Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2022 – 02:22 pm GMT

PDB ID	:	7QDP
Title	:	Crystal structure of FLT3 T343I in complex with the canonical ligand FL
Authors	:	Pannecoucke, E.; Savvides, S.N.
Deposited on	:	2021-11-27
Resolution	:	3.69 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 (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 (1)) were used in the production of this report:

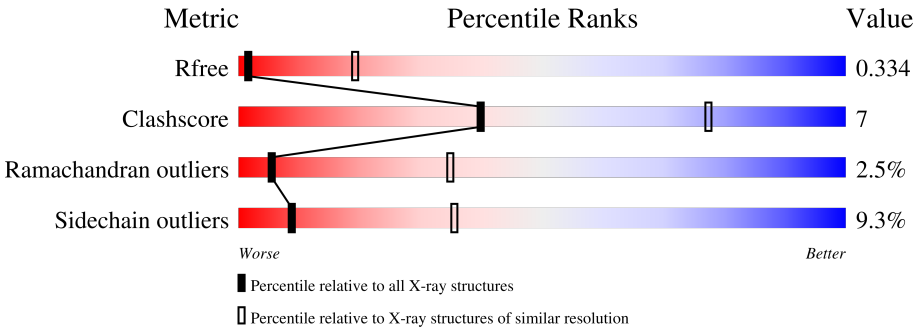
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.69 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

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%

Mol	Chain	Length	Quality of chain
1	A	155	84% 9% • 6%
1	B	155	77% 9% 14%
1	C	155	77% 9% 14%
1	D	155	73% 12% • 14%
2	E	582	47% 9% • 43%
2	F	582	54% 14% • 29%
2	G	582	49% 10% • 39%

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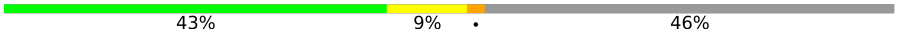
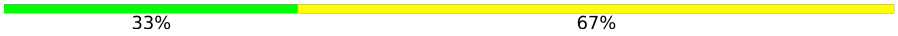
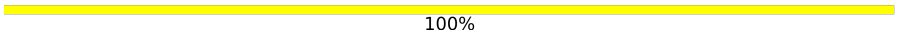
Mol	Chain	Length	Quality of chain
2	H	582	
3	I	3	
4	J	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13508 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	145	Total	C	N	O	S	0	0	0
			1050	665	181	196	8			
1	B	134	Total	C	N	O	S	0	0	0
			937	595	164	169	9			
1	C	133	Total	C	N	O	S	0	0	0
			935	594	159	175	7			
1	D	134	Total	C	N	O	S	0	0	0
			1024	652	178	186	8			

There are 84 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
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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	332	Total	C	N	O	S	0	0	0
			2163	1371	376	400	16			
2	F	413	Total	C	N	O	S	0	1	0
			2783	1750	483	530	20			
2	G	353	Total	C	N	O	S	6	1	0
			2391	1500	421	448	22			
2	H	316	Total	C	N	O	S	0	1	0
			2102	1333	367	389	13			

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	227	MET	THR	variant	UNP P36888
E	343	ILE	THR	engineered mutation	UNP P36888
E	542	GLY	-	expression tag	UNP P36888
E	543	SER	-	expression tag	UNP P36888
E	544	SER	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
E	545	GLY	-	expression tag	UNP P36888
E	546	LEU	-	expression tag	UNP P36888
E	547	VAL	-	expression tag	UNP P36888
E	548	PRO	-	expression tag	UNP P36888
E	549	ARG	-	expression tag	UNP P36888
E	550	GLY	-	expression tag	UNP P36888
E	551	SER	-	expression tag	UNP P36888
E	552	GLY	-	expression tag	UNP P36888
E	553	GLY	-	expression tag	UNP P36888
E	554	SER	-	expression tag	UNP P36888
E	555	GLY	-	expression tag	UNP P36888
E	556	GLY	-	expression tag	UNP P36888
E	557	SER	-	expression tag	UNP P36888
E	558	GLY	-	expression tag	UNP P36888
E	559	LEU	-	expression tag	UNP P36888
E	560	ASN	-	expression tag	UNP P36888
E	561	ASP	-	expression tag	UNP P36888
E	562	ILE	-	expression tag	UNP P36888
E	563	PHE	-	expression tag	UNP P36888
E	564	GLU	-	expression tag	UNP P36888
E	565	ALA	-	expression tag	UNP P36888
E	566	GLN	-	expression tag	UNP P36888
E	567	LYS	-	expression tag	UNP P36888
E	568	ILE	-	expression tag	UNP P36888
E	569	GLU	-	expression tag	UNP P36888
E	570	TRP	-	expression tag	UNP P36888
E	571	HIS	-	expression tag	UNP P36888
E	572	GLU	-	expression tag	UNP P36888
E	573	GLY	-	expression tag	UNP P36888
E	574	ARG	-	expression tag	UNP P36888
E	575	THR	-	expression tag	UNP P36888
E	576	LYS	-	expression tag	UNP P36888
E	577	HIS	-	expression tag	UNP P36888
E	578	HIS	-	expression tag	UNP P36888
E	579	HIS	-	expression tag	UNP P36888
E	580	HIS	-	expression tag	UNP P36888
E	581	HIS	-	expression tag	UNP P36888
E	582	HIS	-	expression tag	UNP P36888
F	227	MET	THR	variant	UNP P36888
F	343	ILE	THR	engineered mutation	UNP P36888
F	542	GLY	-	expression tag	UNP P36888
F	543	SER	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
G	227	MET	THR	variant	UNP P36888
G	343	ILE	THR	engineered mutation	UNP P36888
G	542	GLY	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
G	543	SER	-	expression tag	UNP P36888
G	544	SER	-	expression tag	UNP P36888
G	545	GLY	-	expression tag	UNP P36888
G	546	LEU	-	expression tag	UNP P36888
G	547	VAL	-	expression tag	UNP P36888
G	548	PRO	-	expression tag	UNP P36888
G	549	ARG	-	expression tag	UNP P36888
G	550	GLY	-	expression tag	UNP P36888
G	551	SER	-	expression tag	UNP P36888
G	552	GLY	-	expression tag	UNP P36888
G	553	GLY	-	expression tag	UNP P36888
G	554	SER	-	expression tag	UNP P36888
G	555	GLY	-	expression tag	UNP P36888
G	556	GLY	-	expression tag	UNP P36888
G	557	SER	-	expression tag	UNP P36888
G	558	GLY	-	expression tag	UNP P36888
G	559	LEU	-	expression tag	UNP P36888
G	560	ASN	-	expression tag	UNP P36888
G	561	ASP	-	expression tag	UNP P36888
G	562	ILE	-	expression tag	UNP P36888
G	563	PHE	-	expression tag	UNP P36888
G	564	GLU	-	expression tag	UNP P36888
G	565	ALA	-	expression tag	UNP P36888
G	566	GLN	-	expression tag	UNP P36888
G	567	LYS	-	expression tag	UNP P36888
G	568	ILE	-	expression tag	UNP P36888
G	569	GLU	-	expression tag	UNP P36888
G	570	TRP	-	expression tag	UNP P36888
G	571	HIS	-	expression tag	UNP P36888
G	572	GLU	-	expression tag	UNP P36888
G	573	GLY	-	expression tag	UNP P36888
G	574	ARG	-	expression tag	UNP P36888
G	575	THR	-	expression tag	UNP P36888
G	576	LYS	-	expression tag	UNP P36888
G	577	HIS	-	expression tag	UNP P36888
G	578	HIS	-	expression tag	UNP P36888
G	579	HIS	-	expression tag	UNP P36888
G	580	HIS	-	expression tag	UNP P36888
G	581	HIS	-	expression tag	UNP P36888
G	582	HIS	-	expression tag	UNP P36888
H	227	MET	THR	variant	UNP P36888
H	343	ILE	THR	engineered mutation	UNP P36888

