



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:56 PM UTC

PDB ID : 7QDP / pdb_00007qdp
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 ⓘ symbol.

The types of validation reports are described at

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

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

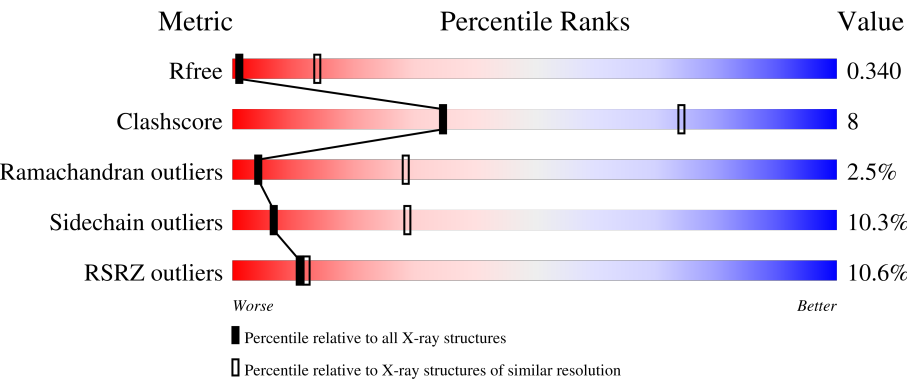
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	10% 83%10%6%
1	B	155	5% 77%9%14%
1	C	155	7% 77%9%14%
1	D	155	10% 73%12%14%
2	E	582	7% 46%9%43%

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Mol	Chain	Length	Quality of chain
2	F	582	6% 54% 15% • 29%
2	G	582	9% 48% 11% • 39%
2	H	582	6% 42% 10% • 46%
3	I	3	33% 67%
4	J	2	100%

2 Entry composition

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

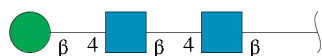
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Chain	Residue	Modelled	Actual	Comment	Reference
H	542	GLY	-	expression tag	UNP P36888
H	543	SER	-	expression tag	UNP P36888
H	544	SER	-	expression tag	UNP P36888
H	545	GLY	-	expression tag	UNP P36888
H	546	LEU	-	expression tag	UNP P36888
H	547	VAL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



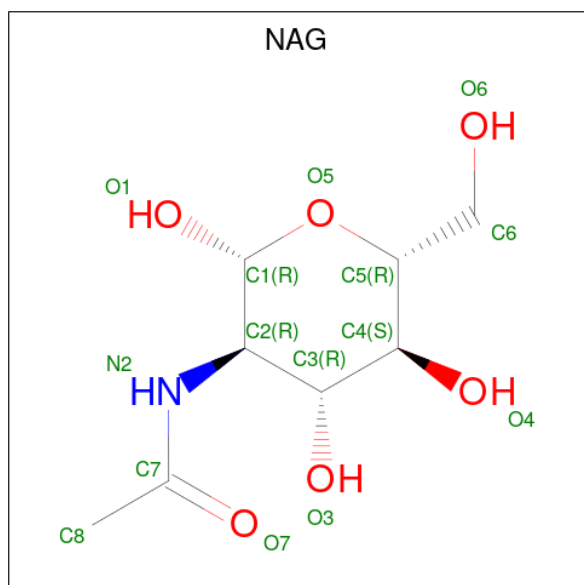
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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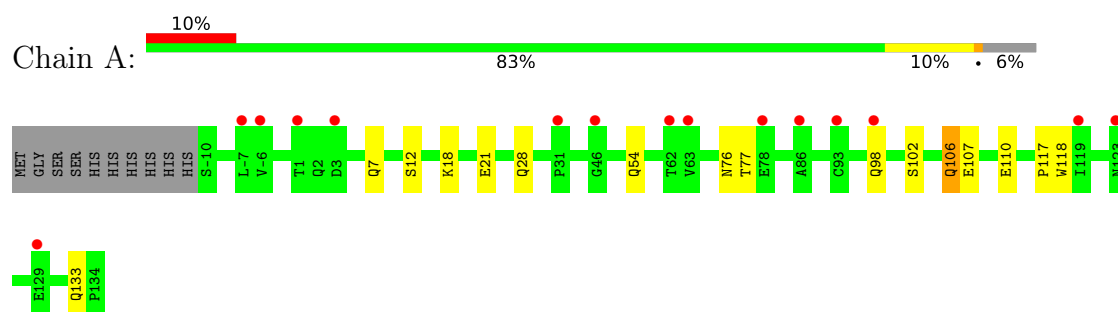
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

