



wwPDB X-ray Structure Validation Summary Report ⓘ

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 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-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

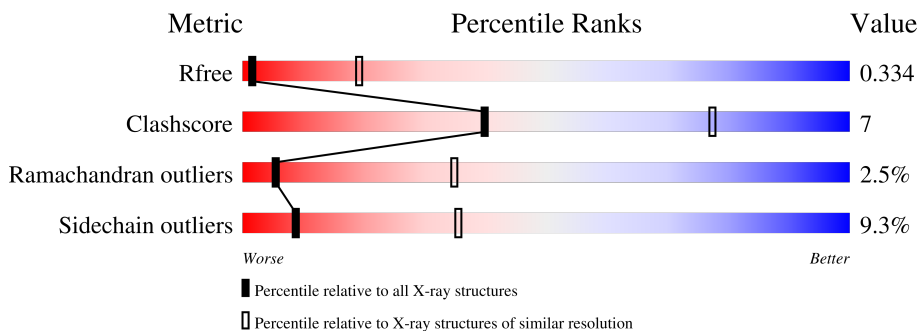
1 Overall quality at a glance

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.



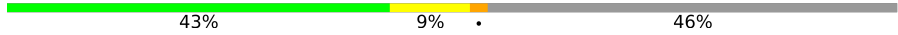

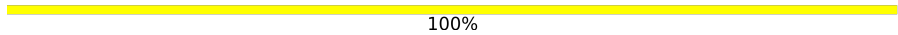
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

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 $\leq 5\%$.

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

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Mol	Chain	Length	Quality of chain
2	H	582	 43% 9% 46%
3	I	3	 33% 67%
4	J	2	 100%

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
			Total	C	N	O	S			
1	A	145	1050	665	181	196	8	0	0	0
1	B	134	937	595	164	169	9	0	0	0
1	C	133	935	594	159	175	7	0	0	0
1	D	134	1024	652	178	186	8	0	0	0

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

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

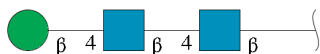
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Chain	Residue	Modelled	Actual	Comment	Reference
H	542	GLY	-	expression tag	UNP P36888
H	543	SER	-	expression tag	UNP P36888
H	544	SER	-	expression tag	UNP P36888
H	545	GLY	-	expression tag	UNP P36888
H	546	LEU	-	expression tag	UNP P36888
H	547	VAL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



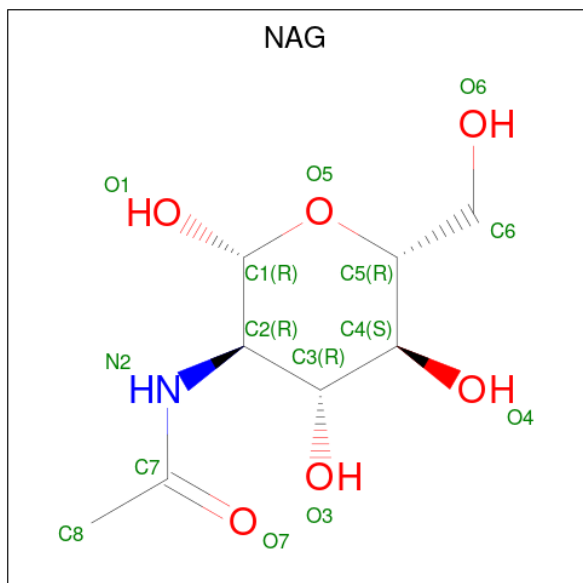
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	39	22	2	15	0	0	0

- 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: C₈H₁₅NO₆).



