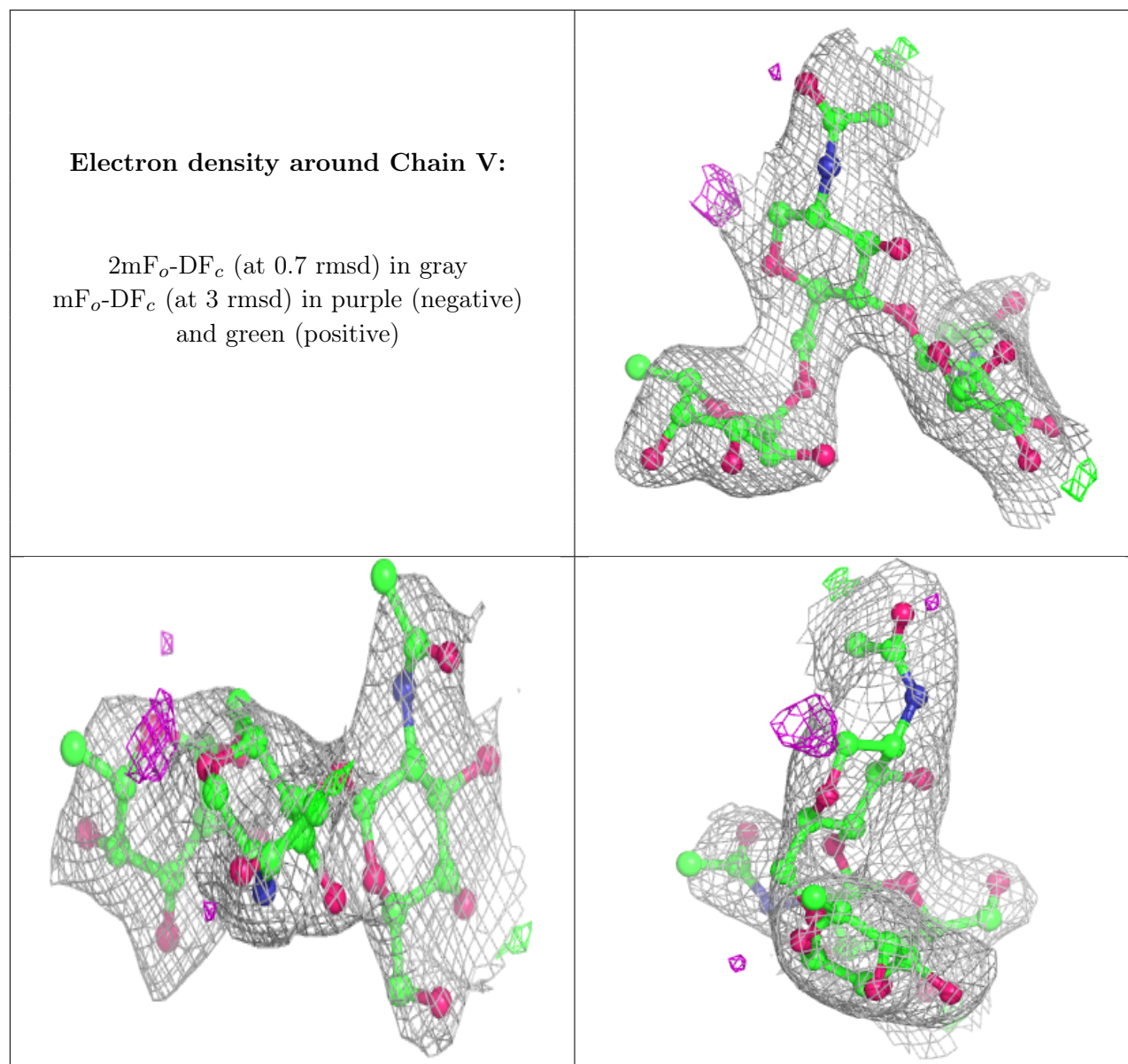
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain U:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
10	NAG	Q	401	14/15	0.64	0.16	97,110,120,121	0
10	NAG	L	401	14/15	0.69	0.16	92,103,111,113	0
11	FUC	O	501	10/11	0.76	0.17	75,83,94,99	0
8	D10	A	401	10/10	0.88	0.18	40,44,54,56	0
8	D10	A	402	10/10	0.88	0.22	52,61,72,74	0

