wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2023 – 01:37 pm BST

PDB ID	:	7ZV9
Title	:	Crystal structure of FLT3 in complex with a monomeric FLT3 Ligand variant
Authors	:	Pannecoucke, E.; Savvides, S.N.
Deposited on	:	2022-05-14
Resolution	:	4.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

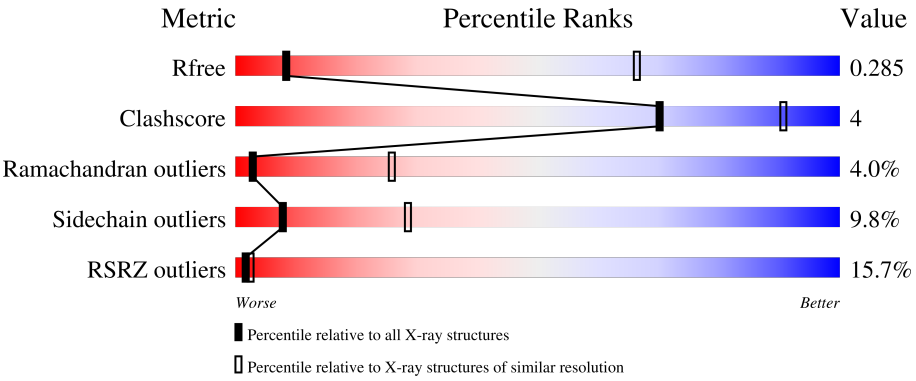
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 <=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	155	8% 74% 12% • 14%
1	C	155	3% 75% 10% • 14%
1	E	155	6% 77% 7% • 14%
1	G	155	7% 74% 9% • • 14%
1	I	155	7% 78% 8% • 13%

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Mol	Chain	Length	Quality of chain
1	K	155	2% 77% 11% 12%
1	M	155	4% 79% 7% 14%
1	O	155	5% 79% 8% 14%
2	B	582	14% 62% 10% 27%
2	D	582	14% 63% 9% 27%
2	F	582	14% 63% 8% 28%
2	H	582	11% 64% 9% 27%
2	J	582	14% 63% 8% 28%
2	L	582	15% 64% 10% 26%
2	N	582	15% 64% 9% 26%
2	P	582	12% 63% 9% 27%
3	Q	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	50% 50%
3	U	2	100%
3	V	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26691 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 Fms-related tyrosine kinase 3 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	1	0
			915	563	163	181	8			
1	C	134	Total	C	N	O	S	0	1	0
			879	532	162	178	7			
1	E	134	Total	C	N	O	S	0	1	0
			844	504	159	174	7			
1	G	134	Total	C	N	O	S	0	0	0
			884	541	161	176	6			
1	I	135	Total	C	N	O	S	0	1	0
			907	554	162	183	8			
1	K	137	Total	C	N	O	S	0	0	0
			892	544	163	177	8			
1	M	134	Total	C	N	O	S	0	0	0
			908	561	158	181	8			
1	O	134	Total	C	N	O	S	0	1	0
			919	571	160	181	7			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P49771
A	-19	GLY	-	expression tag	UNP P49771
A	-18	SER	-	expression tag	UNP P49771
A	-17	SER	-	expression tag	UNP P49771
A	-16	HIS	-	expression tag	UNP P49771
A	-15	HIS	-	expression tag	UNP P49771
A	-14	HIS	-	expression tag	UNP P49771
A	-13	HIS	-	expression tag	UNP P49771
A	-12	HIS	-	expression tag	UNP P49771
A	-11	HIS	-	expression tag	UNP P49771
A	-10	SER	-	expression tag	UNP P49771
A	-9	SER	-	expression tag	UNP P49771
A	-8	GLY	-	expression tag	UNP P49771

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP P49771
A	-6	VAL	-	expression tag	UNP P49771
A	-5	PRO	-	expression tag	UNP P49771
A	-4	ARG	-	expression tag	UNP P49771
A	-3	GLY	-	expression tag	UNP P49771
A	-2	SER	-	expression tag	UNP P49771
A	-1	HIS	-	expression tag	UNP P49771
A	0	MET	-	expression tag	UNP P49771
A	27	ASP	LEU	engineered mutation	UNP P49771
C	-20	MET	-	initiating methionine	UNP P49771
C	-19	GLY	-	expression tag	UNP P49771
C	-18	SER	-	expression tag	UNP P49771
C	-17	SER	-	expression tag	UNP P49771
C	-16	HIS	-	expression tag	UNP P49771
C	-15	HIS	-	expression tag	UNP P49771
C	-14	HIS	-	expression tag	UNP P49771
C	-13	HIS	-	expression tag	UNP P49771
C	-12	HIS	-	expression tag	UNP P49771
C	-11	HIS	-	expression tag	UNP P49771
C	-10	SER	-	expression tag	UNP P49771
C	-9	SER	-	expression tag	UNP P49771
C	-8	GLY	-	expression tag	UNP P49771
C	-7	LEU	-	expression tag	UNP P49771
C	-6	VAL	-	expression tag	UNP P49771
C	-5	PRO	-	expression tag	UNP P49771
C	-4	ARG	-	expression tag	UNP P49771
C	-3	GLY	-	expression tag	UNP P49771
C	-2	SER	-	expression tag	UNP P49771
C	-1	HIS	-	expression tag	UNP P49771
C	0	MET	-	expression tag	UNP P49771
C	27	ASP	LEU	engineered mutation	UNP P49771
E	-20	MET	-	initiating methionine	UNP P49771
E	-19	GLY	-	expression tag	UNP P49771
E	-18	SER	-	expression tag	UNP P49771
E	-17	SER	-	expression tag	UNP P49771
E	-16	HIS	-	expression tag	UNP P49771
E	-15	HIS	-	expression tag	UNP P49771
E	-14	HIS	-	expression tag	UNP P49771
E	-13	HIS	-	expression tag	UNP P49771
E	-12	HIS	-	expression tag	UNP P49771
E	-11	HIS	-	expression tag	UNP P49771
E	-10	SER	-	expression tag	UNP P49771

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	SER	-	expression tag	UNP P49771
E	-8	GLY	-	expression tag	UNP P49771
E	-7	LEU	-	expression tag	UNP P49771
E	-6	VAL	-	expression tag	UNP P49771
E	-5	PRO	-	expression tag	UNP P49771
E	-4	ARG	-	expression tag	UNP P49771
E	-3	GLY	-	expression tag	UNP P49771
E	-2	SER	-	expression tag	UNP P49771
E	-1	HIS	-	expression tag	UNP P49771
E	0	MET	-	expression tag	UNP P49771
E	27	ASP	LEU	engineered mutation	UNP P49771
G	-20	MET	-	initiating methionine	UNP P49771
G	-19	GLY	-	expression tag	UNP P49771
G	-18	SER	-	expression tag	UNP P49771
G	-17	SER	-	expression tag	UNP P49771
G	-16	HIS	-	expression tag	UNP P49771
G	-15	HIS	-	expression tag	UNP P49771
G	-14	HIS	-	expression tag	UNP P49771
G	-13	HIS	-	expression tag	UNP P49771
G	-12	HIS	-	expression tag	UNP P49771
G	-11	HIS	-	expression tag	UNP P49771
G	-10	SER	-	expression tag	UNP P49771
G	-9	SER	-	expression tag	UNP P49771
G	-8	GLY	-	expression tag	UNP P49771
G	-7	LEU	-	expression tag	UNP P49771
G	-6	VAL	-	expression tag	UNP P49771
G	-5	PRO	-	expression tag	UNP P49771
G	-4	ARG	-	expression tag	UNP P49771
G	-3	GLY	-	expression tag	UNP P49771
G	-2	SER	-	expression tag	UNP P49771
G	-1	HIS	-	expression tag	UNP P49771
G	0	MET	-	expression tag	UNP P49771
G	27	ASP	LEU	engineered mutation	UNP P49771
I	-20	MET	-	initiating methionine	UNP P49771
I	-19	GLY	-	expression tag	UNP P49771
I	-18	SER	-	expression tag	UNP P49771
I	-17	SER	-	expression tag	UNP P49771
I	-16	HIS	-	expression tag	UNP P49771
I	-15	HIS	-	expression tag	UNP P49771
I	-14	HIS	-	expression tag	UNP P49771
I	-13	HIS	-	expression tag	UNP P49771
I	-12	HIS	-	expression tag	UNP P49771

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP P49771
I	-10	SER	-	expression tag	UNP P49771
I	-9	SER	-	expression tag	UNP P49771
I	-8	GLY	-	expression tag	UNP P49771
I	-7	LEU	-	expression tag	UNP P49771
I	-6	VAL	-	expression tag	UNP P49771
I	-5	PRO	-	expression tag	UNP P49771
I	-4	ARG	-	expression tag	UNP P49771
I	-3	GLY	-	expression tag	UNP P49771
I	-2	SER	-	expression tag	UNP P49771
I	-1	HIS	-	expression tag	UNP P49771
I	0	MET	-	expression tag	UNP P49771
I	27	ASP	LEU	engineered mutation	UNP P49771
K	-20	MET	-	initiating methionine	UNP P49771
K	-19	GLY	-	expression tag	UNP P49771
K	-18	SER	-	expression tag	UNP P49771
K	-17	SER	-	expression tag	UNP P49771
K	-16	HIS	-	expression tag	UNP P49771
K	-15	HIS	-	expression tag	UNP P49771
K	-14	HIS	-	expression tag	UNP P49771
K	-13	HIS	-	expression tag	UNP P49771
K	-12	HIS	-	expression tag	UNP P49771
K	-11	HIS	-	expression tag	UNP P49771
K	-10	SER	-	expression tag	UNP P49771
K	-9	SER	-	expression tag	UNP P49771
K	-8	GLY	-	expression tag	UNP P49771
K	-7	LEU	-	expression tag	UNP P49771
K	-6	VAL	-	expression tag	UNP P49771
K	-5	PRO	-	expression tag	UNP P49771
K	-4	ARG	-	expression tag	UNP P49771
K	-3	GLY	-	expression tag	UNP P49771
K	-2	SER	-	expression tag	UNP P49771
K	-1	HIS	-	expression tag	UNP P49771
K	0	MET	-	expression tag	UNP P49771
K	27	ASP	LEU	engineered mutation	UNP P49771
M	-20	MET	-	initiating methionine	UNP P49771
M	-19	GLY	-	expression tag	UNP P49771
M	-18	SER	-	expression tag	UNP P49771
M	-17	SER	-	expression tag	UNP P49771
M	-16	HIS	-	expression tag	UNP P49771
M	-15	HIS	-	expression tag	UNP P49771
M	-14	HIS	-	expression tag	UNP P49771

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-13	HIS	-	expression tag	UNP P49771
M	-12	HIS	-	expression tag	UNP P49771
M	-11	HIS	-	expression tag	UNP P49771
M	-10	SER	-	expression tag	UNP P49771
M	-9	SER	-	expression tag	UNP P49771
M	-8	GLY	-	expression tag	UNP P49771
M	-7	LEU	-	expression tag	UNP P49771
M	-6	VAL	-	expression tag	UNP P49771
M	-5	PRO	-	expression tag	UNP P49771
M	-4	ARG	-	expression tag	UNP P49771
M	-3	GLY	-	expression tag	UNP P49771
M	-2	SER	-	expression tag	UNP P49771
M	-1	HIS	-	expression tag	UNP P49771
M	0	MET	-	expression tag	UNP P49771
M	27	ASP	LEU	engineered mutation	UNP P49771
O	-20	MET	-	initiating methionine	UNP P49771
O	-19	GLY	-	expression tag	UNP P49771
O	-18	SER	-	expression tag	UNP P49771
O	-17	SER	-	expression tag	UNP P49771
O	-16	HIS	-	expression tag	UNP P49771
O	-15	HIS	-	expression tag	UNP P49771
O	-14	HIS	-	expression tag	UNP P49771
O	-13	HIS	-	expression tag	UNP P49771
O	-12	HIS	-	expression tag	UNP P49771
O	-11	HIS	-	expression tag	UNP P49771
O	-10	SER	-	expression tag	UNP P49771
O	-9	SER	-	expression tag	UNP P49771
O	-8	GLY	-	expression tag	UNP P49771
O	-7	LEU	-	expression tag	UNP P49771
O	-6	VAL	-	expression tag	UNP P49771
O	-5	PRO	-	expression tag	UNP P49771
O	-4	ARG	-	expression tag	UNP P49771
O	-3	GLY	-	expression tag	UNP P49771
O	-2	SER	-	expression tag	UNP P49771
O	-1	HIS	-	expression tag	UNP P49771
O	0	MET	-	expression tag	UNP P49771
O	27	ASP	LEU	engineered mutation	UNP P49771