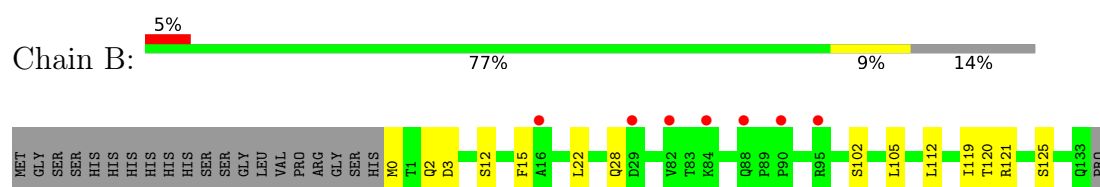
3 Residue-property plots [i](#)

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 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.

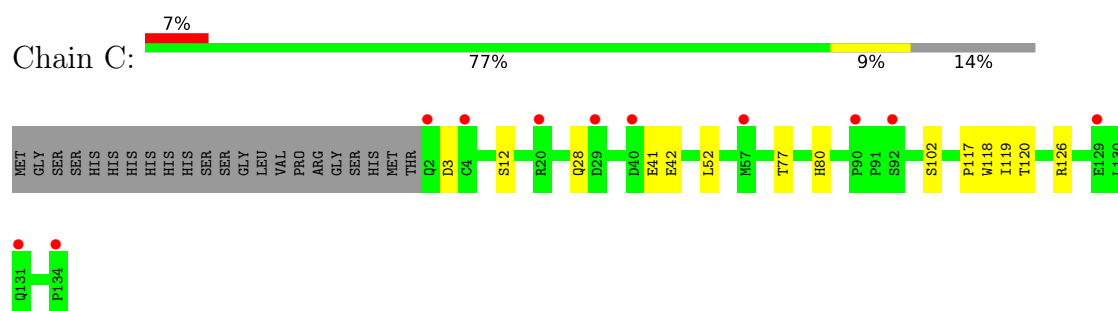
- Molecule 1: Fms-related tyrosine kinase 3 ligand



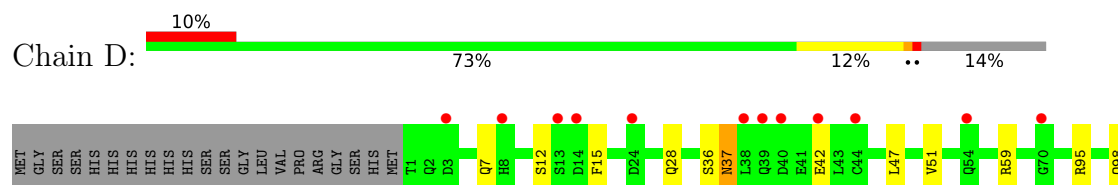
- Molecule 1: Fms-related tyrosine kinase 3 ligand