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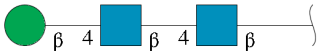
Chain	Residue	Modelled	Actual	Comment	Reference
H	542	GLY	-	expression tag	UNP P36888
H	543	SER	-	expression tag	UNP P36888
H	544	SER	-	expression tag	UNP P36888
H	545	GLY	-	expression tag	UNP P36888
H	546	LEU	-	expression tag	UNP P36888
H	547	VAL	-	expression tag	UNP P36888
H	548	PRO	-	expression tag	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
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

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

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

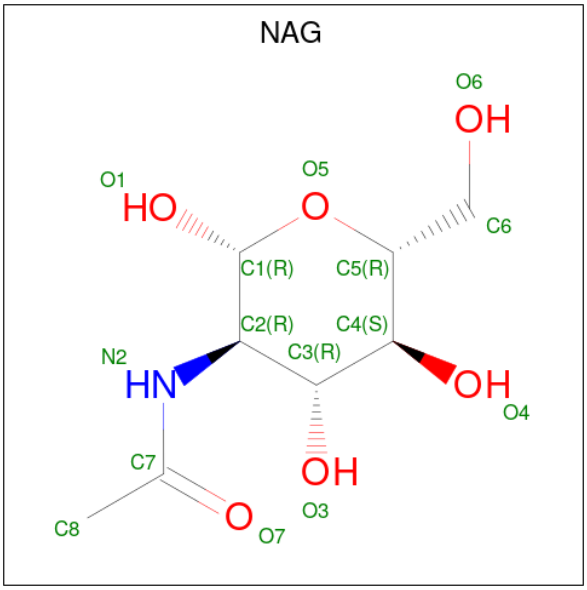


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	39	22	2	15	0	0	0

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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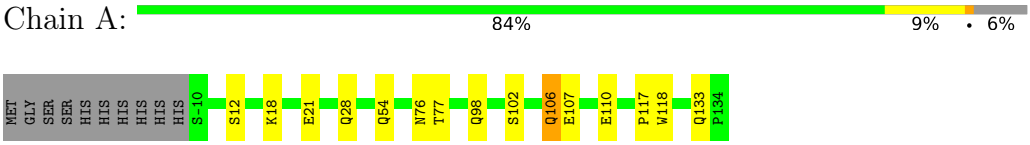
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

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. 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. 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.

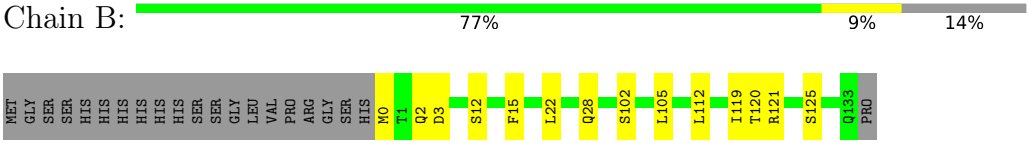
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain A:



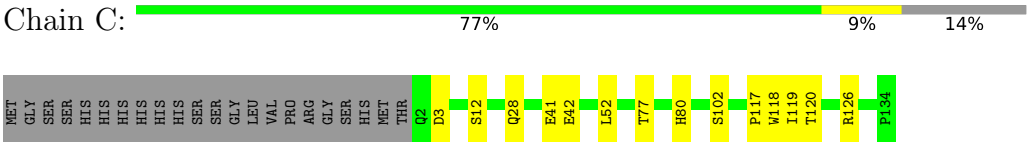
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain B:



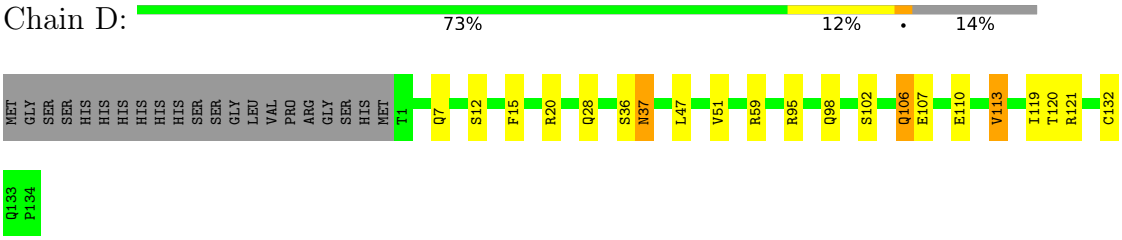
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain C:



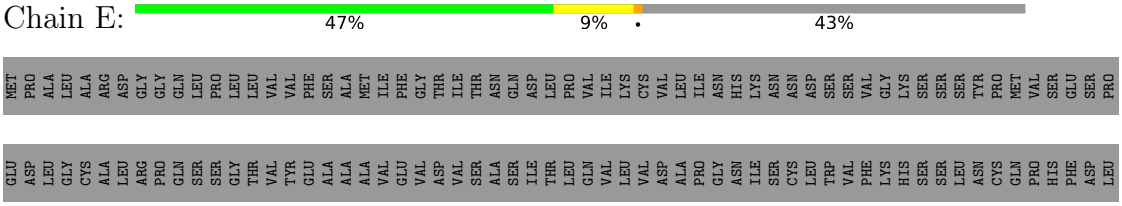
• Molecule 1: Fms-related tyrosine kinase 3 ligand

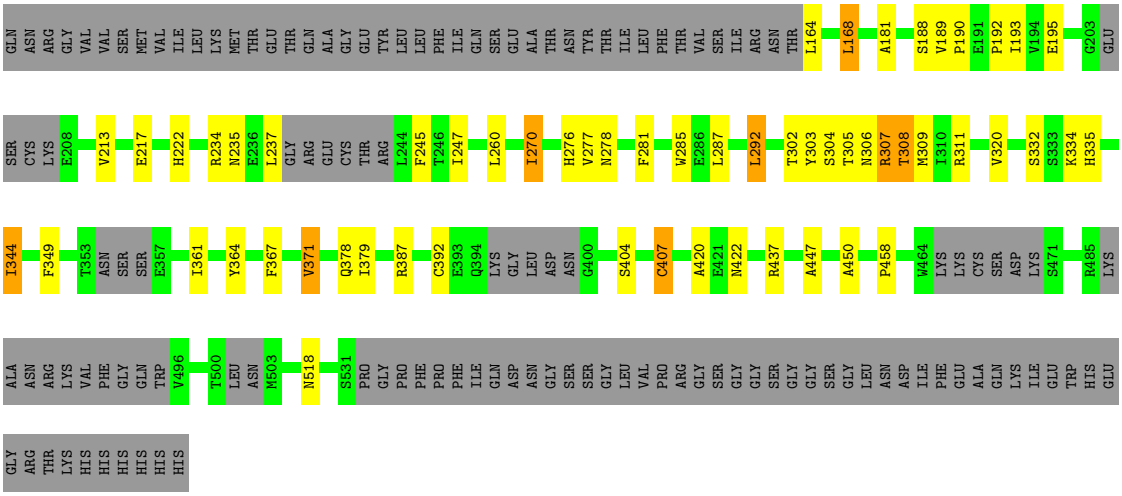
Chain D:



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

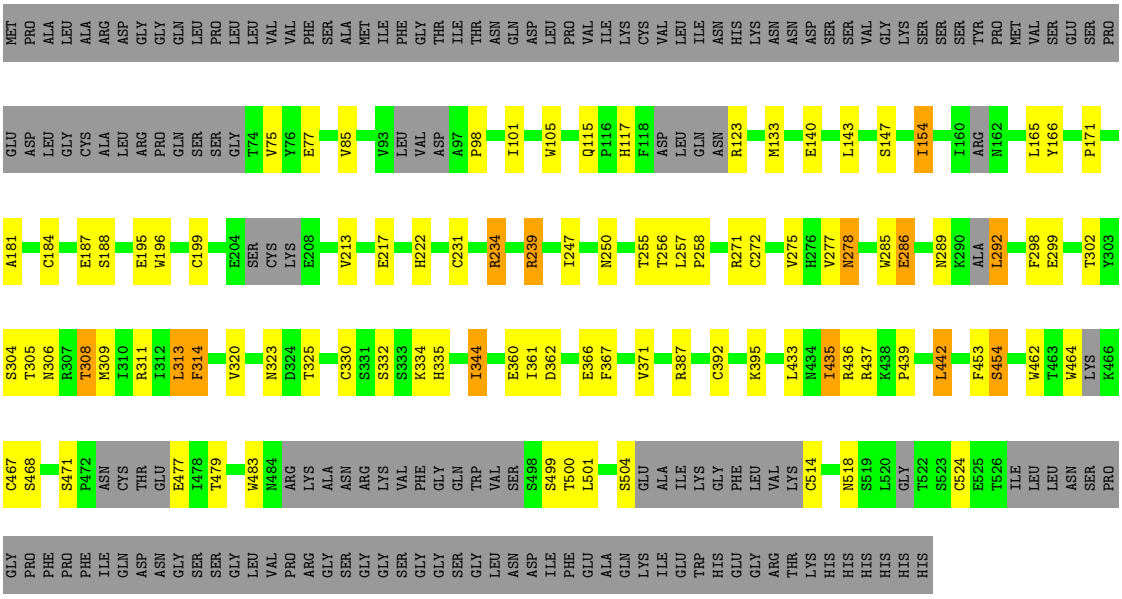
Chain E:





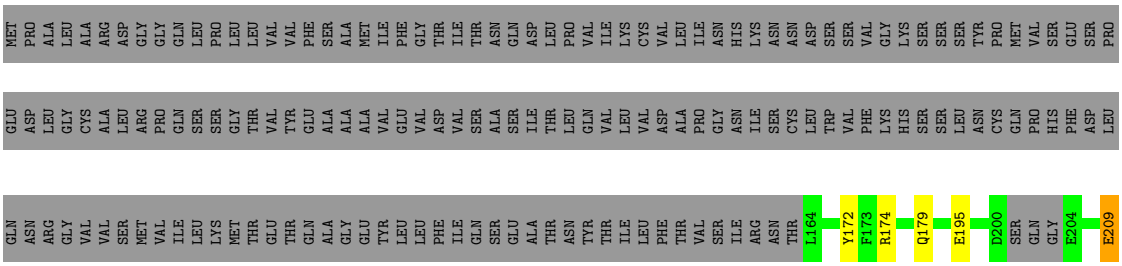
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

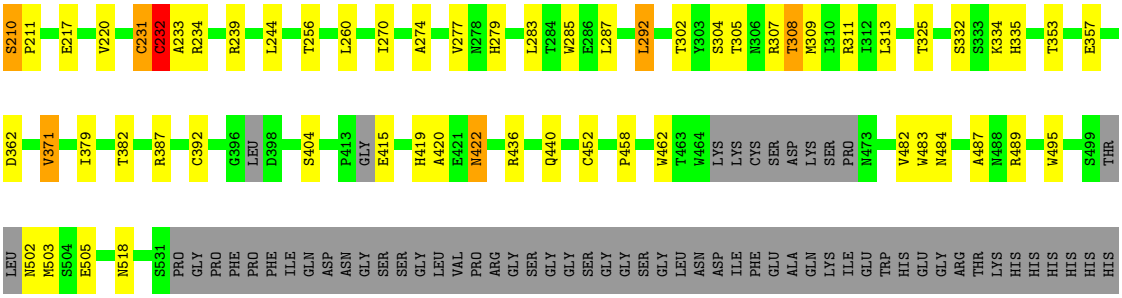
Chain F:



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

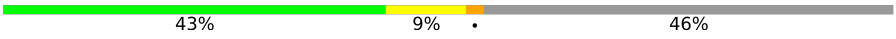
Chain G:

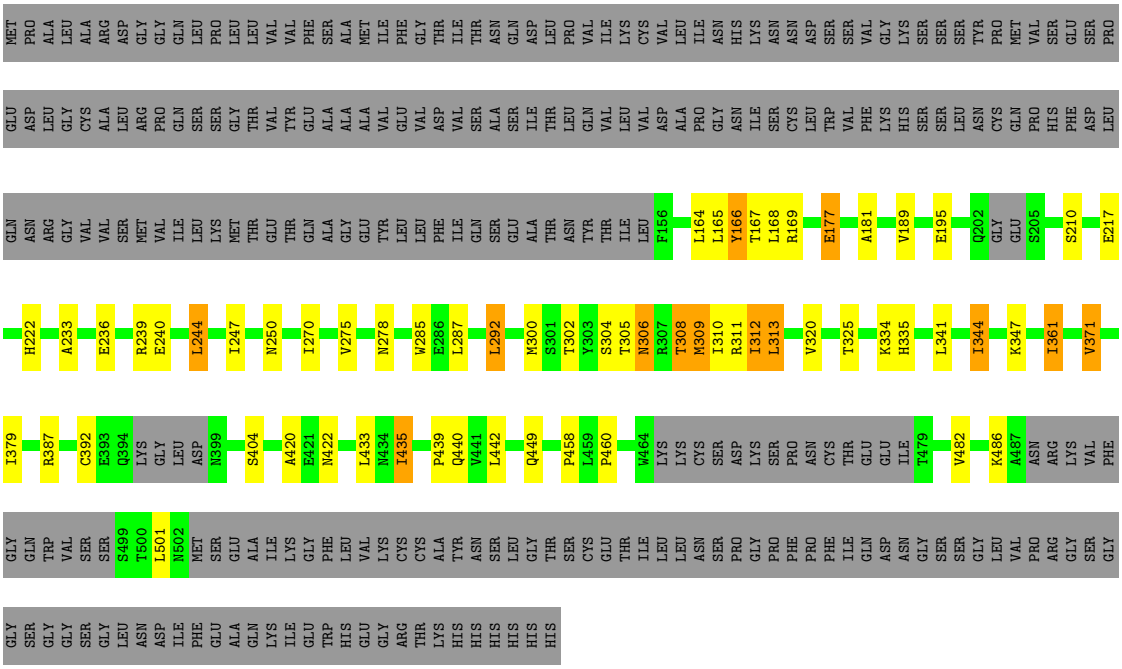




• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

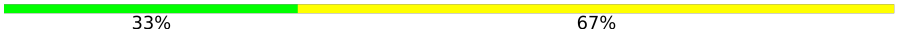
Chain H:





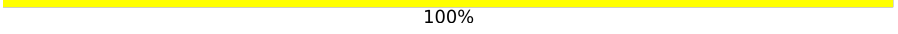
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	102.43Å 113.38Å 123.22Å 105.37° 109.47° 108.22°	Depositor
Resolution (Å)	48.58 – 3.69 48.58 – 3.69	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.58-3.69) 94.4 (48.58-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.67Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.257 , 0.277 0.313 , 0.334	Depositor DCC
R_{free} test set	2298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	143.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13508	wwPDB-VP
Average B, all atoms (Å^2)	237.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

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

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	0.29	0/1071	0.48	0/1467
1	B	0.30	0/956	0.50	0/1313
1	C	0.32	0/956	0.49	0/1314
1	D	0.33	0/1045	0.52	0/1423
2	E	0.33	0/2205	0.59	0/3033
2	F	0.36	0/2838	0.61	0/3887
2	G	0.33	0/2440	0.59	0/3343
2	H	0.37	0/2146	0.63	0/2954
All	All	0.34	0/13657	0.57	0/18734

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	E	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	189	VAL	Peptide,Mainchain

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	1050	0	959	13	0
1	B	937	0	822	7	0
1	C	935	0	806	6	0
1	D	1024	0	986	13	0
2	E	2163	0	1673	35	0
2	F	2783	0	2168	56	0
2	G	2391	0	1873	33	0
2	H	2102	0	1641	27	0
3	I	39	0	34	0	0
4	J	28	0	25	0	0
5	E	14	0	13	0	0
5	F	28	0	26	2	0
5	H	14	0	13	0	0
All	All	13508	0	11039	180	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 7.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:437:ARG:HA	2:E:458:PRO:HD2	1.12	1.09
2:G:436:ARG:HA	2:G:458:PRO:HG2	1.35	1.08
2:F:271:ARG:HA	2:F:314:PHE:HB3	1.34	1.06
1:A:77:THR:HG22	2:E:307:ARG:HE	1.15	1.05
2:F:462:TRP:HE1	2:F:501:LEU:HD13	1.22	1.03
1:B:22:LEU:HD22	1:B:105:LEU:HD11	1.46	0.97
2:E:437:ARG:HA	2:E:458:PRO:CD	1.94	0.96
2:F:462:TRP:CD1	2:F:501:LEU:HD22	2.04	0.93
2:H:304:SER:HB2	2:H:310:ILE:HD11	1.56	0.87
2:E:437:ARG:CA	2:E:458:PRO:HD2	2.01	0.87
2:F:299:GLU:HB3	2:F:313:LEU:HD12	1.61	0.83
1:D:37:ASN:HD21	1:D:95:ARG:H	1.26	0.82
2:F:483:TRP:CD1	2:F:501:LEU:HD12	2.16	0.81
1:A:77:THR:HG22	2:E:307:ARG:NE	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:462:TRP:NE1	2:F:501:LEU:HD13	1.97	0.79
2:E:164:LEU:HA	2:E:234:ARG:HB3	1.65	0.78
2:F:101:ILE:HA	2:F:147:SER:HB2	1.64	0.77
1:D:106:GLN:HE21	1:D:106:GLN:HA	1.50	0.76
2:F:462:TRP:HE1	2:F:501:LEU:CD1	2.00	0.75
2:F:286:GLU:HB2	2:F:289:ASN:HA	1.68	0.75
1:A:106:GLN:HE21	1:A:106:GLN:HA	1.52	0.74
2:E:181:ALA:HB2	2:E:222:HIS:CD2	2.22	0.74
2:F:234:ARG:HG2	2:F:239:ARG:HB3	1.70	0.73
2:F:332:SER:HB3	2:F:335:HIS:HB2	1.68	0.73
1:A:107:GLU:HA	1:A:110:GLU:HG2	1.72	0.72
2:H:435:ILE:CB	2:H:460:PRO:HG2	2.19	0.72
2:G:231:CYS:O	2:G:232:CYS:HB2	1.90	0.71
2:G:233:ALA:HA	2:G:239:ARG:CG	2.23	0.69
2:E:192:PRO:HA	2:E:235:ASN:HB2	1.75	0.68
2:F:362:ASP:HA	2:F:437:ARG:HE	1.59	0.68
2:F:464:TRP:CD1	2:F:479:THR:HG23	2.29	0.67
2:H:181:ALA:HB2	2:H:222:HIS:CE1	2.29	0.67
2:F:462:TRP:NE1	2:F:501:LEU:HD22	2.10	0.67
1:A:77:THR:CG2	2:E:307:ARG:HE	2.00	0.66
2:G:233:ALA:HA	2:G:239:ARG:HG2	1.78	0.66
1:D:37:ASN:ND2	1:D:95:ARG:H	1.93	0.66
2:G:172:TYR:HE1	2:G:174:ARG:HE	1.45	0.65
2:H:486:LYS:CB	2:H:501:LEU:HA	2.27	0.64
2:H:166:TYR:HA	2:H:189:VAL:HB	1.79	0.64
2:F:271:ARG:CA	2:F:314:PHE:HB3	2.20	0.63
1:B:2:GLN:HA	1:B:125:SER:HB3	1.79	0.62
2:G:487:ALA:HB3	2:G:489:ARG:HE	1.64	0.61
2:E:168:LEU:HB2	2:E:237:LEU:HD13	1.82	0.60
2:F:454:SER:H	2:F:500:THR:HA	1.66	0.60
1:A:54:GLN:HE21	1:A:76:ASN:HD21	1.51	0.58
1:B:22:LEU:HD22	1:B:105:LEU:CD1	2.28	0.58
2:E:320:VAL:HB	2:E:344:ILE:HD12	1.86	0.57
2:F:362:ASP:HA	2:F:437:ARG:NE	2.18	0.57
2:G:436:ARG:HA	2:G:458:PRO:CG	2.24	0.57
2:G:379:ILE:HD13	2:G:420:ALA:HB1	1.87	0.57
2:H:379:ILE:HD13	2:H:420:ALA:HB1	1.86	0.56
2:H:250:ASN:HD21	2:H:275:VAL:H	1.53	0.56
2:H:167:THR:HG22	2:H:189:VAL:HG23	1.88	0.56
2:E:379:ILE:HD13	2:E:420:ALA:HB1	1.87	0.56
2:E:245:PHE:HD2	2:E:270:ILE:HG23	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:210:SER:N	2:G:211:PRO:HD3	2.21	0.55
2:F:464:TRP:CD1	2:F:479:THR:CG2	2.90	0.55
2:F:256:THR:O	2:F:258:PRO:HD3	2.07	0.55
2:F:271:ARG:HA	2:F:314:PHE:CB	2.23	0.55
2:G:195:GLU:O	2:G:231:CYS:O	2.25	0.55
1:C:119:ILE:HG23	1:C:120:THR:HG23	1.89	0.54
1:B:119:ILE:HG23	1:B:120:THR:HG23	1.89	0.54
1:D:119:ILE:HG23	1:D:120:THR:HG23	1.90	0.54
2:H:181:ALA:HB2	2:H:222:HIS:ND1	2.21	0.54
2:G:209:GLU:HB3	2:G:211:PRO:HD3	1.89	0.53
2:E:276:HIS:HE1	2:E:278:ASN:ND2	2.07	0.53
1:D:37:ASN:HD22	1:D:37:ASN:H	1.55	0.53
2:E:276:HIS:CE1	2:E:278:ASN:ND2	2.77	0.52
2:E:245:PHE:CD2	2:E:270:ILE:HG23	2.45	0.52
2:F:98:PRO:HG3	2:F:123:ARG:HA	1.92	0.52
2:H:304:SER:O	2:H:306:ASN:O	2.28	0.52