- Molecule 2 is a protein called Receptor-type tyrosine-protein kinase FLT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			2440	1517	445	467	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	422	Total	C	N	O	S	0	0	0
			2400	1494	446	449	11			
2	F	420	Total	C	N	O	S	0	0	0
			2430	1520	445	453	12			
2	H	423	Total	C	N	O	S	0	0	0
			2389	1474	449	454	12			
2	J	417	Total	C	N	O	S	0	0	0
			2372	1473	441	446	12			
2	L	430	Total	C	N	O	S	0	0	0
			2453	1527	451	464	11			
2	N	428	Total	C	N	O	S	0	0	0
			2418	1504	448	456	10			
2	P	427	Total	C	N	O	S	0	0	0
			2417	1500	445	459	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	227	MET	THR	conflict	UNP P36888
B	542	GLY	-	expression tag	UNP P36888
B	543	SER	-	expression tag	UNP P36888
B	544	SER	-	expression tag	UNP P36888
B	545	GLY	-	expression tag	UNP P36888
B	546	LEU	-	expression tag	UNP P36888
B	547	VAL	-	expression tag	UNP P36888
B	548	PRO	-	expression tag	UNP P36888
B	549	ARG	-	expression tag	UNP P36888
B	550	GLY	-	expression tag	UNP P36888
B	551	SER	-	expression tag	UNP P36888
B	552	GLY	-	expression tag	UNP P36888
B	553	GLY	-	expression tag	UNP P36888
B	554	SER	-	expression tag	UNP P36888
B	555	GLY	-	expression tag	UNP P36888
B	556	GLY	-	expression tag	UNP P36888
B	557	SER	-	expression tag	UNP P36888
B	558	GLY	-	expression tag	UNP P36888
B	559	LEU	-	expression tag	UNP P36888
B	560	ASN	-	expression tag	UNP P36888
B	561	ASP	-	expression tag	UNP P36888
B	562	ILE	-	expression tag	UNP P36888
B	563	PHE	-	expression tag	UNP P36888
B	564	GLU	-	expression tag	UNP P36888
B	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	GLN	-	expression tag	UNP P36888
B	567	LYS	-	expression tag	UNP P36888
B	568	ILE	-	expression tag	UNP P36888
B	569	GLU	-	expression tag	UNP P36888
B	570	TRP	-	expression tag	UNP P36888
B	571	HIS	-	expression tag	UNP P36888
B	572	GLU	-	expression tag	UNP P36888
B	573	GLY	-	expression tag	UNP P36888
B	574	ARG	-	expression tag	UNP P36888
B	575	THR	-	expression tag	UNP P36888
B	576	LYS	-	expression tag	UNP P36888
B	577	HIS	-	expression tag	UNP P36888
B	578	HIS	-	expression tag	UNP P36888
B	579	HIS	-	expression tag	UNP P36888
B	580	HIS	-	expression tag	UNP P36888
B	581	HIS	-	expression tag	UNP P36888
B	582	HIS	-	expression tag	UNP P36888
D	227	MET	THR	conflict	UNP P36888
D	542	GLY	-	expression tag	UNP P36888
D	543	SER	-	expression tag	UNP P36888
D	544	SER	-	expression tag	UNP P36888
D	545	GLY	-	expression tag	UNP P36888
D	546	LEU	-	expression tag	UNP P36888
D	547	VAL	-	expression tag	UNP P36888
D	548	PRO	-	expression tag	UNP P36888
D	549	ARG	-	expression tag	UNP P36888
D	550	GLY	-	expression tag	UNP P36888
D	551	SER	-	expression tag	UNP P36888
D	552	GLY	-	expression tag	UNP P36888
D	553	GLY	-	expression tag	UNP P36888
D	554	SER	-	expression tag	UNP P36888
D	555	GLY	-	expression tag	UNP P36888
D	556	GLY	-	expression tag	UNP P36888
D	557	SER	-	expression tag	UNP P36888
D	558	GLY	-	expression tag	UNP P36888
D	559	LEU	-	expression tag	UNP P36888
D	560	ASN	-	expression tag	UNP P36888
D	561	ASP	-	expression tag	UNP P36888
D	562	ILE	-	expression tag	UNP P36888
D	563	PHE	-	expression tag	UNP P36888
D	564	GLU	-	expression tag	UNP P36888
D	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
D	566	GLN	-	expression tag	UNP P36888
D	567	LYS	-	expression tag	UNP P36888
D	568	ILE	-	expression tag	UNP P36888
D	569	GLU	-	expression tag	UNP P36888
D	570	TRP	-	expression tag	UNP P36888
D	571	HIS	-	expression tag	UNP P36888
D	572	GLU	-	expression tag	UNP P36888
D	573	GLY	-	expression tag	UNP P36888
D	574	ARG	-	expression tag	UNP P36888
D	575	THR	-	expression tag	UNP P36888
D	576	LYS	-	expression tag	UNP P36888
D	577	HIS	-	expression tag	UNP P36888
D	578	HIS	-	expression tag	UNP P36888
D	579	HIS	-	expression tag	UNP P36888
D	580	HIS	-	expression tag	UNP P36888
D	581	HIS	-	expression tag	UNP P36888
D	582	HIS	-	expression tag	UNP P36888
F	227	MET	THR	conflict	UNP P36888
F	542	GLY	-	expression tag	UNP P36888
F	543	SER	-	expression tag	UNP P36888
F	544	SER	-	expression tag	UNP P36888
F	545	GLY	-	expression tag	UNP P36888
F	546	LEU	-	expression tag	UNP P36888
F	547	VAL	-	expression tag	UNP P36888
F	548	PRO	-	expression tag	UNP P36888
F	549	ARG	-	expression tag	UNP P36888
F	550	GLY	-	expression tag	UNP P36888
F	551	SER	-	expression tag	UNP P36888
F	552	GLY	-	expression tag	UNP P36888
F	553	GLY	-	expression tag	UNP P36888
F	554	SER	-	expression tag	UNP P36888
F	555	GLY	-	expression tag	UNP P36888
F	556	GLY	-	expression tag	UNP P36888
F	557	SER	-	expression tag	UNP P36888
F	558	GLY	-	expression tag	UNP P36888
F	559	LEU	-	expression tag	UNP P36888
F	560	ASN	-	expression tag	UNP P36888
F	561	ASP	-	expression tag	UNP P36888
F	562	ILE	-	expression tag	UNP P36888
F	563	PHE	-	expression tag	UNP P36888
F	564	GLU	-	expression tag	UNP P36888
F	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
F	566	GLN	-	expression tag	UNP P36888
F	567	LYS	-	expression tag	UNP P36888
F	568	ILE	-	expression tag	UNP P36888
F	569	GLU	-	expression tag	UNP P36888
F	570	TRP	-	expression tag	UNP P36888
F	571	HIS	-	expression tag	UNP P36888
F	572	GLU	-	expression tag	UNP P36888
F	573	GLY	-	expression tag	UNP P36888
F	574	ARG	-	expression tag	UNP P36888
F	575	THR	-	expression tag	UNP P36888
F	576	LYS	-	expression tag	UNP P36888
F	577	HIS	-	expression tag	UNP P36888
F	578	HIS	-	expression tag	UNP P36888
F	579	HIS	-	expression tag	UNP P36888
F	580	HIS	-	expression tag	UNP P36888
F	581	HIS	-	expression tag	UNP P36888
F	582	HIS	-	expression tag	UNP P36888
H	227	MET	THR	conflict	UNP P36888
H	542	GLY	-	expression tag	UNP P36888
H	543	SER	-	expression tag	UNP P36888
H	544	SER	-	expression tag	UNP P36888
H	545	GLY	-	expression tag	UNP P36888
H	546	LEU	-	expression tag	UNP P36888
H	547	VAL	-	expression tag	UNP P36888
H	548	PRO	-	expression tag	UNP P36888
H	549	ARG	-	expression tag	UNP P36888
H	550	GLY	-	expression tag	UNP P36888
H	551	SER	-	expression tag	UNP P36888
H	552	GLY	-	expression tag	UNP P36888
H	553	GLY	-	expression tag	UNP P36888
H	554	SER	-	expression tag	UNP P36888
H	555	GLY	-	expression tag	UNP P36888
H	556	GLY	-	expression tag	UNP P36888
H	557	SER	-	expression tag	UNP P36888
H	558	GLY	-	expression tag	UNP P36888
H	559	LEU	-	expression tag	UNP P36888
H	560	ASN	-	expression tag	UNP P36888
H	561	ASP	-	expression tag	UNP P36888
H	562	ILE	-	expression tag	UNP P36888
H	563	PHE	-	expression tag	UNP P36888
H	564	GLU	-	expression tag	UNP P36888
H	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
H	566	GLN	-	expression tag	UNP P36888
H	567	LYS	-	expression tag	UNP P36888
H	568	ILE	-	expression tag	UNP P36888
H	569	GLU	-	expression tag	UNP P36888
H	570	TRP	-	expression tag	UNP P36888
H	571	HIS	-	expression tag	UNP P36888
H	572	GLU	-	expression tag	UNP P36888
H	573	GLY	-	expression tag	UNP P36888
H	574	ARG	-	expression tag	UNP P36888
H	575	THR	-	expression tag	UNP P36888
H	576	LYS	-	expression tag	UNP P36888
H	577	HIS	-	expression tag	UNP P36888
H	578	HIS	-	expression tag	UNP P36888
H	579	HIS	-	expression tag	UNP P36888
H	580	HIS	-	expression tag	UNP P36888
H	581	HIS	-	expression tag	UNP P36888
H	582	HIS	-	expression tag	UNP P36888
J	227	MET	THR	conflict	UNP P36888
J	542	GLY	-	expression tag	UNP P36888
J	543	SER	-	expression tag	UNP P36888
J	544	SER	-	expression tag	UNP P36888
J	545	GLY	-	expression tag	UNP P36888
J	546	LEU	-	expression tag	UNP P36888
J	547	VAL	-	expression tag	UNP P36888
J	548	PRO	-	expression tag	UNP P36888
J	549	ARG	-	expression tag	UNP P36888
J	550	GLY	-	expression tag	UNP P36888
J	551	SER	-	expression tag	UNP P36888
J	552	GLY	-	expression tag	UNP P36888
J	553	GLY	-	expression tag	UNP P36888
J	554	SER	-	expression tag	UNP P36888
J	555	GLY	-	expression tag	UNP P36888
J	556	GLY	-	expression tag	UNP P36888
J	557	SER	-	expression tag	UNP P36888
J	558	GLY	-	expression tag	UNP P36888
J	559	LEU	-	expression tag	UNP P36888
J	560	ASN	-	expression tag	UNP P36888
J	561	ASP	-	expression tag	UNP P36888
J	562	ILE	-	expression tag	UNP P36888
J	563	PHE	-	expression tag	UNP P36888
J	564	GLU	-	expression tag	UNP P36888
J	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
J	566	GLN	-	expression tag	UNP P36888
J	567	LYS	-	expression tag	UNP P36888
J	568	ILE	-	expression tag	UNP P36888
J	569	GLU	-	expression tag	UNP P36888
J	570	TRP	-	expression tag	UNP P36888
J	571	HIS	-	expression tag	UNP P36888
J	572	GLU	-	expression tag	UNP P36888
J	573	GLY	-	expression tag	UNP P36888
J	574	ARG	-	expression tag	UNP P36888
J	575	THR	-	expression tag	UNP P36888
J	576	LYS	-	expression tag	UNP P36888
J	577	HIS	-	expression tag	UNP P36888
J	578	HIS	-	expression tag	UNP P36888
J	579	HIS	-	expression tag	UNP P36888
J	580	HIS	-	expression tag	UNP P36888
J	581	HIS	-	expression tag	UNP P36888
J	582	HIS	-	expression tag	UNP P36888
L	227	MET	THR	conflict	UNP P36888
L	542	GLY	-	expression tag	UNP P36888
L	543	SER	-	expression tag	UNP P36888
L	544	SER	-	expression tag	UNP P36888
L	545	GLY	-	expression tag	UNP P36888
L	546	LEU	-	expression tag	UNP P36888
L	547	VAL	-	expression tag	UNP P36888
L	548	PRO	-	expression tag	UNP P36888
L	549	ARG	-	expression tag	UNP P36888
L	550	GLY	-	expression tag	UNP P36888
L	551	SER	-	expression tag	UNP P36888
L	552	GLY	-	expression tag	UNP P36888
L	553	GLY	-	expression tag	UNP P36888
L	554	SER	-	expression tag	UNP P36888
L	555	GLY	-	expression tag	UNP P36888
L	556	GLY	-	expression tag	UNP P36888
L	557	SER	-	expression tag	UNP P36888
L	558	GLY	-	expression tag	UNP P36888
L	559	LEU	-	expression tag	UNP P36888
L	560	ASN	-	expression tag	UNP P36888
L	561	ASP	-	expression tag	UNP P36888
L	562	ILE	-	expression tag	UNP P36888
L	563	PHE	-	expression tag	UNP P36888
L	564	GLU	-	expression tag	UNP P36888
L	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
L	566	GLN	-	expression tag	UNP P36888
L	567	LYS	-	expression tag	UNP P36888
L	568	ILE	-	expression tag	UNP P36888
L	569	GLU	-	expression tag	UNP P36888
L	570	TRP	-	expression tag	UNP P36888
L	571	HIS	-	expression tag	UNP P36888
L	572	GLU	-	expression tag	UNP P36888
L	573	GLY	-	expression tag	UNP P36888
L	574	ARG	-	expression tag	UNP P36888
L	575	THR	-	expression tag	UNP P36888
L	576	LYS	-	expression tag	UNP P36888
L	577	HIS	-	expression tag	UNP P36888
L	578	HIS	-	expression tag	UNP P36888
L	579	HIS	-	expression tag	UNP P36888
L	580	HIS	-	expression tag	UNP P36888
L	581	HIS	-	expression tag	UNP P36888
L	582	HIS	-	expression tag	UNP P36888
N	227	MET	THR	conflict	UNP P36888
N	542	GLY	-	expression tag	UNP P36888
N	543	SER	-	expression tag	UNP P36888
N	544	SER	-	expression tag	UNP P36888
N	545	GLY	-	expression tag	UNP P36888
N	546	LEU	-	expression tag	UNP P36888
N	547	VAL	-	expression tag	UNP P36888
N	548	PRO	-	expression tag	UNP P36888
N	549	ARG	-	expression tag	UNP P36888
N	550	GLY	-	expression tag	UNP P36888
N	551	SER	-	expression tag	UNP P36888
N	552	GLY	-	expression tag	UNP P36888
N	553	GLY	-	expression tag	UNP P36888
N	554	SER	-	expression tag	UNP P36888
N	555	GLY	-	expression tag	UNP P36888
N	556	GLY	-	expression tag	UNP P36888
N	557	SER	-	expression tag	UNP P36888
N	558	GLY	-	expression tag	UNP P36888
N	559	LEU	-	expression tag	UNP P36888
N	560	ASN	-	expression tag	UNP P36888
N	561	ASP	-	expression tag	UNP P36888
N	562	ILE	-	expression tag	UNP P36888
N	563	PHE	-	expression tag	UNP P36888
N	564	GLU	-	expression tag	UNP P36888
N	565	ALA	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
N	566	GLN	-	expression tag	UNP P36888
N	567	LYS	-	expression tag	UNP P36888
N	568	ILE	-	expression tag	UNP P36888
N	569	GLU	-	expression tag	UNP P36888
N	570	TRP	-	expression tag	UNP P36888
N	571	HIS	-	expression tag	UNP P36888
N	572	GLU	-	expression tag	UNP P36888
N	573	GLY	-	expression tag	UNP P36888
N	574	ARG	-	expression tag	UNP P36888
N	575	THR	-	expression tag	UNP P36888
N	576	LYS	-	expression tag	UNP P36888
N	577	HIS	-	expression tag	UNP P36888
N	578	HIS	-	expression tag	UNP P36888
N	579	HIS	-	expression tag	UNP P36888
N	580	HIS	-	expression tag	UNP P36888
N	581	HIS	-	expression tag	UNP P36888
N	582	HIS	-	expression tag	UNP P36888
P	227	MET	THR	conflict	UNP P36888
P	542	GLY	-	expression tag	UNP P36888
P	543	SER	-	expression tag	UNP P36888
P	544	SER	-	expression tag	UNP P36888
P	545	GLY	-	expression tag	UNP P36888
P	546	LEU	-	expression tag	UNP P36888
P	547	VAL	-	expression tag	UNP P36888
P	548	PRO	-	expression tag	UNP P36888
P	549	ARG	-	expression tag	UNP P36888
P	550	GLY	-	expression tag	UNP P36888
P	551	SER	-	expression tag	UNP P36888
P	552	GLY	-	expression tag	UNP P36888
P	553	GLY	-	expression tag	UNP P36888
P	554	SER	-	expression tag	UNP P36888
P	555	GLY	-	expression tag	UNP P36888
P	556	GLY	-	expression tag	UNP P36888
P	557	SER	-	expression tag	UNP P36888
P	558	GLY	-	expression tag	UNP P36888
P	559	LEU	-	expression tag	UNP P36888
P	560	ASN	-	expression tag	UNP P36888
P	561	ASP	-	expression tag	UNP P36888
P	562	ILE	-	expression tag	UNP P36888
P	563	PHE	-	expression tag	UNP P36888
P	564	GLU	-	expression tag	UNP P36888
P	565	ALA	-	expression tag	UNP P36888