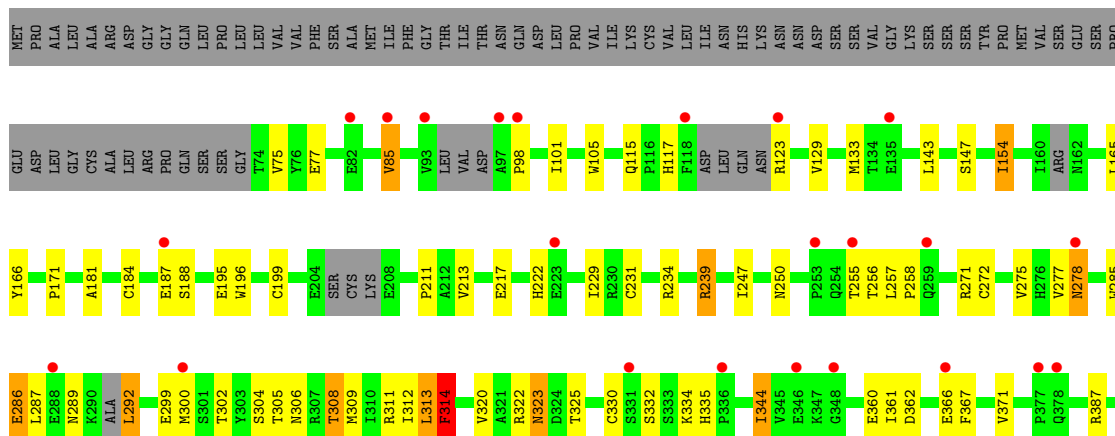


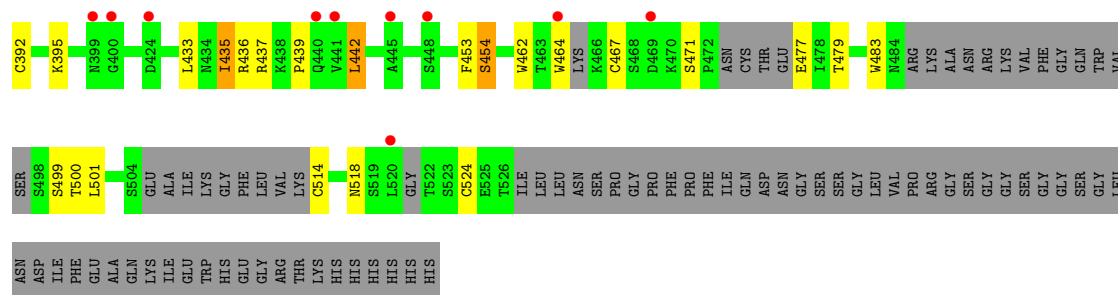
- Molecule 1: Fms-related tyrosine kinase 3 ligand



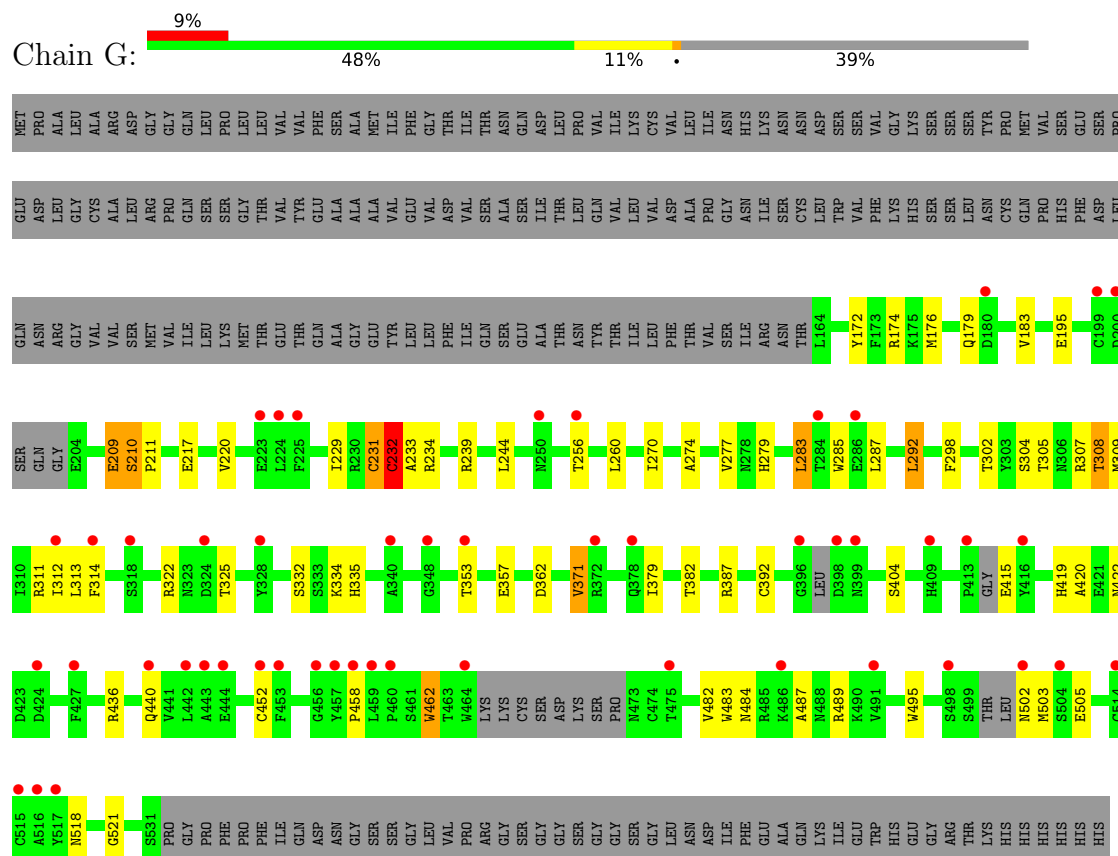
- Molecule 1: Fms-related tyrosine kinase 3 ligand