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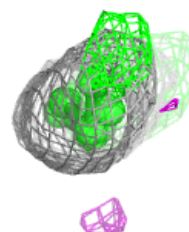
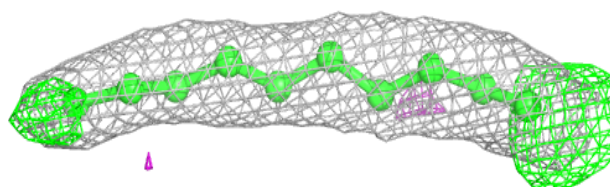
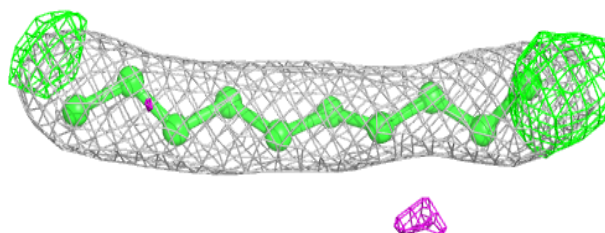
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	D10	G	401	10/10	0.88	0.23	57,61,64,65	0
8	D10	Q	403	10/10	0.90	0.22	68,72,75,76	0
8	D10	G	402	10/10	0.90	0.22	64,67,81,83	0
8	D10	L	403	10/10	0.91	0.18	55,61,78,79	0
9	EDO	R	301	4/4	0.93	0.11	58,60,60,62	0
8	D10	Q	402	10/10	0.93	0.15	50,57,58,59	0
8	D10	L	402	10/10	0.94	0.14	53,55,61,63	0
9	EDO	H	301	4/4	0.94	0.09	63,66,67,68	0
9	EDO	D	200	4/4	0.96	0.08	42,48,50,52	0
9	EDO	M	301	4/4	0.96	0.08	52,58,59,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

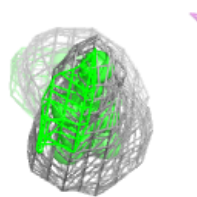
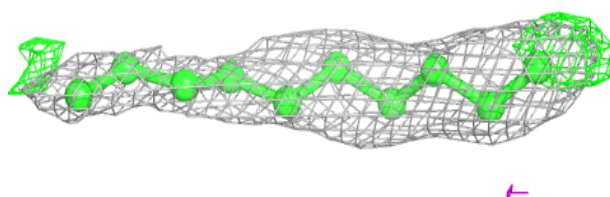
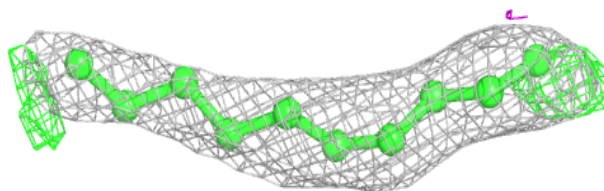
Electron density around D10 A 401:

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

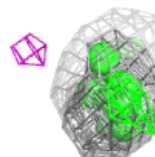
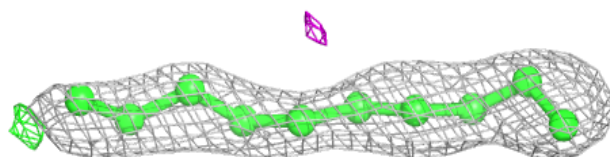
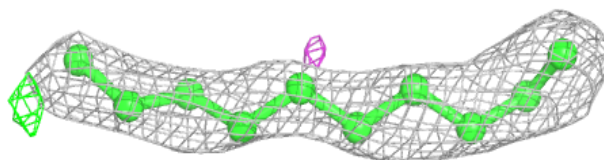


Electron density around D10 A 402:

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

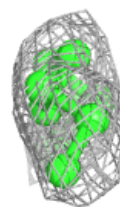
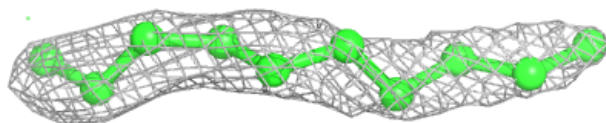
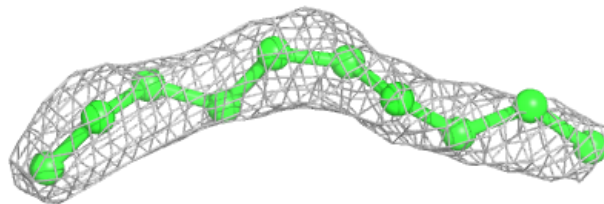
**Electron density around D10 G 401:**

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

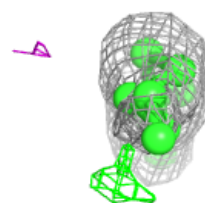
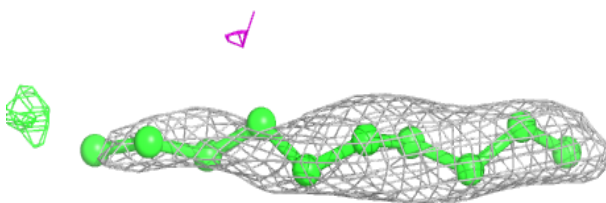
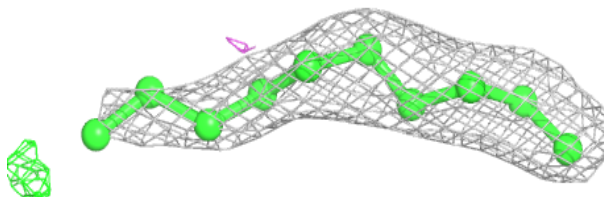


Electron density around D10 Q 403:

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

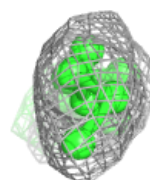
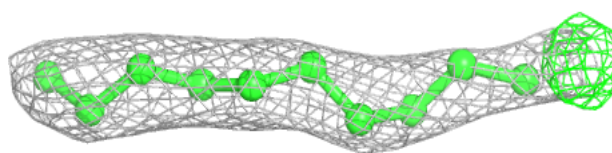
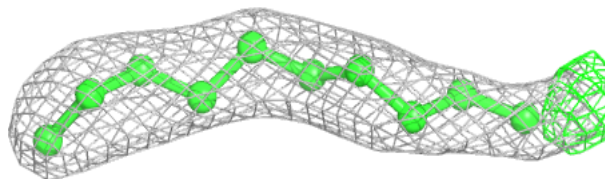
**Electron density around D10 G 402:**

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

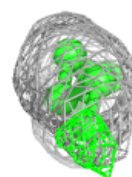
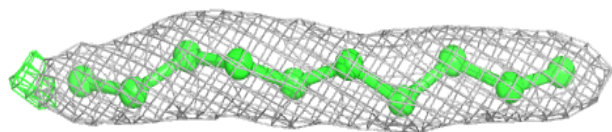
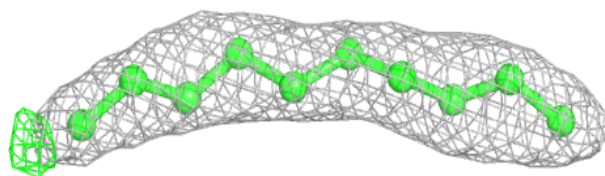


Electron density around D10 L 403:

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

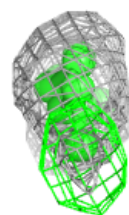
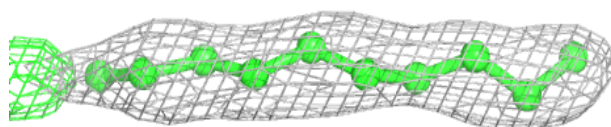
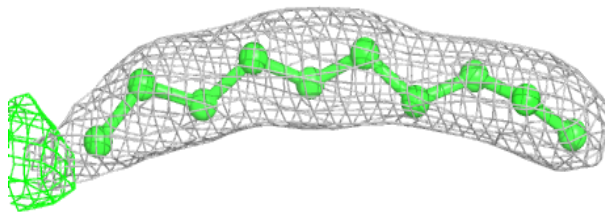
**Electron density around D10 Q 402:**

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



Electron density around D10 L 402:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.