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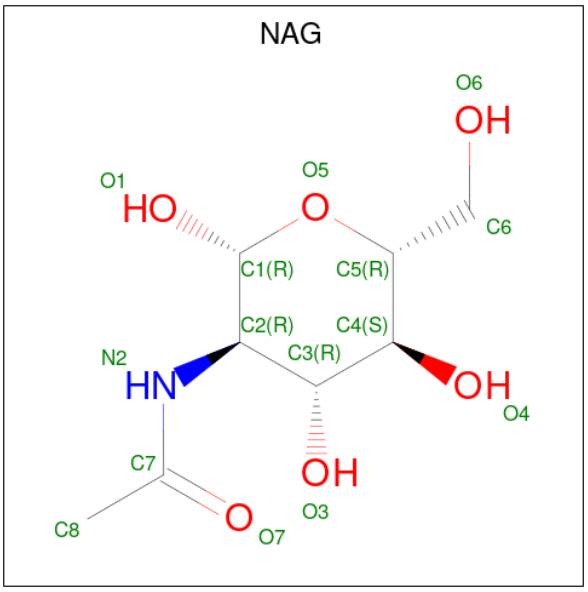
Chain	Residue	Modelled	Actual	Comment	Reference
P	566	GLN	-	expression tag	UNP P36888
P	567	LYS	-	expression tag	UNP P36888
P	568	ILE	-	expression tag	UNP P36888
P	569	GLU	-	expression tag	UNP P36888
P	570	TRP	-	expression tag	UNP P36888
P	571	HIS	-	expression tag	UNP P36888
P	572	GLU	-	expression tag	UNP P36888
P	573	GLY	-	expression tag	UNP P36888
P	574	ARG	-	expression tag	UNP P36888
P	575	THR	-	expression tag	UNP P36888
P	576	LYS	-	expression tag	UNP P36888
P	577	HIS	-	expression tag	UNP P36888
P	578	HIS	-	expression tag	UNP P36888
P	579	HIS	-	expression tag	UNP P36888
P	580	HIS	-	expression tag	UNP P36888
P	581	HIS	-	expression tag	UNP P36888
P	582	HIS	-	expression tag	UNP P36888

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	28	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



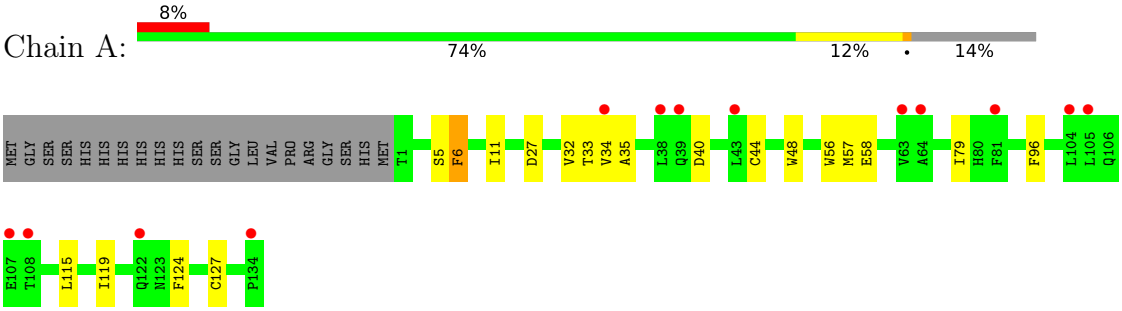
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	14	0
4	B	1	Total C N O 14 8 1 5	14	0
4	H	1	Total C N O 14 8 1 5	14	0
4	P	1	Total C N O 14 8 1 5	14	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

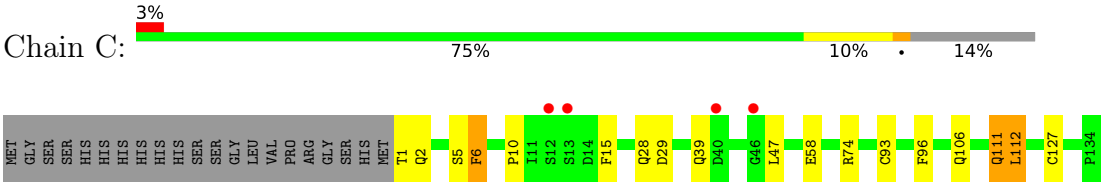
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain A:



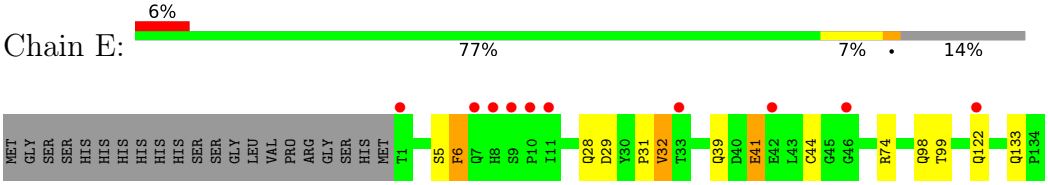
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain C:



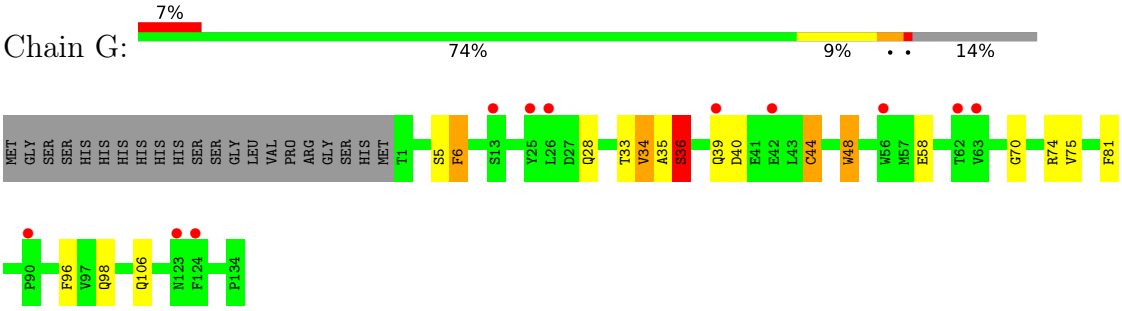
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain E:

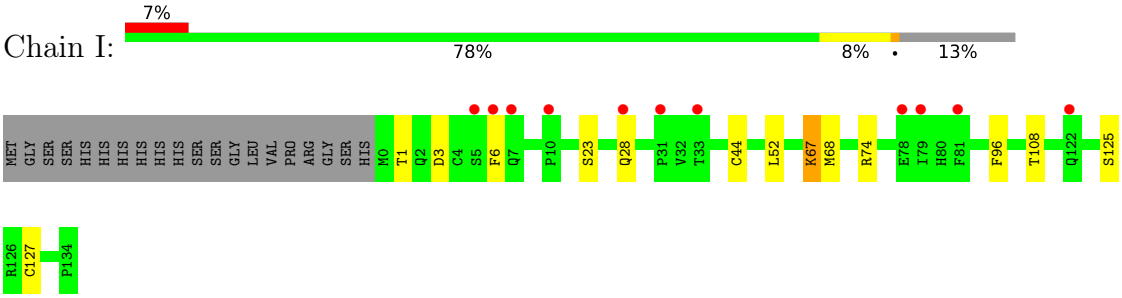


• Molecule 1: Fms-related tyrosine kinase 3 ligand

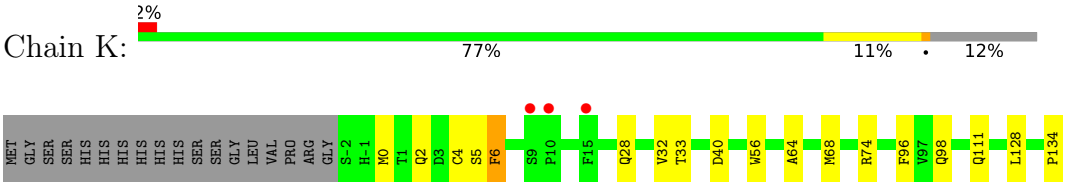
Chain G:



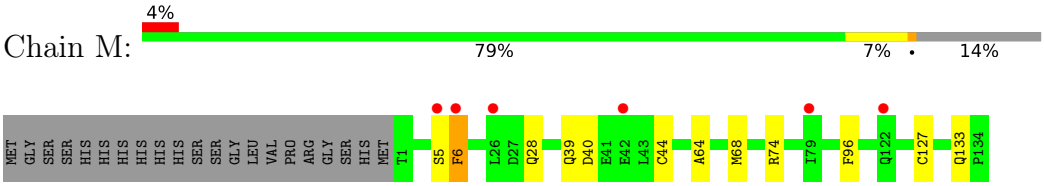
• Molecule 1: Fms-related tyrosine kinase 3 ligand



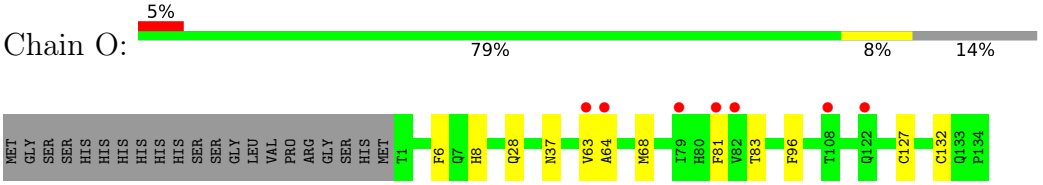
• Molecule 1: Fms-related tyrosine kinase 3 ligand



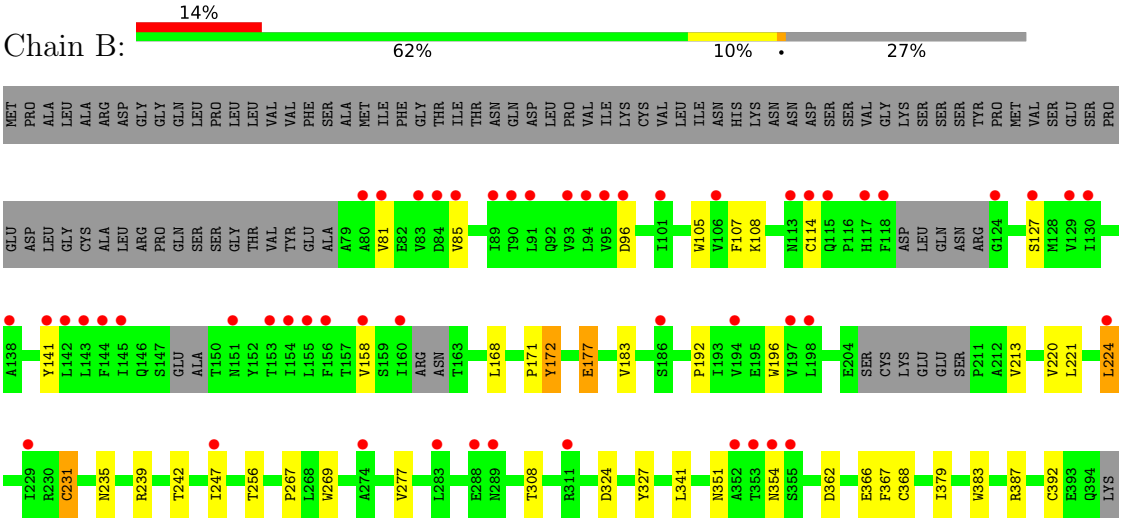
• Molecule 1: Fms-related tyrosine kinase 3 ligand

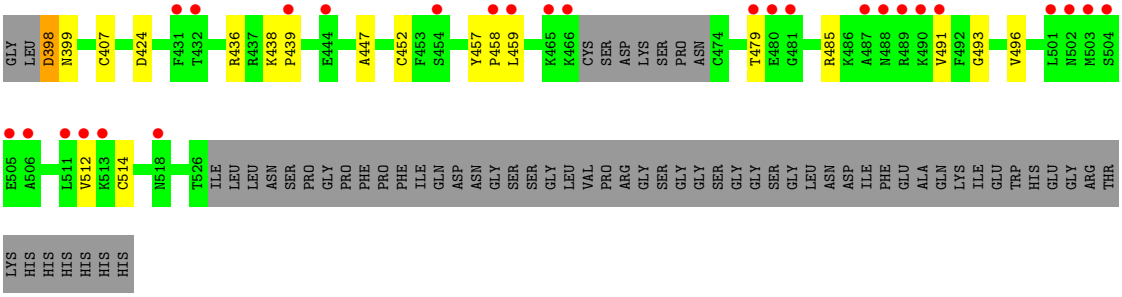


• Molecule 1: Fms-related tyrosine kinase 3 ligand



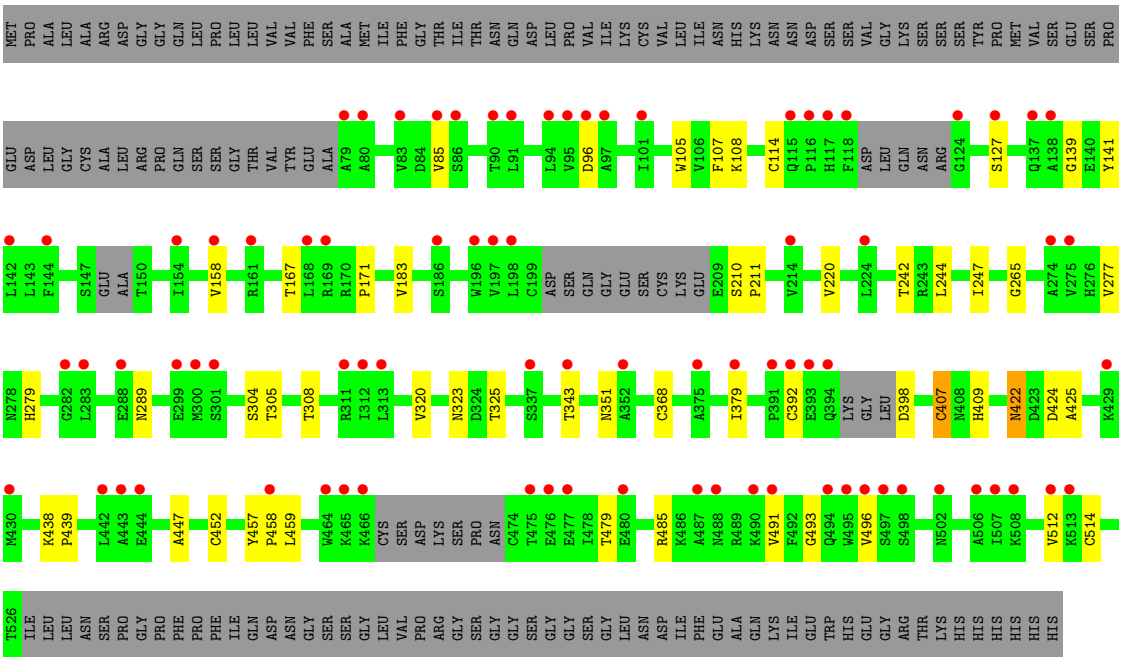
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3





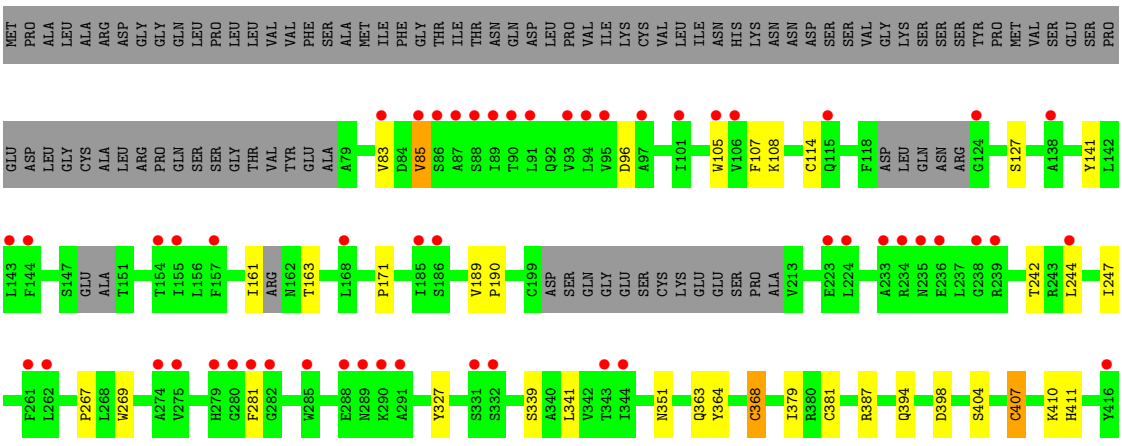
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

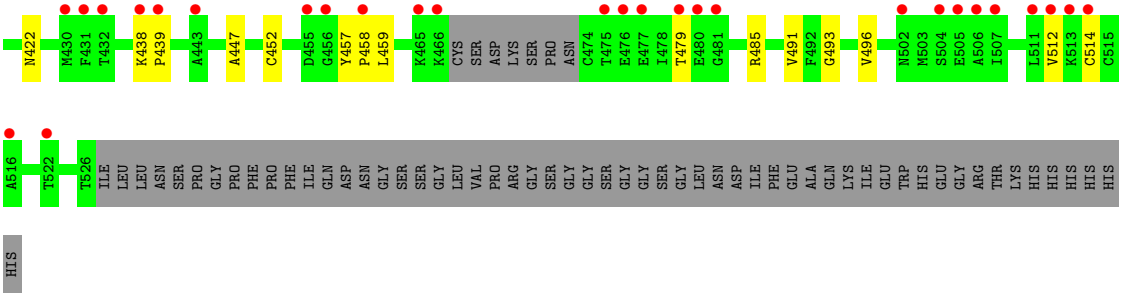
Chain D:



• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

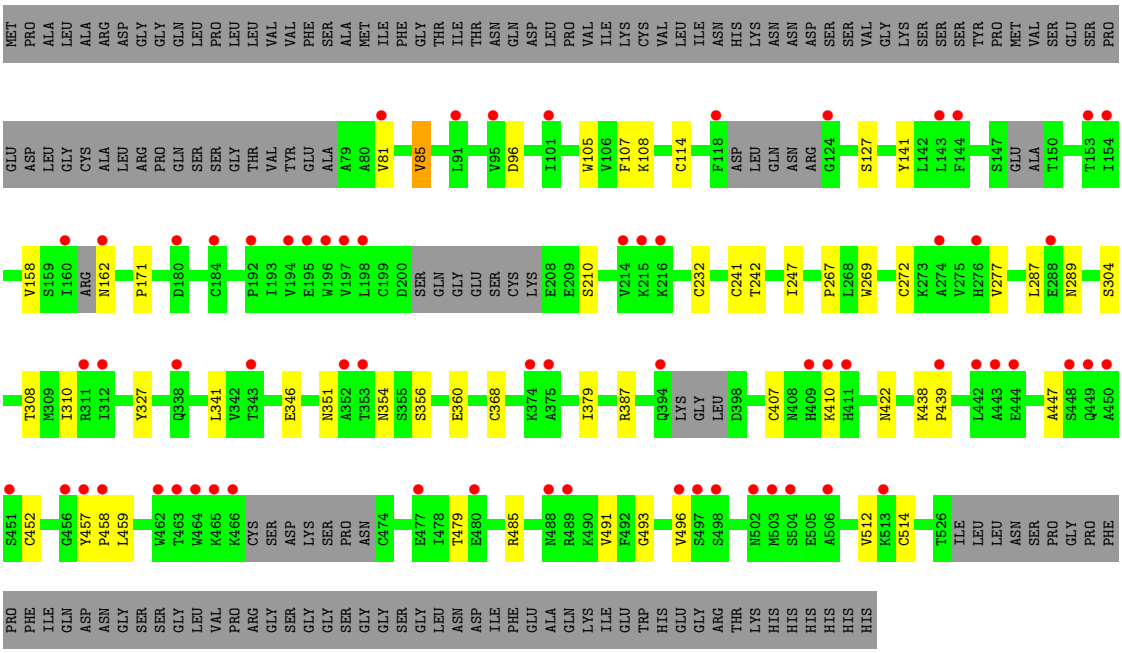
Chain F:





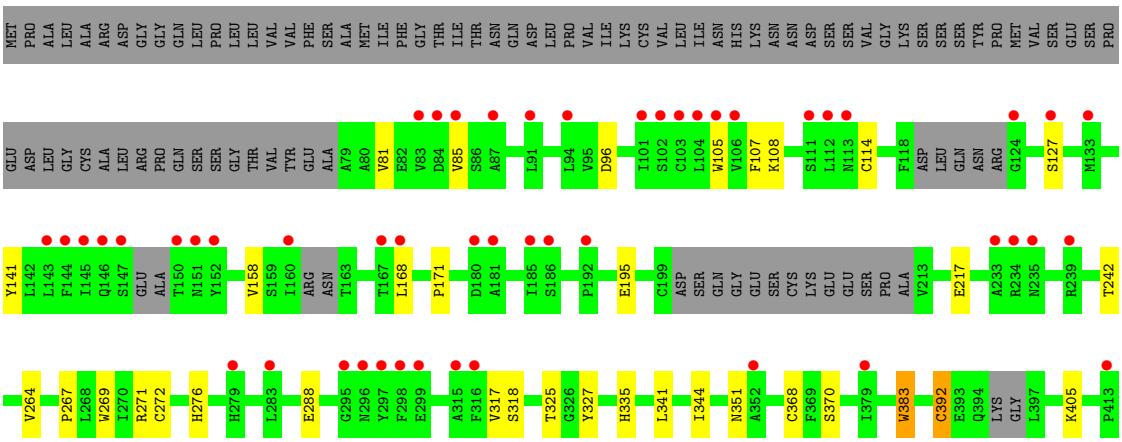
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

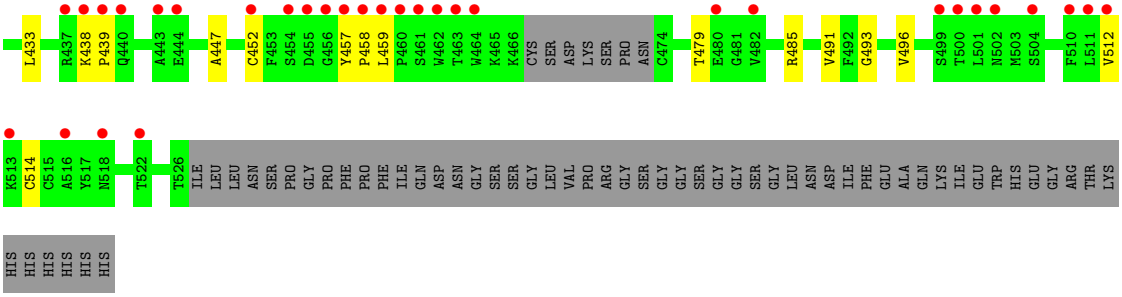
Chain H:



• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

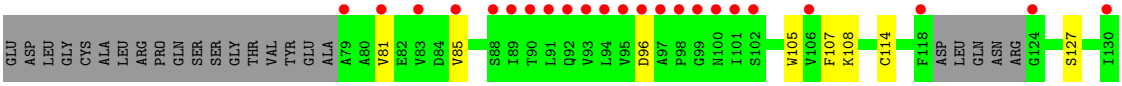
Chain J:

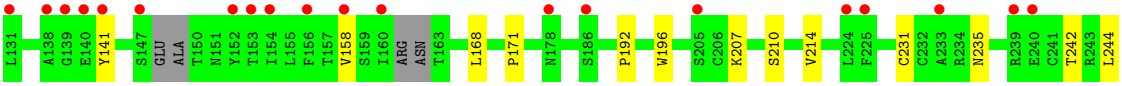


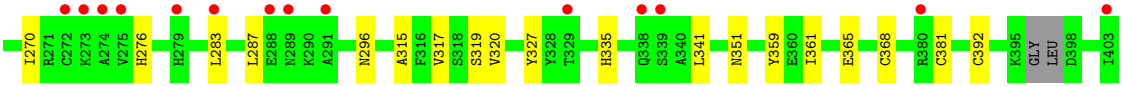


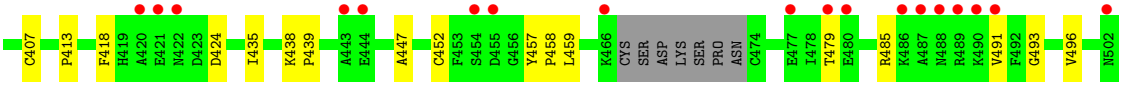
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

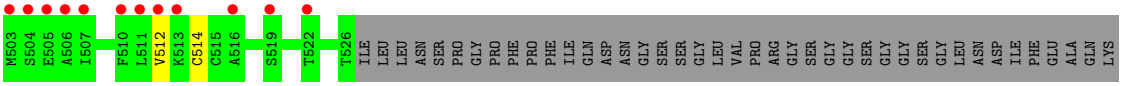
Chain L:

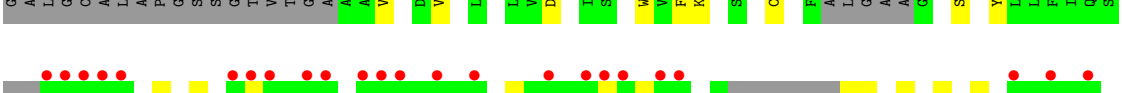


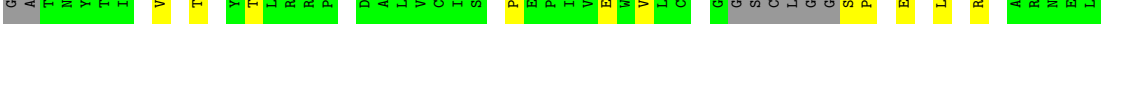






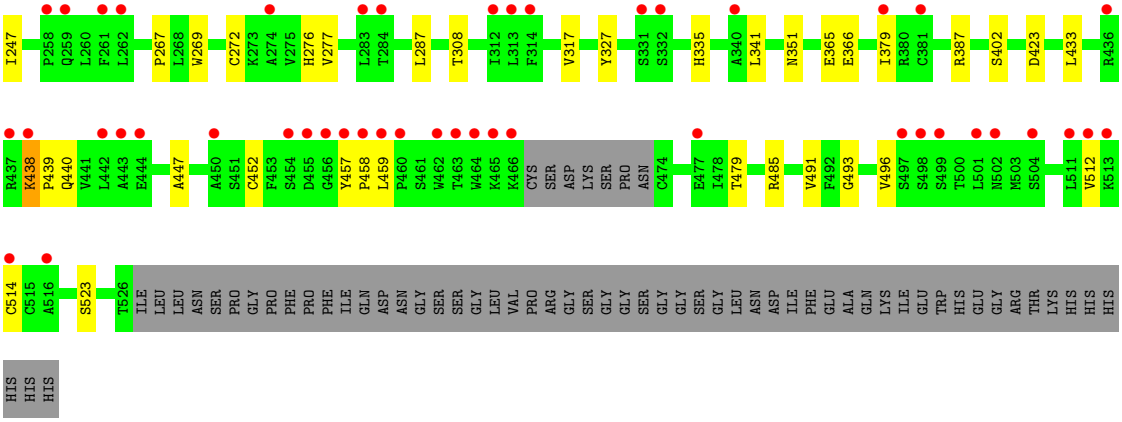






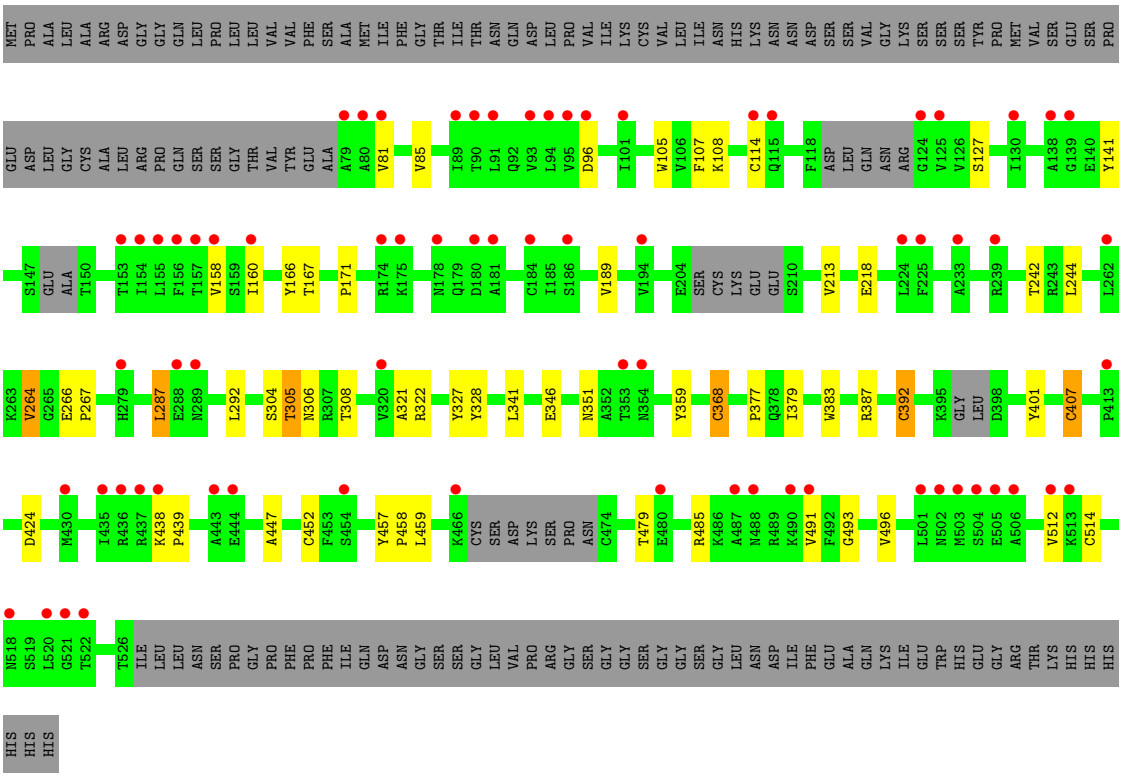
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