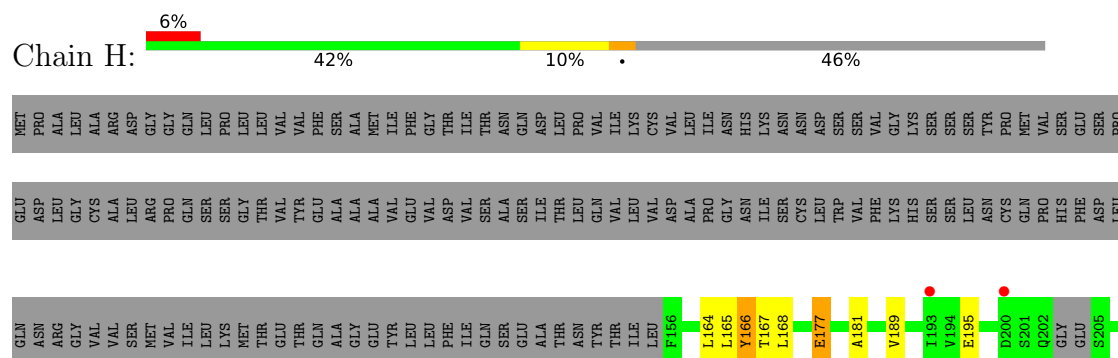


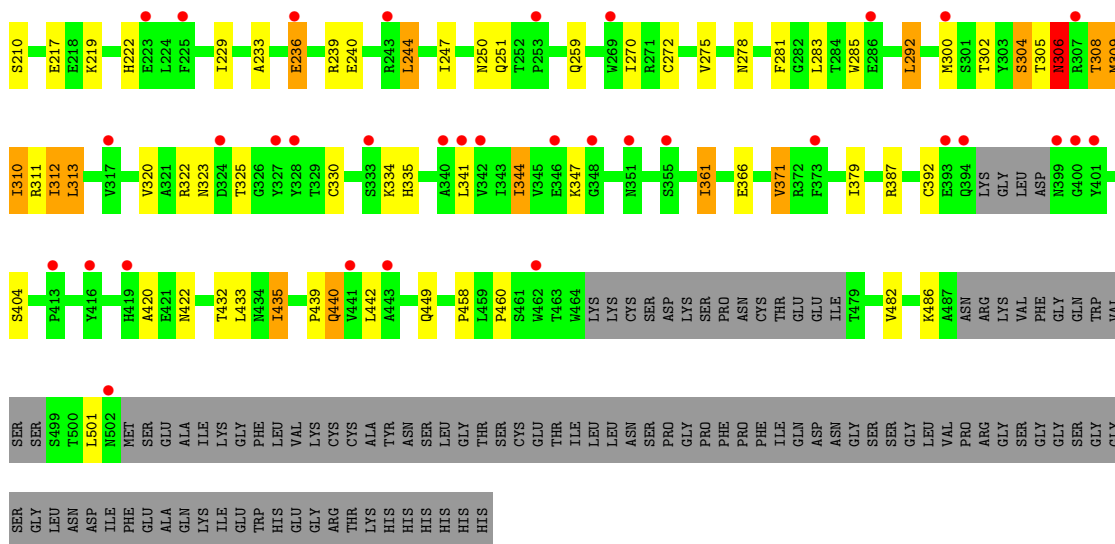


• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

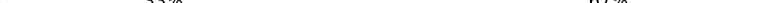


• Molecule 2: Receptor-type tyrosine-protein kinase FLT3





- 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:  33% 67%



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

Chain J: 100%



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 0.319 , 0.340	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)	0.26 , 217.2	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	0.90	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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/1071	0.95	0/1467
1	B	0.59	0/956	1.00	0/1313
1	C	0.62	0/956	1.00	0/1314
1	D	0.60	0/1045	1.01	1/1423 (0.1%)
2	E	0.71	0/2205	1.11	5/3033 (0.2%)
2	F	0.73	0/2838	1.13	9/3887 (0.2%)
2	G	0.69	0/2440	1.11	6/3343 (0.2%)
2	H	0.75	0/2146	1.17	14/2954 (0.5%)
All	All	0.69	0/13657	1.09	35/18734 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	2