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: 



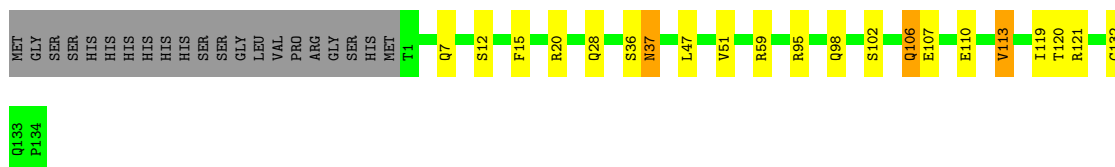
- Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain C: 



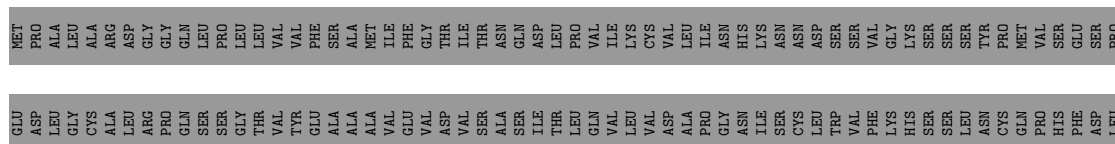
- Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain D: 



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

Chain E: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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.

The worst 5 of 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

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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	367	PHE
2	G	277	VAL
2	H	361	ILE
2	F	392	CYS
2	G	179	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	488	ASN
2	H	276	HIS
2	H	449	GLN
2	H	278	ASN
1	D	106	GLN

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](#)

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.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

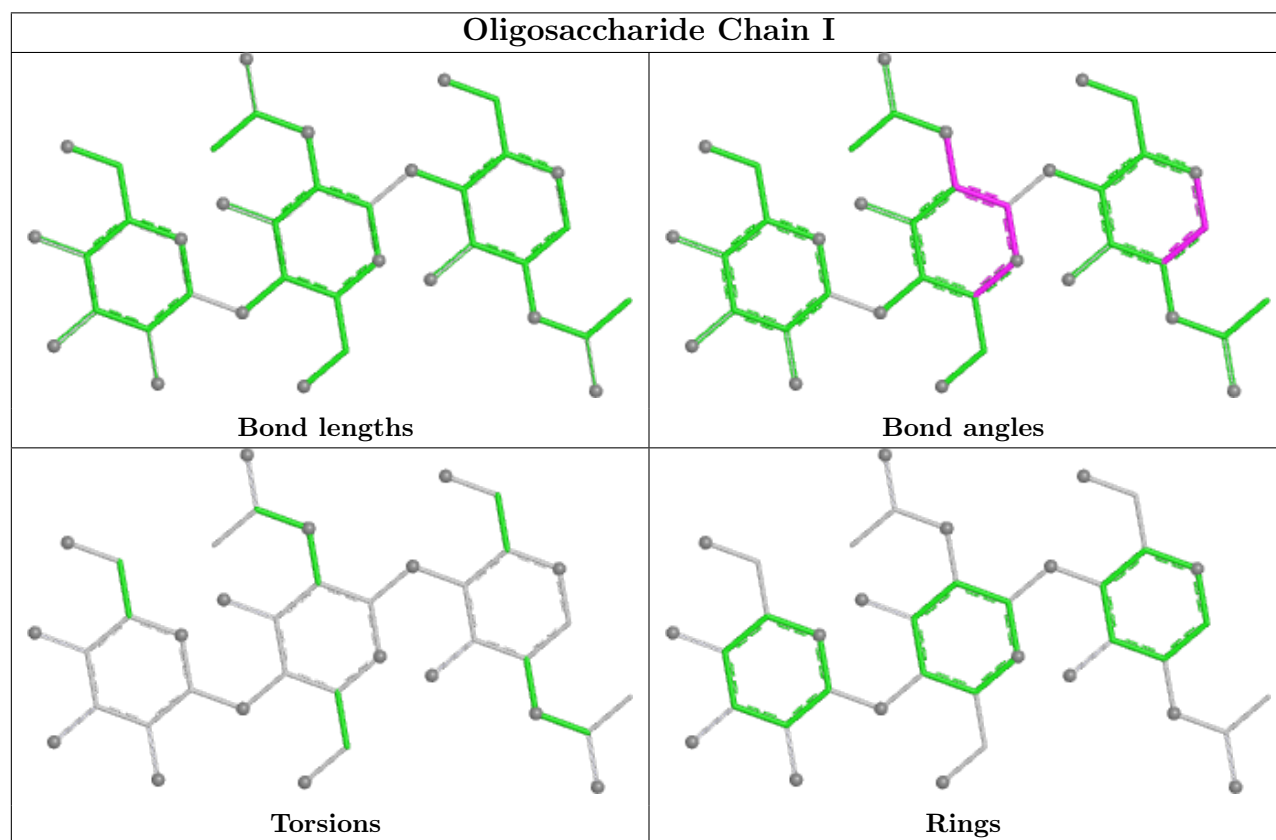
All (1) torsion outliers are listed below:

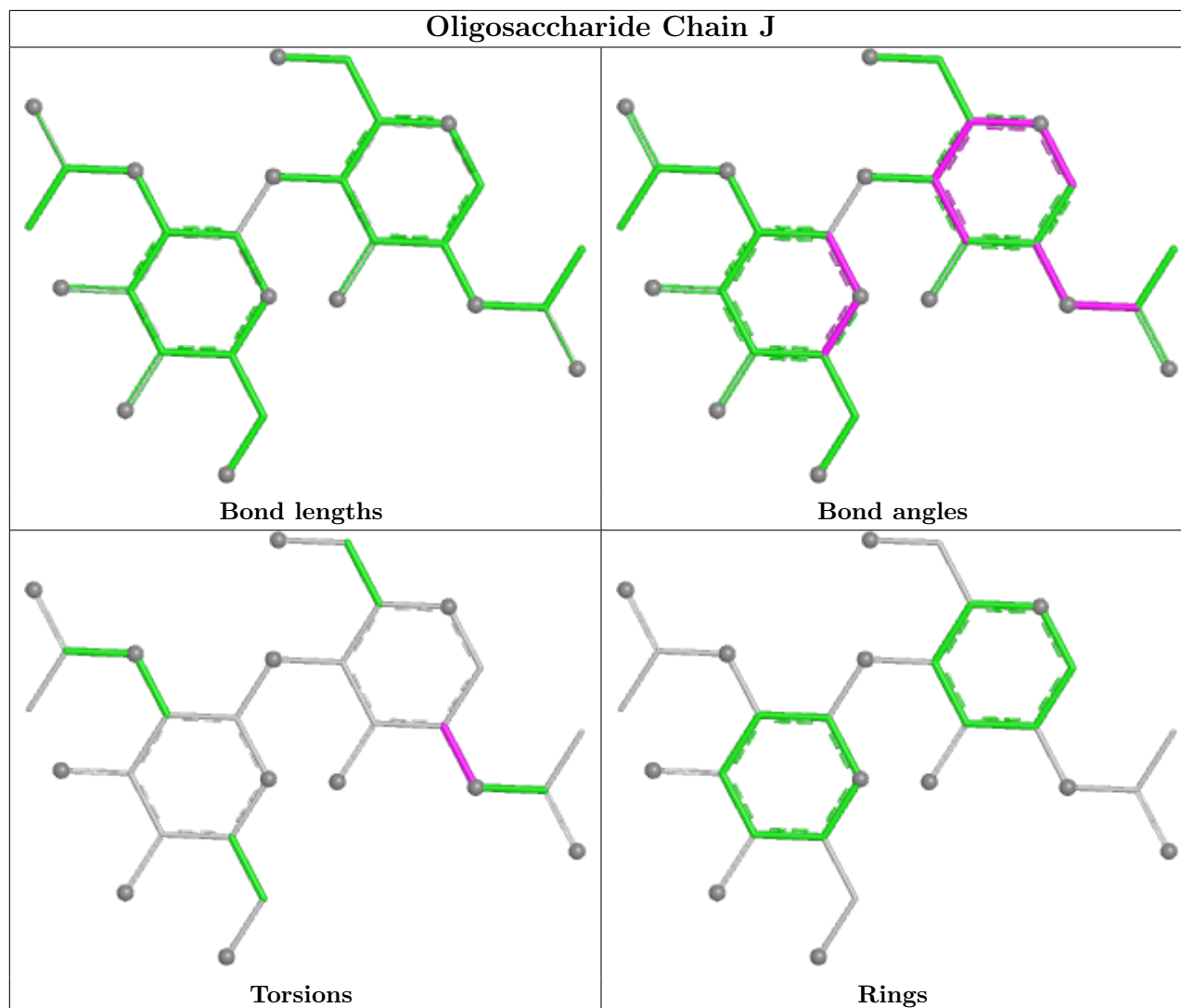
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C1-C2-N2-C7

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.