Chain N:



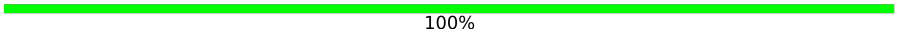
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

Chain P:



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

Chain Q:

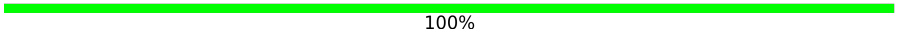


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain S:

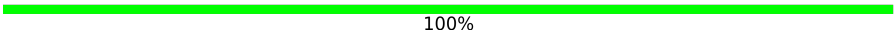


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

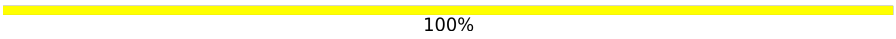
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	139.21Å 139.22Å 143.69Å 90.02° 90.03° 89.99°	Depositor
Resolution (Å)	47.90 – 4.51 47.90 – 4.51	Depositor EDS
% Data completeness (in resolution range)	66.2 (47.90-4.51) 66.0 (47.90-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 4.45Å)	Xtriage
Refinement program	BUSTER 2.10.3, PHENIX 1.20-4459, PDB-REDO	Depositor
R, R_{free}	0.278 , 0.291 0.299 , 0.285	Depositor DCC
R_{free} test set	2027 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	214.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 462.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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Property	Value	Source
Estimated twinning fraction	0.027 for h,-l,k 0.027 for h,l,-k 0.027 for l,k,-h 0.027 for -l,k,h 0.387 for k,-h,l 0.387 for -k,h,l 0.029 for k,-l,-h 0.029 for -l,h,-k 0.026 for -l,-h,k 0.026 for -k,l,-h 0.025 for l,-h,-k 0.025 for -k,-l,h 0.028 for k,l,h 0.028 for l,h,k 0.390 for h,-k,-l 0.390 for -h,k,-l 0.387 for -h,-k,l 0.389 for k,h,-l 0.389 for -k,-h,-l 0.035 for -l,-k,-h 0.037 for l,-k,h 0.030 for -h,-l,-k 0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	26691	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/933	0.45	0/1277
1	C	0.27	0/896	0.50	0/1235
1	E	0.24	0/858	0.48	0/1183
1	G	0.26	0/903	0.50	0/1247
1	I	0.55	1/926 (0.1%)	0.77	3/1273 (0.2%)
1	K	0.26	0/911	0.47	0/1256
1	M	0.23	0/930	0.47	0/1281
1	O	0.24	0/941	0.46	0/1294
2	B	0.26	0/2470	0.48	2/3425 (0.1%)
2	D	0.25	0/2429	0.46	0/3369
2	F	0.25	0/2464	0.46	0/3408
2	H	0.26	0/2415	0.44	0/3347
2	J	0.25	0/2401	0.44	0/3331
2	L	0.26	0/2483	0.45	0/3447
2	N	0.26	0/2449	0.46	0/3398
2	P	0.26	0/2444	0.46	0/3391
All	All	0.27	1/26853 (0.0%)	0.47	5/37162 (0.0%)

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
2	B	0	3
2	D	0	4
2	F	0	4
2	H	0	3
2	J	0	3
2	L	0	4
2	N	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	23[A]	SER	C-N	-15.00	0.99	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	23[A]	SER	C-N-CA	-13.96	86.79	121.70
1	I	23[A]	SER	O-C-N	12.12	142.09	122.70
1	I	23[A]	SER	CA-C-N	-10.11	94.97	117.20
2	B	172	TYR	CA-CB-CG	5.43	123.73	113.40
2	B	398	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	438	LYS	Peptide
2	B	457	TYR	Peptide
2	B	459	LEU	Peptide
2	D	210	SER	Peptide
2	D	438	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	915	0	715	11	0
1	C	879	0	656	4	0
1	E	844	0	578	5	0
1	G	884	0	661	5	0
1	I	907	0	697	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	892	0	649	10	0
1	M	908	0	684	3	0
1	O	919	0	723	3	0
2	B	2440	0	1569	18	0
2	D	2400	0	1501	15	0
2	F	2430	0	1573	15	0
2	H	2389	0	1489	12	0
2	J	2372	0	1484	14	0
2	L	2453	0	1562	18	0
2	N	2418	0	1505	12	0
2	P	2417	0	1534	16	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
4	B	28	0	26	0	0
4	H	14	0	13	0	0
4	P	14	0	13	0	0
All	All	26691	0	17782	160	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.

The worst 5 of 160 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:K:32:VAL:HG13	1:K:56:TRP:CD2	2.06	0.90
1:A:32:VAL:HG13	1:A:56:TRP:CD2	2.09	0.87
1:A:33:THR:N	1:A:34:VAL:N	2.26	0.84
2:B:398:ASP:OD1	2:B:399:ASN:N	2.12	0.81
2:B:399:ASN:O	2:B:399:ASN:OD1	1.98	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/155 (83%)	126 (98%)	1 (1%)	2 (2%)	9	45
1	C	132/155 (85%)	126 (96%)	4 (3%)	2 (2%)	10	46
1	E	132/155 (85%)	126 (96%)	3 (2%)	3 (2%)	6	37
1	G	132/155 (85%)	124 (94%)	4 (3%)	4 (3%)	4	31
1	I	133/155 (86%)	124 (93%)	7 (5%)	2 (2%)	10	46
1	K	135/155 (87%)	128 (95%)	5 (4%)	2 (2%)	10	46
1	M	132/155 (85%)	126 (96%)	4 (3%)	2 (2%)	10	46
1	O	132/155 (85%)	129 (98%)	3 (2%)	0	100	100
2	B	409/582 (70%)	351 (86%)	39 (10%)	19 (5%)	2	24
2	D	410/582 (70%)	345 (84%)	47 (12%)	18 (4%)	2	25
2	F	410/582 (70%)	339 (83%)	54 (13%)	17 (4%)	3	25
2	H	409/582 (70%)	347 (85%)	43 (10%)	19 (5%)	2	24
2	J	403/582 (69%)	336 (83%)	52 (13%)	15 (4%)	3	28
2	L	418/582 (72%)	352 (84%)	46 (11%)	20 (5%)	2	23
2	N	418/582 (72%)	350 (84%)	45 (11%)	23 (6%)	2	21
2	P	415/582 (71%)	348 (84%)	43 (10%)	24 (6%)	1	20
All	All	4349/5896 (74%)	3777 (87%)	400 (9%)	172 (4%)	3	26

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
2	B	85	VAL
2	B	367	PHE
2	B	439	PRO
2	B	458	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/142 (54%)	74 (96%)	3 (4%)	32 57
1	C	69/142 (49%)	56 (81%)	13 (19%)	1 10
1	E	57/142 (40%)	52 (91%)	5 (9%)	10 33
1	G	70/142 (49%)	58 (83%)	12 (17%)	2 13
1	I	76/142 (54%)	68 (90%)	8 (10%)	7 26
1	K	67/142 (47%)	59 (88%)	8 (12%)	5 23
1	M	75/142 (53%)	70 (93%)	5 (7%)	16 43
1	O	79/142 (56%)	72 (91%)	7 (9%)	9 33
2	B	109/515 (21%)	97 (89%)	12 (11%)	6 25
2	D	94/515 (18%)	85 (90%)	9 (10%)	8 29
2	F	107/515 (21%)	99 (92%)	8 (8%)	13 40
2	H	95/515 (18%)	85 (90%)	10 (10%)	7 26
2	J	96/515 (19%)	87 (91%)	9 (9%)	8 30
2	L	103/515 (20%)	96 (93%)	7 (7%)	16 42
2	N	95/515 (18%)	88 (93%)	7 (7%)	13 40
2	P	101/515 (20%)	90 (89%)	11 (11%)	6 25
All	All	1370/5256 (26%)	1236 (90%)	134 (10%)	8 28

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	433	LEU
1	O	81	PHE
2	P	368	CYS
2	F	398	ASP
2	F	381	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	335	HIS
2	L	335	HIS
2	F	351	ASN
1	E	98	GLN
2	J	335	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	Q	1	2,3	14,14,15	0.33	0	17,19,21	0.67	0
3	NAG	Q	2	3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	R	1	2,3	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
3	NAG	R	2	3	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	S	1	2,3	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	T	1	2,3	14,14,15	0.33	0	17,19,21	0.64	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.57	1 (5%)
3	NAG	U	1	2,3	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	U	2	3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	V	1	2,3	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
3	NAG	V	2	3	14,14,15	0.28	0	17,19,21	0.57	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	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(^{o})	Ideal(^{o})
3	V	1	NAG	O5-C1-C2	-2.71	107.01	111.29
3	R	1	NAG	O5-C1-C2	-2.07	108.02	111.29
3	V	2	NAG	C1-O5-C5	2.02	114.93	112.19
3	T	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

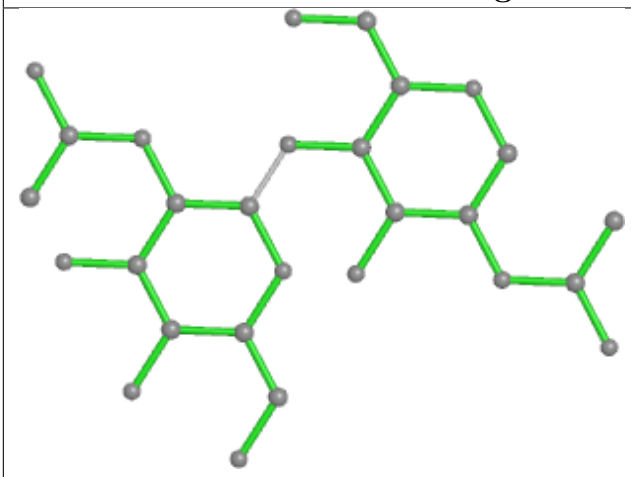
There are no torsion outliers.

There are no ring outliers.