2:F:514:CYS:N	2:F:524:CYS:HG	2.08	0.52
1:B:28:GLN:HG3	1:B:102:SER:HB3	1.92	0.51
1:D:15:PHE:HZ	1:D:113:VAL:HG13	1.76	0.51
2:F:467:CYS:HB2	2:F:477:GLU:HB3	1.92	0.51
1:A:107:GLU:HA	1:A:110:GLU:CG	2.39	0.51
2:G:482:VAL:HG21	2:G:505:GLU:HB3	1.92	0.51
1:C:12:SER:HB2	2:G:302:THR:HA	1.93	0.51
2:G:285:TRP:NE1	2:G:313:LEU:O	2.41	0.51
1:C:77:THR:HG22	2:G:307:ARG:HG2	1.93	0.50
2:F:247:ILE:HD12	2:F:285:TRP:HH2	1.76	0.50
2:F:184:CYS:HG	2:F:231:CYS:HG	1.58	0.50
2:F:250:ASN:HB3	2:F:275:VAL:H	1.77	0.50
1:D:7:GLN:NE2	1:D:7:GLN:H	2.08	0.50
2:E:234:ARG:HG3	2:E:235:ASN:H	1.76	0.50
2:F:181:ALA:HB2	2:F:222:HIS:ND1	2.27	0.50
1:C:28:GLN:HG3	1:C:102:SER:HB3	1.92	0.50
2:F:285:TRP:CD1	2:F:313:LEU:HD23	2.47	0.50
1:A:18:LYS:NZ	2:E:303:TYR:HB2	2.27	0.50
1:A:28:GLN:HG3	1:A:102:SER:HB3	1.93	0.49
1:D:28:GLN:HG3	1:D:102:SER:HB3	1.94	0.49
2:F:323:ASN:HB2	5:F:601:NAG:O5	2.12	0.49
2:F:277:VAL:HG22	2:F:308:THR:HG23	1.93	0.49
2:G:279:HIS:O	2:G:311:ARG:NH2	2.44	0.49
2:F:101:ILE:CA	2:F:147:SER:HB2	2.38	0.49
2:F:439:PRO:HB3	2:F:518:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:382:THR:CB	2:G:419:HIS:CE1	2.96	0.48
2:H:304:SER:HB3	2:H:308:THR:HB	1.95	0.48
2:G:210:SER:H	2:G:211:PRO:HD3	1.77	0.48
2:F:277:VAL:O	2:F:278:ASN:CB	2.61	0.48
2:F:77:GLU:HB2	2:F:154:ILE:HG23	1.95	0.48
2:F:105:TRP:CD2	2:F:143:LEU:HD13	2.49	0.48
2:G:195:GLU:HA	2:G:217:GLU:HA	1.96	0.48
2:F:514:CYS:O	2:F:524:CYS:SG	2.71	0.47
2:H:379:ILE:HG22	2:H:422:ASN:HB3	1.97	0.47
1:B:12:SER:HB2	2:F:302:THR:HA	1.96	0.47
1:D:7:GLN:H	1:D:7:GLN:CD	2.17	0.47
2:E:332:SER:CB	2:E:335:HIS:HB2	2.44	0.47
2:H:247:ILE:HD12	2:H:285:TRP:HH2	1.78	0.47
2:F:286:GLU:HB2	2:F:289:ASN:CA	2.40	0.47
2:F:361:ILE:CB	2:F:435:ILE:CB	2.93	0.47
2:G:233:ALA:CA	2:G:239:ARG:HG2	2.45	0.47
2:G:285:TRP:HB3	2:G:292:LEU:HD13	1.97	0.47
2:H:361:ILE:O	2:H:435:ILE:O	2.33	0.47
1:A:54:GLN:NE2	1:A:76:ASN:HD21	2.12	0.46
2:E:247:ILE:HD12	2:E:285:TRP:HH2	1.79	0.46
2:E:195:GLU:HA	2:E:217:GLU:HA	1.98	0.46
2:F:272:CYS:HG	2:F:330:CYS:HG	1.61	0.46
2:F:199:CYS:CB	2:F:213:VAL:CB	2.94	0.46
2:H:275:VAL:HG22	2:H:310:ILE:HG23	1.97	0.46
2:E:379:ILE:HG22	2:E:422:ASN:HB3	1.97	0.46
2:G:233:ALA:HA	2:G:239:ARG:HG3	1.96	0.45
2:H:285:TRP:CD1	2:H:313:LEU:HD23	2.50	0.45
2:G:274:ALA:HB3	2:G:283:LEU:HD11	1.98	0.45
2:F:115:GLN:HE21	2:F:117:HIS:CE1	2.35	0.45
2:H:195:GLU:HA	2:H:217:GLU:HA	1.98	0.45
2:H:309:MET:SD	2:H:311:ARG:NH2	2.90	0.45
2:F:171:PRO:HB3	2:F:184:CYS:SG	2.57	0.44
2:F:304:SER:HB3	2:F:308:THR:HB	2.00	0.44
2:F:442:LEU:HD12	2:F:453:PHE:HD1	1.82	0.44
2:G:332:SER:CB	2:G:335:HIS:HB2	2.47	0.44
2:G:304:SER:HB3	2:G:308:THR:HB	2.00	0.44
2:F:101:ILE:CB	2:F:147:SER:HB2	2.48	0.44
2:F:195:GLU:HA	2:F:217:GLU:HA	1.99	0.44
1:A:106:GLN:HA	1:A:106:GLN:NE2	2.28	0.43
2:H:285:TRP:HB3	2:H:292:LEU:HD13	2.00	0.43
2:E:304:SER:HB3	2:E:308:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:483:TRP:CD1	2:F:501:LEU:CD1	2.96	0.43
1:D:37:ASN:HD22	1:D:37:ASN:N	2.15	0.43
2:F:105:TRP:CE2	2:F:143:LEU:HD13	2.53	0.43
2:G:379:ILE:HG22	2:G:422:ASN:HB3	1.99	0.43
2:G:462:TRP:CD1	2:G:502:ASN:ND2	2.79	0.43
2:F:314:PHE:HD1	2:F:314:PHE:H	1.65	0.43
2:E:447:ALA:O	2:E:450:ALA:O	2.37	0.43
2:H:250:ASN:ND2	2:H:335:HIS:NE2	2.67	0.43
2:E:168:LEU:HD12	2:E:237:LEU:HB3	2.01	0.42
2:H:320:VAL:HB	2:H:344:ILE:HD11	2.01	0.42
2:E:164:LEU:HG	2:E:234:ARG:HD2	2.00	0.42
2:E:285:TRP:HB3	2:E:292:LEU:HD13	2.00	0.42
2:F:187:GLU:O	2:F:188:SER:OG	2.32	0.42
1:C:117:PRO:HG2	1:C:118:TRP:CD1	2.55	0.42
2:E:437:ARG:HA	2:E:458:PRO:CG	2.48	0.42
1:A:12:SER:HB2	2:E:302:THR:HA	2.02	0.42
2:E:281:PHE:CE1	2:E:311:ARG:NH1	2.88	0.42
2:G:415:GLU:HG2	2:G:495:TRP:HH2	1.83	0.42
2:F:323:ASN:CB	5:F:601:NAG:O5	2.68	0.41
2:F:468:SER:HG	2:F:477:GLU:N	2.17	0.41
2:H:371:VAL:HG23	2:H:404:SER:HB3	2.01	0.41
2:E:168:LEU:HD22	2:E:188:SER:HA	2.03	0.41
1:D:107:GLU:HA	1:D:110:GLU:OE1	2.21	0.41
2:G:234:ARG:CB	2:G:239:ARG:HA	2.50	0.41
2:F:285:TRP:HB3	2:F:292:LEU:HD13	2.03	0.41
2:G:371:VAL:HG23	2:G:404:SER:HB3	2.02	0.41
2:H:233:ALA:O	2:H:239:ARG:HA	2.20	0.41
2:F:514:CYS:N	2:F:524:CYS:SG	2.93	0.41
2:H:244:LEU:HD23	2:H:244:LEU:HA	1.92	0.40
1:B:15:PHE:CE2	1:B:112:LEU:CB	3.04	0.40
1:D:47:LEU:O	1:D:51:VAL:HG23	2.21	0.40
2:F:320:VAL:HB	2:F:344:ILE:HD11	2.01	0.40
2:G:452:CYS:HB3	2:G:503:MET:HA	2.02	0.40
2:H:168:LEU:CD2	2:H:240:GLU:HG2	2.51	0.40
2:H:300:MET:HB2	2:H:312:ILE:HG22	2.03	0.40
1:C:80:HIS:CD2	2:G:307:ARG:HD3	2.57	0.40
1:D:12:SER:HB2	2:H:302:THR:HA	2.02	0.40
2:E:371:VAL:HG23	2:E:404:SER:HB3	2.03	0.40
1:A:117:PRO:HG2	1:A:118:TRP:CD1	2.56	0.40
2:E:164:LEU:HG	2:E:234:ARG:HB3	2.04	0.40
2:E:367:PHE:O	2:E:407:CYS:SG	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:ILE:CB	2:E:234:ARG:HG3	2.52	0.40
2:G:483:TRP:CD1	2:G:483:TRP:N	2.89	0.40