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	323	ASN	CA-CB-CG	11.51	124.11	112.60
2	F	323	ASN	OD1-CG-ND2	-7.74	114.86	122.60
2	F	314	PHE	CA-CB-CG	7.32	121.12	113.80
2	E	314	PHE	CA-CB-CG	7.14	120.94	113.80
2	F	323	ASN	CA-CB-CG	6.64	119.24	112.60
2	G	462	TRP	N-CA-C	6.36	119.13	110.55
2	H	322	ARG	CA-C-N	5.97	128.56	120.38
2	H	322	ARG	C-N-CA	5.97	128.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	521	GLY	N-CA-C	5.96	121.72	111.47
2	G	314	PHE	CA-CB-CG	5.79	119.59	113.80
2	E	521	GLY	N-CA-C	5.68	121.32	110.86
2	F	287	LEU	N-CA-C	-5.65	103.99	111.96
2	G	298	PHE	CA-CB-CG	5.62	119.42	113.80
2	E	462	TRP	N-CA-C	5.61	118.78	110.48
1	D	113	VAL	N-CA-CB	5.55	117.04	110.55
2	H	281	PHE	CA-CB-CG	5.47	119.27	113.80
2	H	323	ASN	CB-CG-ND2	-5.47	108.20	116.40
2	H	306	ASN	OD1-CG-ND2	-5.37	117.23	122.60
2	F	211	PRO	CA-C-N	5.33	128.31	119.35
2	F	211	PRO	C-N-CA	5.33	128.31	119.35
2	H	432	THR	CA-C-N	5.32	131.70	121.54
2	H	432	THR	C-N-CA	5.32	131.70	121.54
2	G	322	ARG	CA-C-N	5.24	127.56	120.38
2	G	322	ARG	C-N-CA	5.24	127.56	120.38
2	H	236	GLU	CA-C-N	5.21	127.26	120.28
2	H	236	GLU	C-N-CA	5.21	127.26	120.28
2	H	251	GLN	CA-C-N	5.20	128.04	120.51
2	H	251	GLN	C-N-CA	5.20	128.04	120.51
2	F	323	ASN	CB-CG-ND2	5.14	124.11	116.40
2	E	322	ARG	CA-C-N	5.13	127.41	120.38
2	E	322	ARG	C-N-CA	5.13	127.41	120.38
2	F	322	ARG	CA-C-N	5.09	127.36	120.38
2	F	322	ARG	C-N-CA	5.09	127.36	120.38
2	H	304	SER	CA-C-N	5.01	131.10	121.54
2	H	304	SER	C-N-CA	5.01	131.10	121.54

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 ⓘ

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	37	0
2	H	2102	0	1641	28	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	185	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 8.

All (185) 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
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
2:G:462:TRP:CD1	2:G:502:ASN:HD22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:272:CYS:HG	2:H:330:CYS:HG	1.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:272:CYS:HG	2:F:330:CYS:HG	1.56	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:F:514:CYS:N	2:F:524:CYS:HG	2.06	0.53
2:E:276:HIS:CE1	2:E:278:ASN:ND2	2.77	0.52
1:D:7:GLN:H	1:D:7:GLN:CD	2.17	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
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
2:G:176:MET:HE2	2:G:183:VAL:HG21	1.90	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:H	1:D:7:GLN:NE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:300:MET:HE3	2:F:312:ILE:HD12	1.98	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:462:TRP:CG	2:G:502:ASN:HD22	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:482:VAL:C	2:G:483:TRP:CD1	2.97	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: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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	143/155 (92%)	133 (93%)	10 (7%)	0	100	100
1	B	132/155 (85%)	126 (96%)	5 (4%)	1 (1%)	16	48
1	C	131/155 (84%)	126 (96%)	4 (3%)	1 (1%)	16	48
1	D	132/155 (85%)	127 (96%)	5 (4%)	0	100	100
2	E	316/582 (54%)	277 (88%)	32 (10%)	7 (2%)	5	31
2	F	392/582 (67%)	325 (83%)	54 (14%)	13 (3%)	3	25
2	G	340/582 (58%)	289 (85%)	40 (12%)	11 (3%)	3	25
2	H	307/582 (53%)	254 (83%)	38 (12%)	15 (5%)	1	17
All	All	1893/2948 (64%)	1657 (88%)	188 (10%)	48 (2%)	4	29