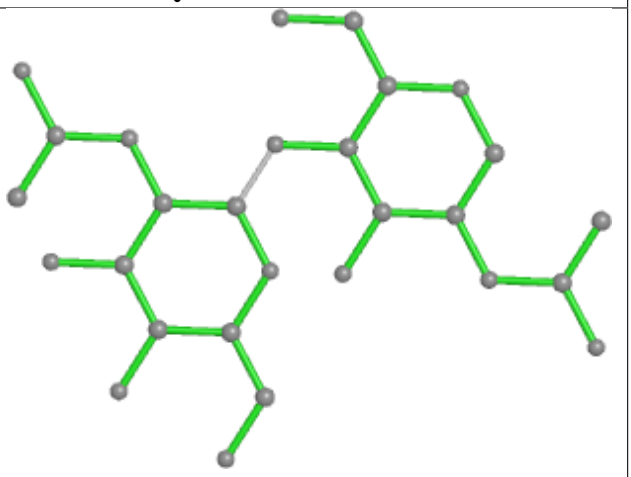
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

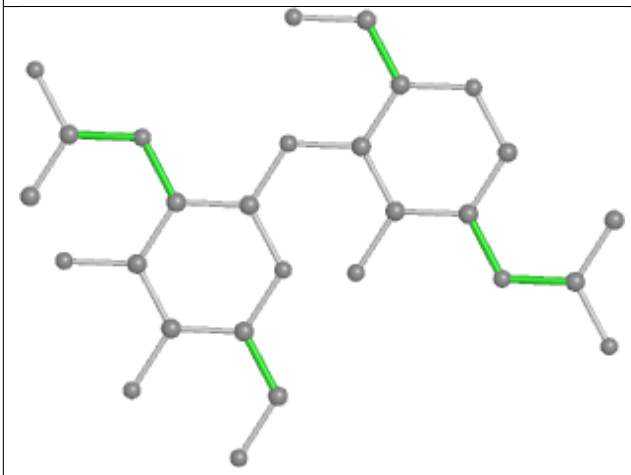
Oligosaccharide Chain Q



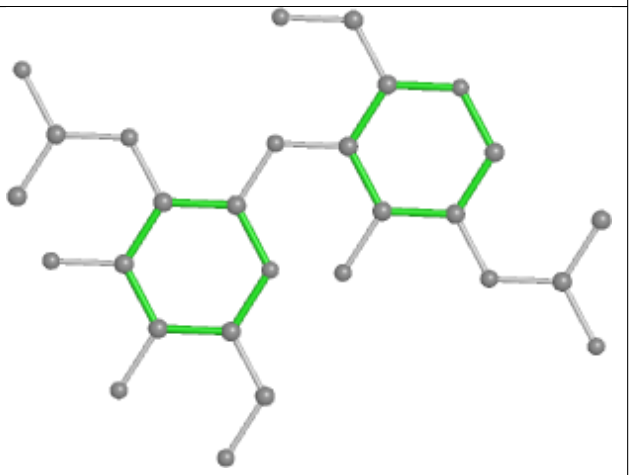
Bond lengths



Bond angles

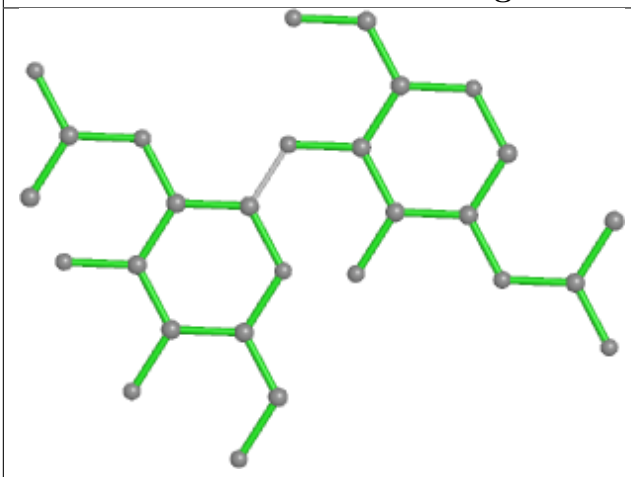


Torsions

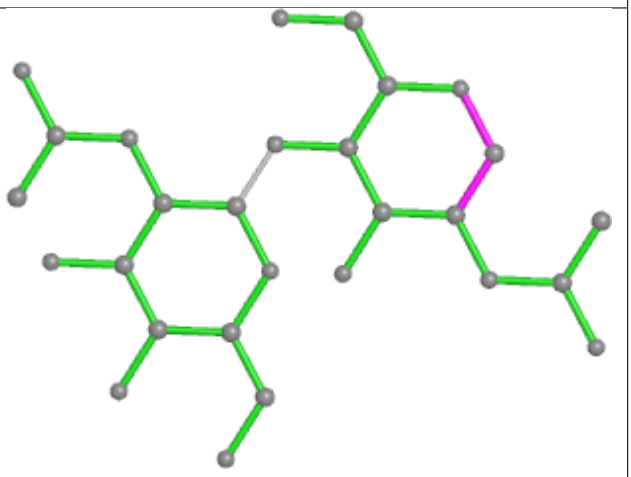


Rings

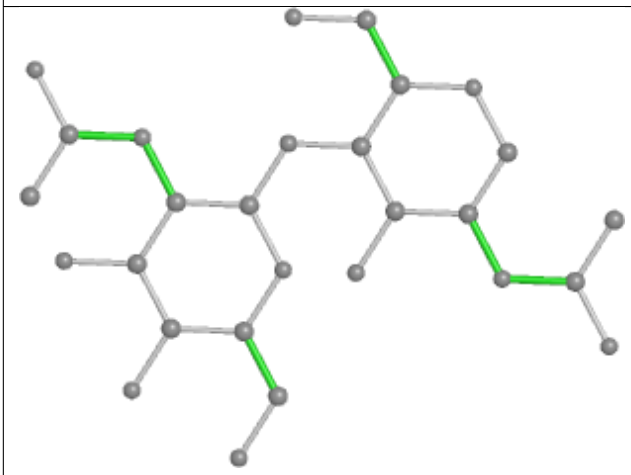
Oligosaccharide Chain R



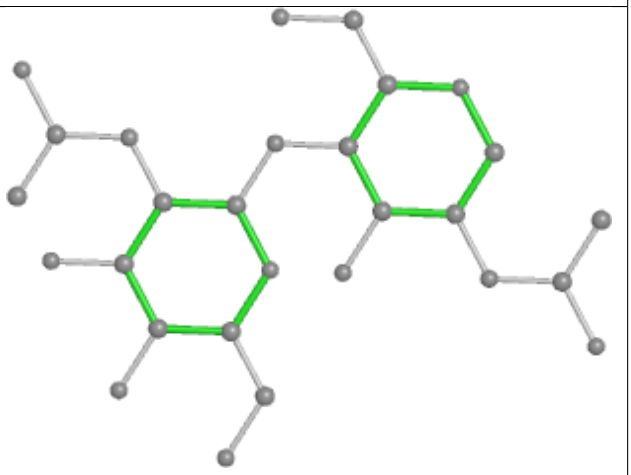
Bond lengths



Bond angles

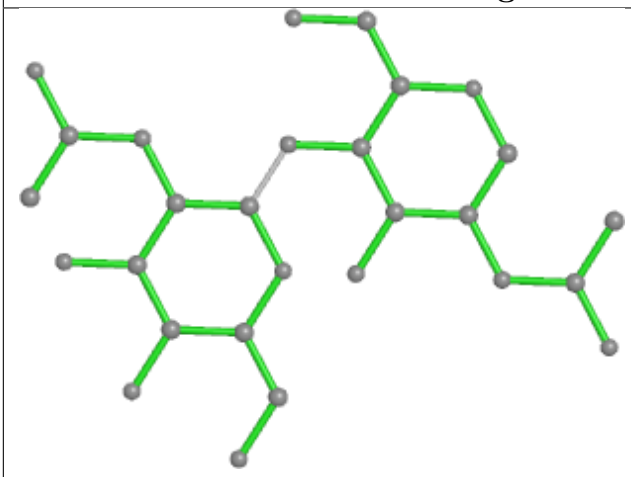


Torsions

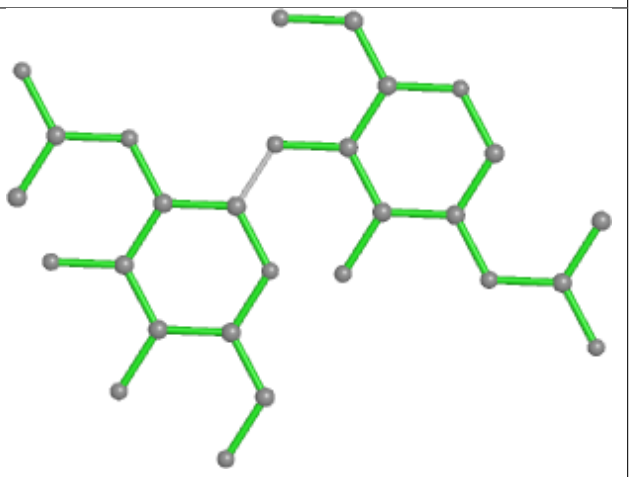


Rings

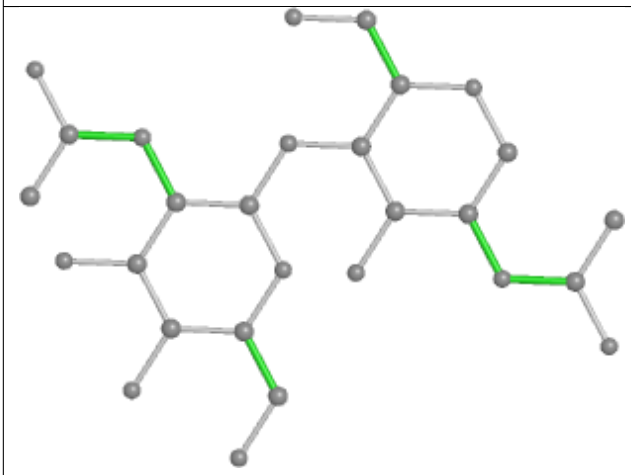
Oligosaccharide Chain S



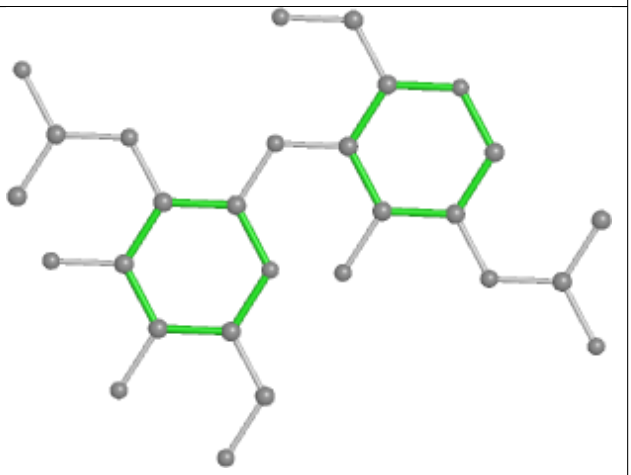
Bond lengths



Bond angles

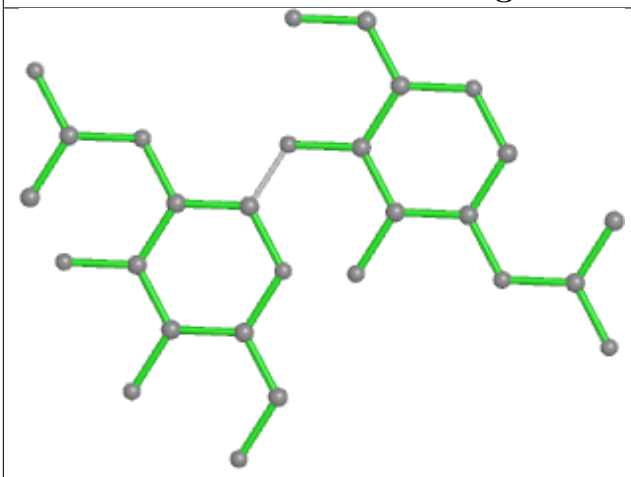


Torsions

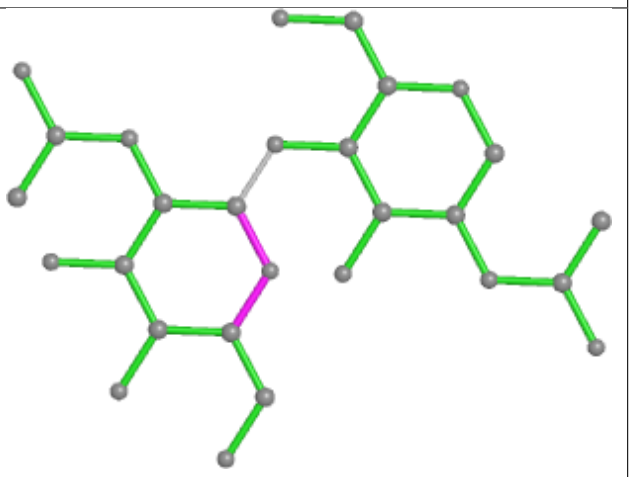


Rings

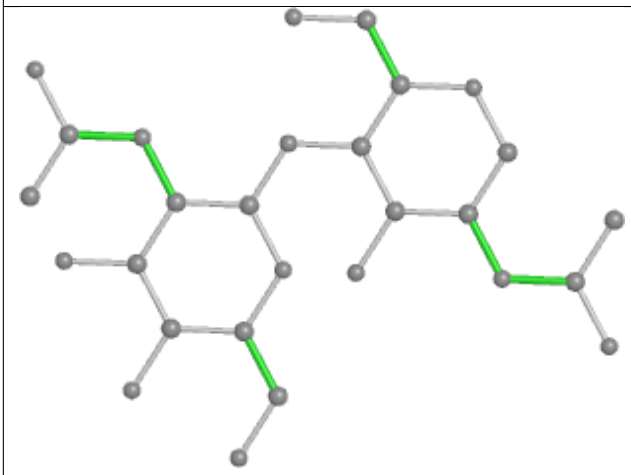
Oligosaccharide Chain T



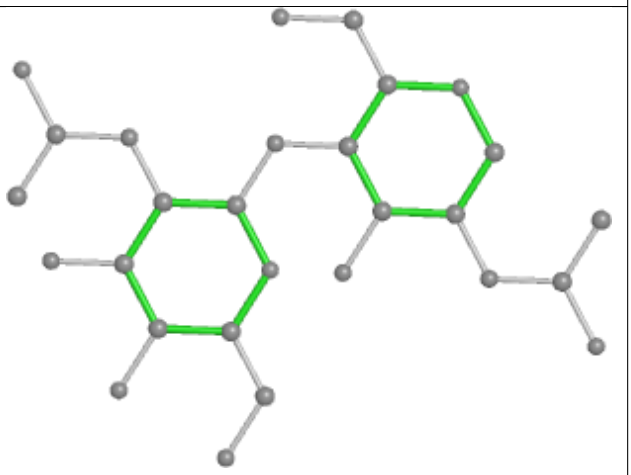
Bond lengths



Bond angles

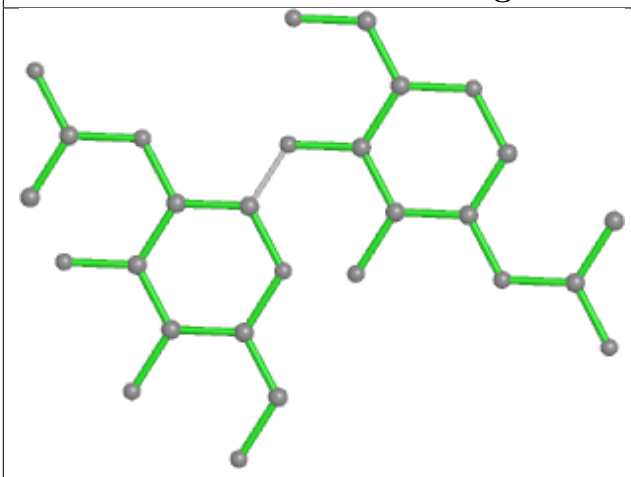


Torsions

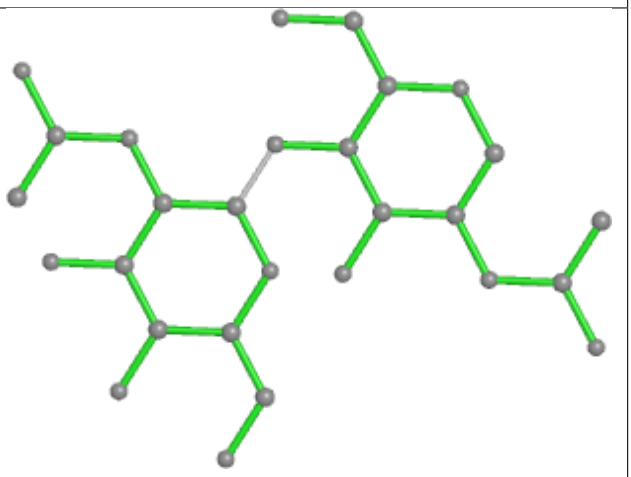


Rings

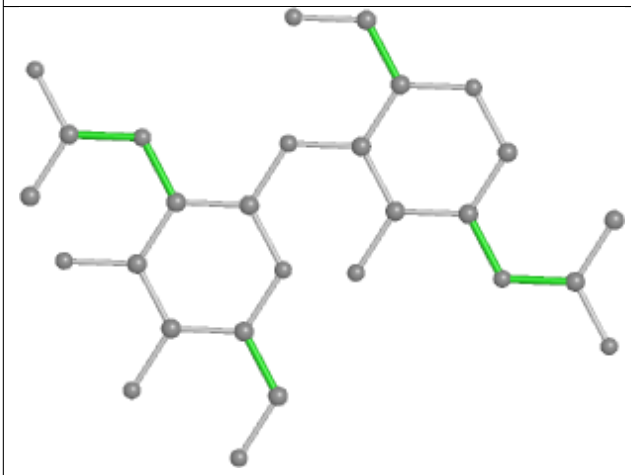
Oligosaccharide Chain U



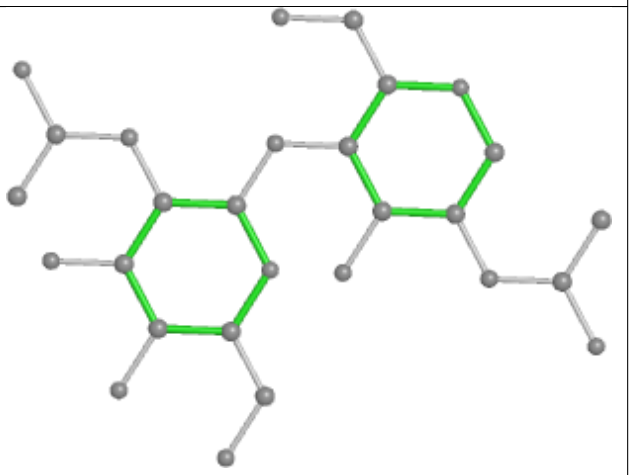
Bond lengths



Bond angles

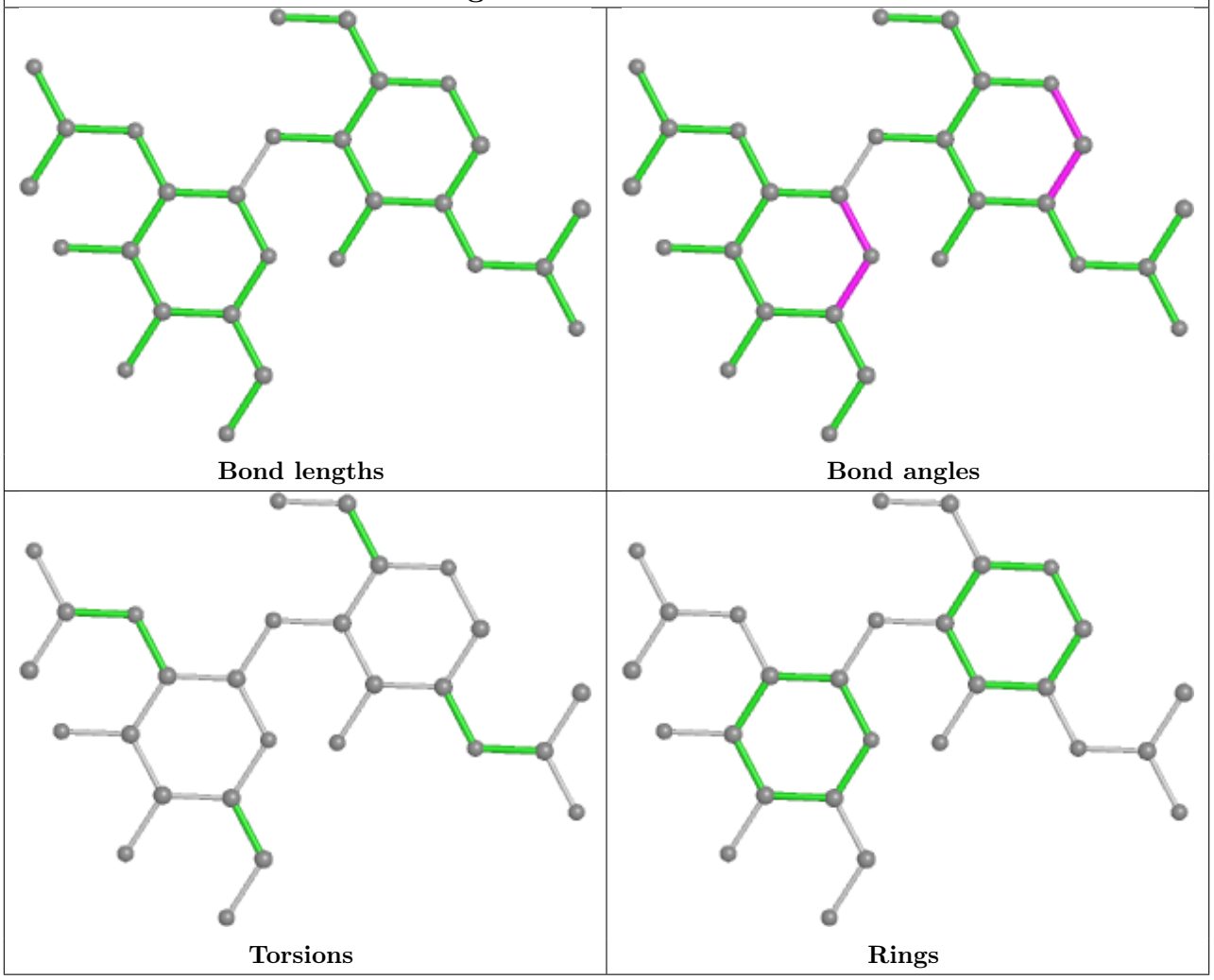


Torsions



Rings

Oligosaccharide Chain V



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	P	601	2	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	B	602	2	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	H	601	2	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	B	601	2	14,14,15	0.33	0	17,19,21	0.47	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