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	143/155 (92%)	133 (93%)	10 (7%)	0	100	100
1	B	132/155 (85%)	126 (96%)	5 (4%)	1 (1%)	19	56
1	C	131/155 (84%)	126 (96%)	4 (3%)	1 (1%)	19	56
1	D	132/155 (85%)	127 (96%)	5 (4%)	0	100	100
2	E	316/582 (54%)	277 (88%)	32 (10%)	7 (2%)	6	37
2	F	392/582 (67%)	325 (83%)	54 (14%)	13 (3%)	4	31
2	G	340/582 (58%)	289 (85%)	40 (12%)	11 (3%)	4	31
2	H	307/582 (53%)	254 (83%)	38 (12%)	15 (5%)	2	22
All	All	1893/2948 (64%)	1657 (88%)	188 (10%)	48 (2%)	5	35

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ASP
2	E	190	PRO
2	E	334	LYS
2	E	364	TYR
2	F	85	VAL
2	F	334	LYS
2	G	334	LYS
2	H	177	GLU

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Mol	Chain	Res	Type
2	H	305	THR
2	H	334	LYS
2	H	433	LEU
2	H	435	ILE
2	H	440	GLN
2	H	458	PRO
1	C	3	ASP
2	E	305	THR
2	E	387	ARG
2	F	278	ASN
2	F	305	THR
2	F	387	ARG
2	F	435	ILE
2	G	231	CYS
2	G	305	THR
2	G	353	THR
2	G	387	ARG
2	H	166	TYR
2	H	306	ASN
2	H	387	ARG
2	F	133	MET
2	G	232	CYS
2	G	256	THR
2	H	236	GLU
2	E	306	ASN
2	F	75	VAL
2	F	436	ARG
2	F	454	SER
2	G	484	ASN
2	F	255	THR
2	G	220	VAL
2	H	347	LYS
2	F	257	LEU
2	G	210	SER
2	G	362	ASP
2	H	210	SER
2	H	482	VAL
2	H	439	PRO
2	E	213	VAL
2	F	471	SER

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	104/142 (73%)	100 (96%)	4 (4%)	33 61
1	B	84/142 (59%)	82 (98%)	2 (2%)	49 71
1	C	86/142 (61%)	82 (95%)	4 (5%)	26 56
1	D	108/142 (76%)	99 (92%)	9 (8%)	11 40
2	E	161/515 (31%)	144 (89%)	17 (11%)	6 30
2	F	217/515 (42%)	188 (87%)	29 (13%)	4 21
2	G	188/515 (36%)	170 (90%)	18 (10%)	8 34
2	H	157/515 (30%)	136 (87%)	21 (13%)	4 21
All	All	1105/2628 (42%)	1001 (91%)	104 (9%)	9 35

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	98	GLN
1	A	106	GLN
1	A	133	GLN
1	B	0	MET
1	B	121	ARG
1	C	41	GLU
1	C	42	GLU
1	C	52	LEU
1	C	126	ARG
1	D	20	ARG
1	D	36	SER
1	D	37	ASN
1	D	59	ARG
1	D	98	GLN
1	D	106	GLN
1	D	113	VAL
1	D	121	ARG
1	D	132	CYS

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Mol	Chain	Res	Type
2	E	168	LEU
2	E	260	LEU
2	E	270	ILE
2	E	277	VAL
2	E	287	LEU
2	E	292	LEU
2	E	307	ARG
2	E	308	THR
2	E	309	MET
2	E	344	ILE
2	E	349	PHE
2	E	361	ILE
2	E	371	VAL
2	E	378	GLN
2	E	392	CYS
2	E	407	CYS
2	E	518	ASN
2	F	140	GLU
2	F	154	ILE
2	F	165	LEU
2	F	166	TYR
2	F	196	TRP
2	F	234	ARG
2	F	239	ARG
2	F	286	GLU
2	F	292	LEU
2	F	298	PHE
2	F	306	ASN
2	F	308	THR
2	F	309	MET
2	F	311	ARG
2	F	313	LEU
2	F	314	PHE
2	F	325	THR
2	F	344	ILE
2	F	360	GLU
2	F	366[A]	GLU
2	F	366[B]	GLU
2	F	367	PHE
2	F	371	VAL
2	F	392	CYS
2	F	395	LYS

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Mol	Chain	Res	Type
2	F	433	LEU
2	F	442	LEU
2	F	499	SER
2	F	504	SER
2	G	179	GLN
2	G	209	GLU
2	G	232	CYS
2	G	244	LEU
2	G	260	LEU
2	G	270	ILE
2	G	277	VAL
2	G	287	LEU
2	G	292	LEU
2	G	308	THR
2	G	309	MET
2	G	325	THR
2	G	357	GLU
2	G	371	VAL
2	G	392	CYS
2	G	422	ASN
2	G	440	GLN
2	G	518	ASN
2	H	164	LEU
2	H	165	LEU
2	H	169	ARG
2	H	177	GLU
2	H	244	LEU
2	H	270	ILE
2	H	278	ASN
2	H	287	LEU
2	H	292	LEU
2	H	308	THR
2	H	309	MET
2	H	312	ILE
2	H	313	LEU
2	H	325	THR
2	H	341	LEU
2	H	344	ILE
2	H	361	ILE
2	H	371	VAL
2	H	392	CYS
2	H	442	LEU