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(°)	Ideal(°)
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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

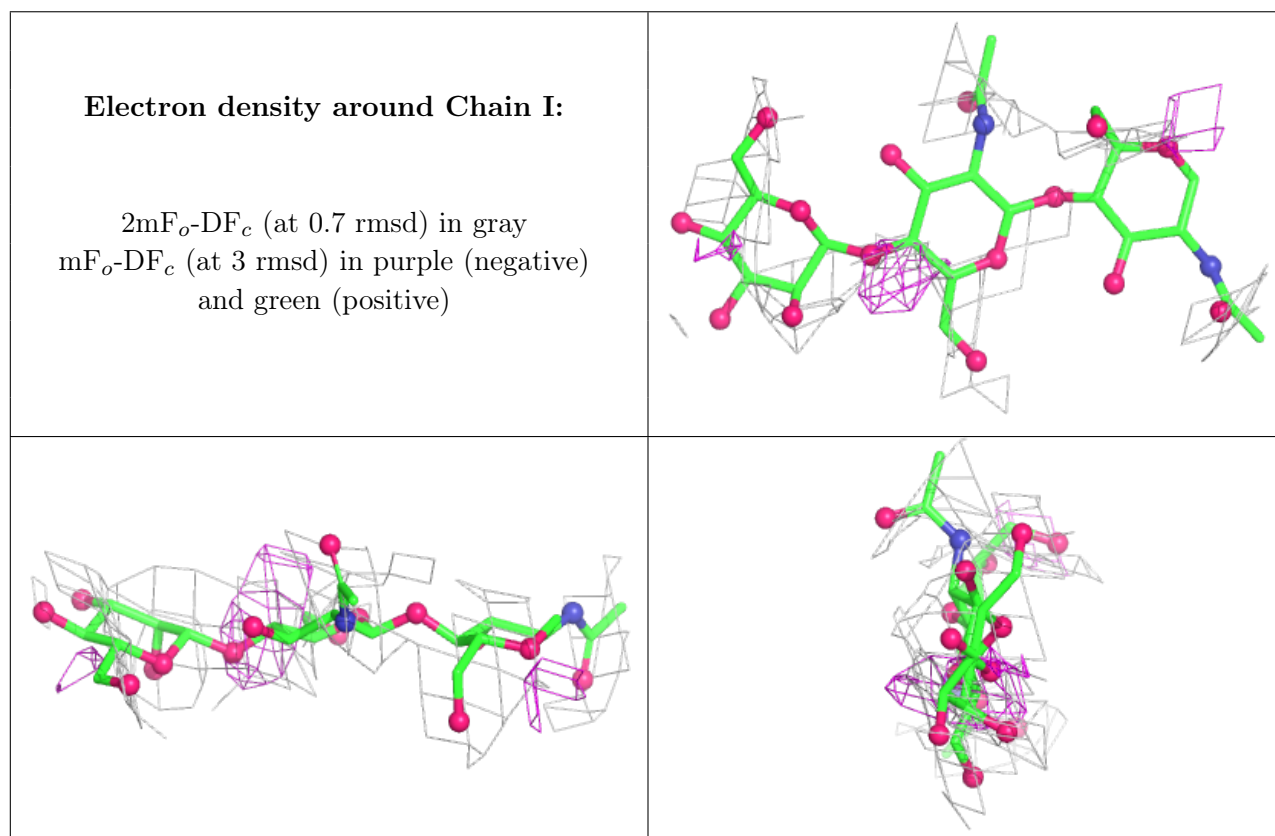
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