4	NAG	P	601	2	-	1/6/23/26	0/1/1/1
4	NAG	B	602	2	-	0/6/23/26	0/1/1/1
4	NAG	H	601	2	-	0/6/23/26	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	33:THR	C	34:VAL	N	3.81
1	A	32:VAL	C	33:THR	N	3.60
1	I	23[A]:SER	C	24:ASP	N	0.99

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, 95^{th} 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	134/155 (86%)	0.45	13 (9%) 7 7	93, 178, 196, 198	0
1	C	134/155 (86%)	0.09	4 (2%) 50 39	97, 173, 194, 196	0
1	E	134/155 (86%)	0.40	10 (7%) 14 12	138, 180, 195, 206	0
1	G	134/155 (86%)	0.25	11 (8%) 11 10	139, 177, 189, 192	0
1	I	135/155 (87%)	0.34	11 (8%) 12 11	146, 179, 188, 192	0
1	K	137/155 (88%)	0.16	3 (2%) 62 52	100, 177, 195, 203	0
1	M	134/155 (86%)	0.21	6 (4%) 33 28	139, 170, 182, 186	0
1	O	134/155 (86%)	0.30	7 (5%) 27 24	145, 175, 191, 193	0
2	B	423/582 (72%)	0.91	79 (18%) 1 2	98, 188, 289, 298	0
2	D	422/582 (72%)	0.81	81 (19%) 1 2	98, 197, 294, 299	0
2	F	420/582 (72%)	0.90	81 (19%) 1 1	145, 197, 290, 299	0
2	H	423/582 (72%)	0.78	66 (15%) 2 2	122, 201, 292, 299	0
2	J	417/582 (71%)	0.96	82 (19%) 1 1	126, 188, 289, 299	0
2	L	430/582 (73%)	1.06	87 (20%) 1 1	146, 207, 293, 299	0
2	N	428/582 (73%)	1.09	87 (20%) 1 1	136, 191, 294, 299	0
2	P	427/582 (73%)	0.82	71 (16%) 1 2	145, 209, 285, 297	0
All	All	4466/5896 (75%)	0.76	699 (15%) 2 2	93, 183, 289, 299	0

The worst 5 of 699 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	458	PRO	19.7
2	L	94	LEU	16.8
2	J	457	TYR	16.7
2	N	457	TYR	16.6
2	L	96	ASP	16.3

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)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.