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Mol	Chain	Res	Type
2	H	449	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	76	ASN
1	A	106	GLN
1	C	80	HIS
1	D	7	GLN
1	D	37	ASN
1	D	106	GLN
1	D	111	GLN
2	E	222	HIS
2	E	278	ASN
2	E	408	ASN
2	F	117	HIS
2	F	518	ASN
2	G	422	ASN
2	G	488	ASN
2	G	494	GLN
2	H	250	ASN
2	H	276	HIS
2	H	278	ASN
2	H	449	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

5 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	I	1	2,3	14,14,15	0.33	0	17,19,21	1.16	1 (5%)
3	NAG	I	2	3	14,14,15	0.35	0	17,19,21	1.05	3 (17%)
3	BMA	I	3	3	11,11,12	0.33	0	15,15,17	0.43	0
4	NAG	J	1	2,4	14,14,15	0.45	0	17,19,21	1.60	3 (17%)
4	NAG	J	2	4	14,14,15	0.31	0	17,19,21	0.73	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	I	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	C1-O5-C5	4.78	118.67	112.19
3	I	1	NAG	O5-C1-C2	-3.66	105.50	111.29
4	J	2	NAG	C1-O5-C5	2.84	116.05	112.19
3	I	2	NAG	C1-O5-C5	2.58	115.69	112.19
4	J	1	NAG	C2-N2-C7	2.56	126.55	122.90
3	I	2	NAG	C1-C2-N2	2.50	114.75	110.49
4	J	1	NAG	C3-C4-C5	2.25	114.25	110.24
3	I	2	NAG	O5-C1-C2	-2.21	107.80	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

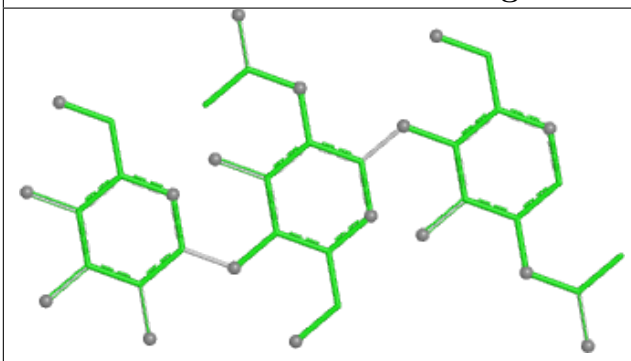
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C1-C2-N2-C7

There are no ring outliers.

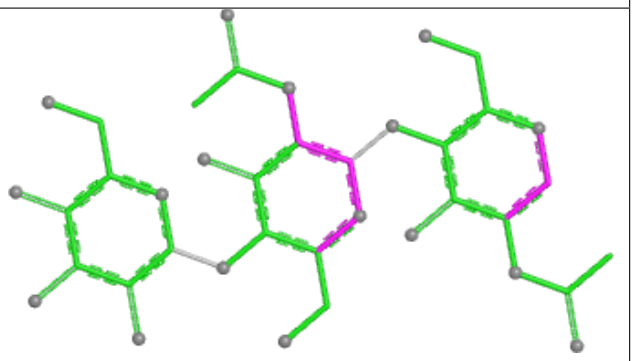
No monomer is involved in short contacts.

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

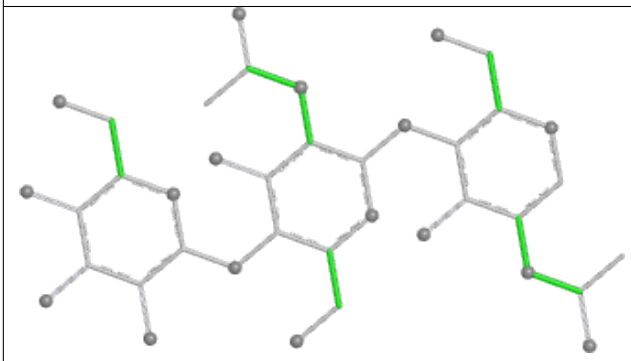
Oligosaccharide Chain I



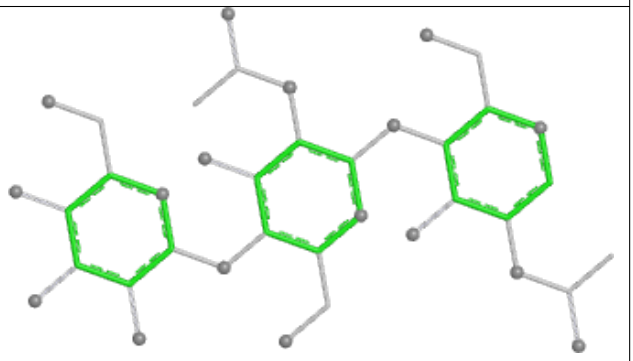
Bond lengths



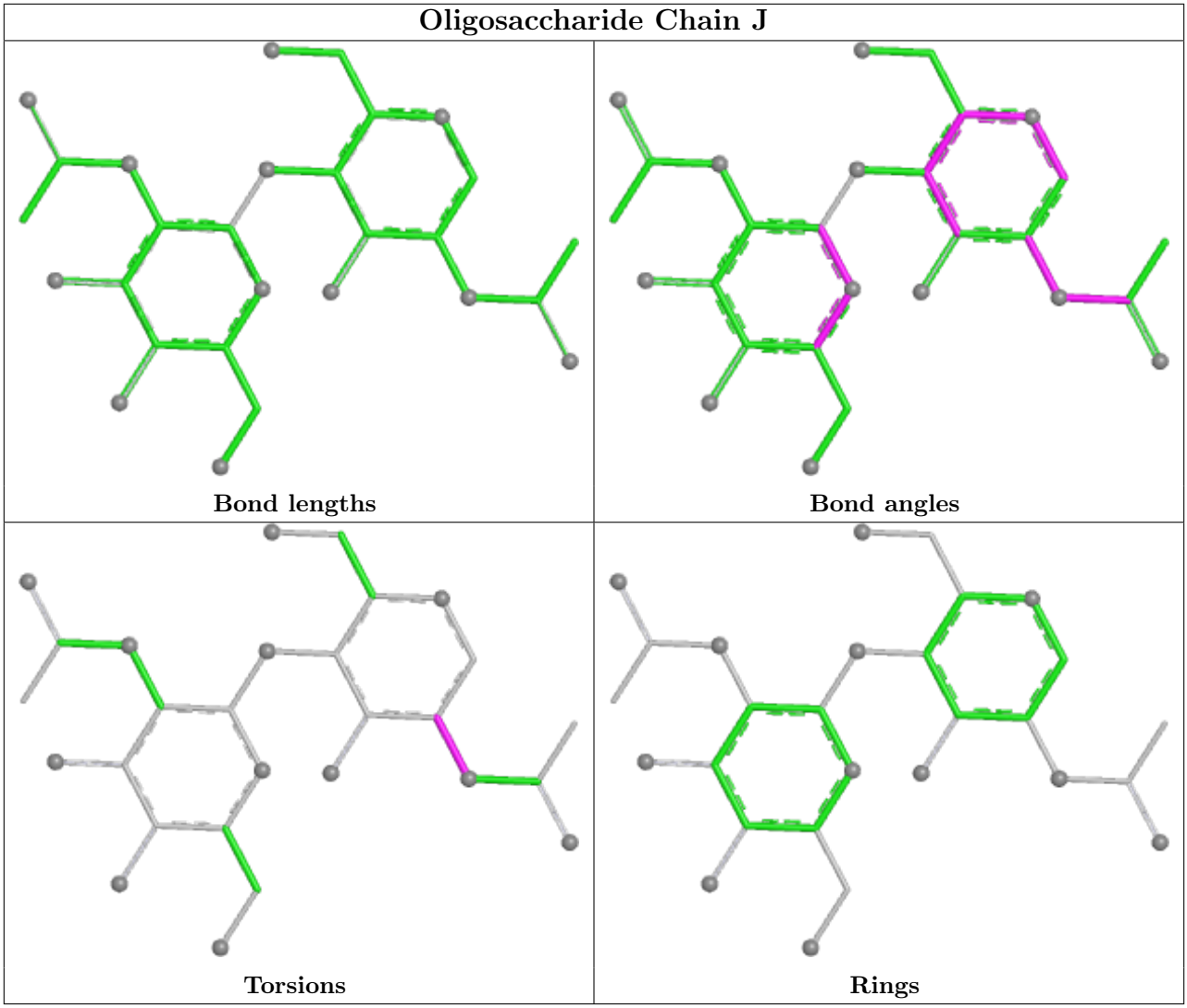
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
5	NAG	F	602	2	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	F	601	2	14,14,15	0.33	0	17,19,21	0.46	0
5	NAG	E	601	2	14,14,15	0.33	0	17,19,21	0.58	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	H	601	2	14,14,15	0.38	0	17,19,21	1.12	2 (11%)