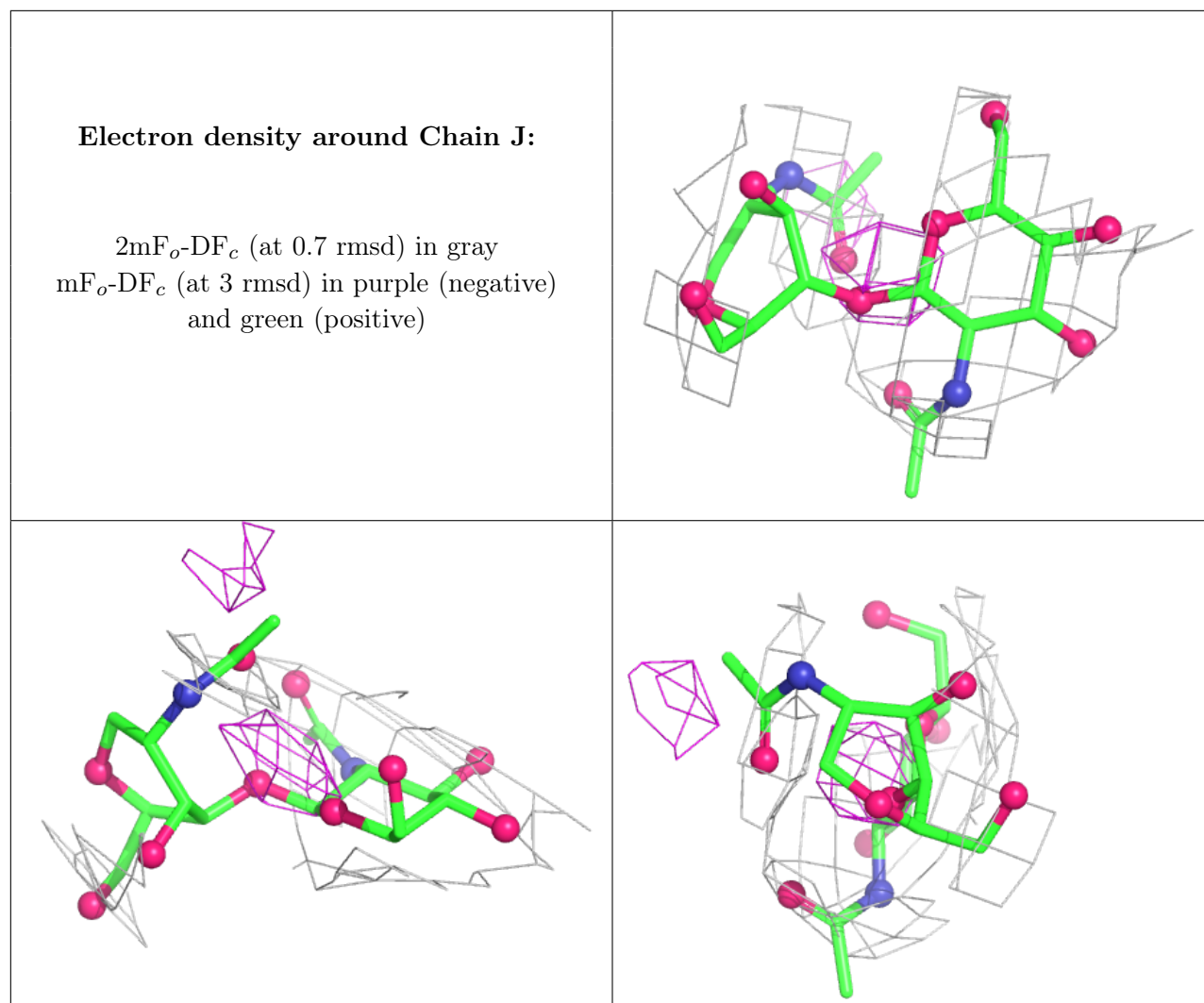
Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

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.





6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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