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
5	NAG	F	602	2	-	0/6/23/26	0/1/1/1
5	NAG	F	601	2	-	2/6/23/26	0/1/1/1
5	NAG	E	601	2	-	0/6/23/26	0/1/1/1
5	NAG	H	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	601	NAG	C1-C2-N2	3.51	116.48	110.49
5	H	601	NAG	C2-N2-C7	2.59	126.59	122.90
5	E	601	NAG	C1-O5-C5	2.17	115.14	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	601	NAG	C1-C2-N2-C7
5	H	601	NAG	O5-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	F	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	601	NAG	2	0

5.7 Other polymers

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
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	504:SER	C	505:GLU	N	3.85

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

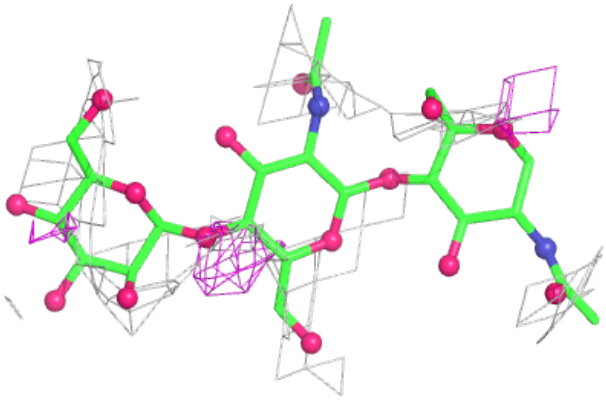
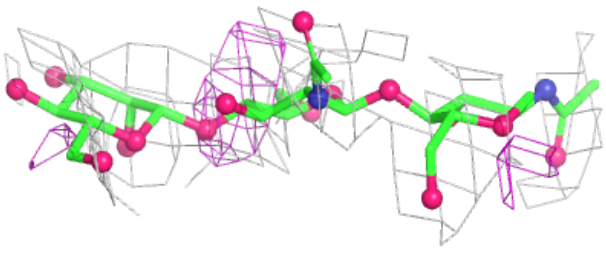
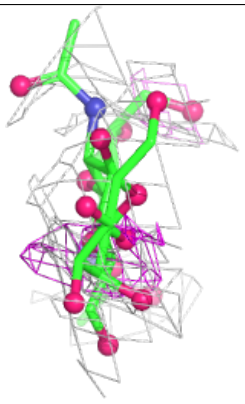
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

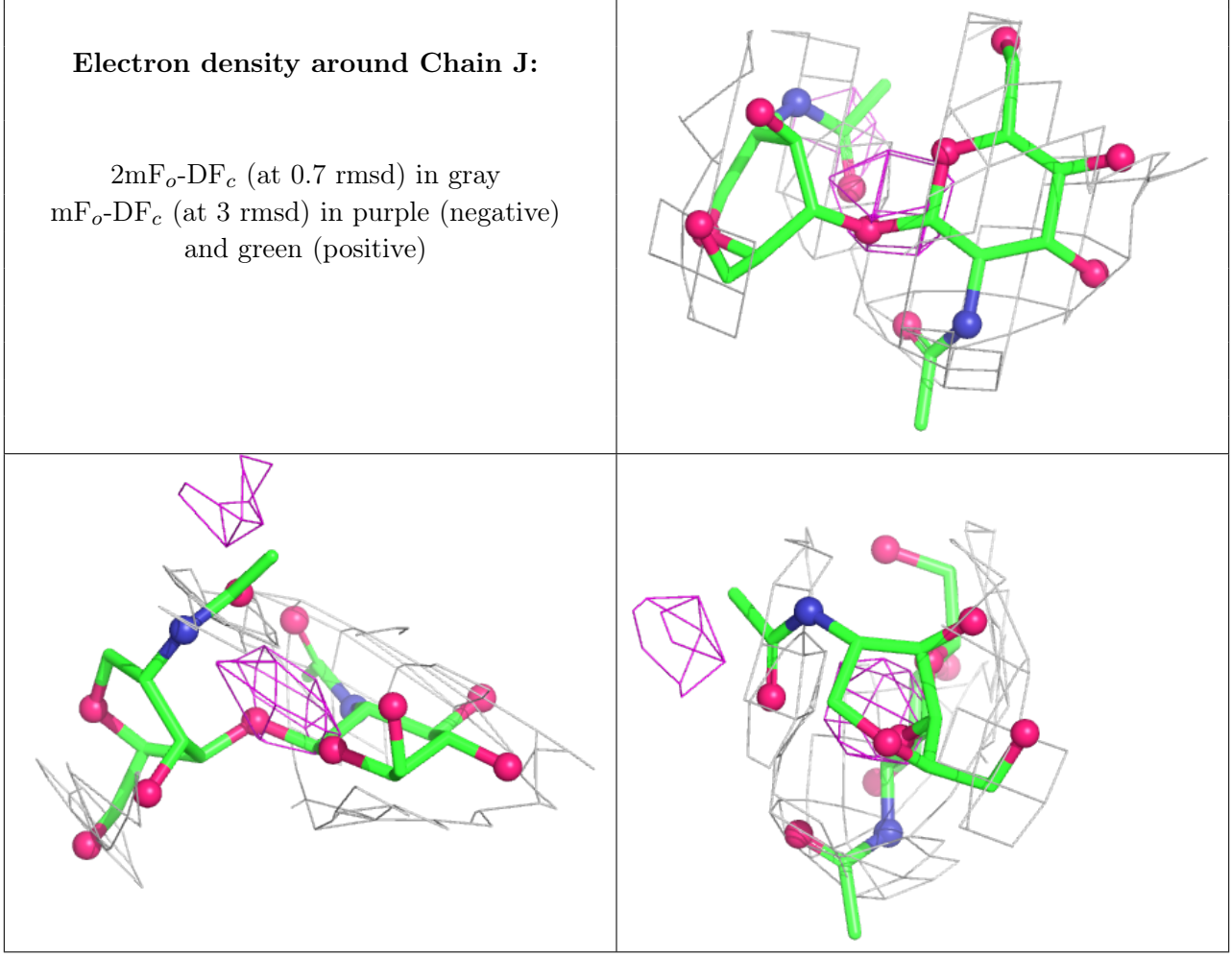
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around Chain J:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.