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
2	H	305	THR
2	H	334	LYS
2	H	433	LEU
2	H	435	ILE
2	H	440	GLN
2	H	458	PRO

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Mol	Chain	Res	Type
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 ⓘ

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%)	99 (95%)	5 (5%)	23	48
1	B	84/142 (59%)	82 (98%)	2 (2%)	43	61
1	C	86/142 (61%)	82 (95%)	4 (5%)	23	48
1	D	108/142 (76%)	99 (92%)	9 (8%)	10	35
2	E	161/515 (31%)	141 (88%)	20 (12%)	4	22
2	F	217/515 (42%)	189 (87%)	28 (13%)	4	21
2	G	188/515 (36%)	168 (89%)	20 (11%)	6	27
2	H	157/515 (30%)	131 (83%)	26 (17%)	2	14
All	All	1105/2628 (42%)	991 (90%)	114 (10%)	7	29

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

Mol	Chain	Res	Type
1	A	7	GLN
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	36	SER
1	D	37	ASN
1	D	42	GLU
1	D	59	ARG
1	D	98	GLN
1	D	106	GLN
1	D	113	VAL
1	D	121	ARG
1	D	132	CYS
2	E	168	LEU
2	E	222	HIS
2	E	229	ILE
2	E	260	LEU
2	E	270	ILE
2	E	277	VAL
2	E	287	LEU

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Mol	Chain	Res	Type
2	E	292	LEU
2	E	307	ARG
2	E	308	THR
2	E	309	MET
2	E	312	ILE
2	E	344	ILE
2	E	345	VAL
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	F	85	VAL
2	F	129	VAL
2	F	154	ILE
2	F	165	LEU
2	F	166	TYR
2	F	196	TRP
2	F	229	ILE
2	F	239	ARG
2	F	286	GLU
2	F	292	LEU
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
2	F	433	LEU
2	F	442	LEU
2	F	499	SER
2	G	179	GLN

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Mol	Chain	Res	Type
2	G	209	GLU
2	G	229	ILE
2	G	232	CYS
2	G	244	LEU
2	G	260	LEU
2	G	270	ILE
2	G	277	VAL
2	G	283	LEU
2	G	287	LEU
2	G	292	LEU
2	G	308	THR
2	G	309	MET
2	G	312	ILE
2	G	325	THR
2	G	357	GLU
2	G	371	VAL
2	G	392	CYS
2	G	440	GLN
2	G	518	ASN
2	H	164	LEU
2	H	165	LEU
2	H	177	GLU
2	H	219	LYS
2	H	229	ILE
2	H	244	LEU
2	H	259	GLN
2	H	270	ILE
2	H	278	ASN
2	H	283	LEU
2	H	292	LEU
2	H	308	THR
2	H	309	MET
2	H	310	ILE
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	366	GLU
2	H	371	VAL
2	H	392	CYS

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Mol	Chain	Res	Type
2	H	440	GLN
2	H	442	LEU
2	H	449	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	8	HIS
1	A	76	ASN
1	A	106	GLN
1	B	39	GLN
1	B	111	GLN
1	B	131	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	276	HIS
2	E	278	ASN
2	E	351	ASN
2	E	378	GLN
2	E	408	ASN
2	F	109	HIS
2	F	117	HIS
2	F	202	GLN
2	F	250	ASN
2	F	502	ASN
2	F	518	ASN
2	G	179	GLN
2	G	278	ASN
2	G	422	ASN
2	G	488	ASN
2	G	494	GLN
2	H	222	HIS
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	3,2	14,14,15	0.34	0	17,19,21	1.18	1 (5%)
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	1.10	3 (17%)
3	BMA	I	3	3	11,11,12	0.32	0	15,15,17	0.42	0
4	NAG	J	1	4,2	14,14,15	0.47	0	17,19,21	1.64	4 (23%)
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.74	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	3,2	-	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	4,2	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	4.84	118.67	112.19
3	I	1	NAG	O5-C1-C2	-3.74	105.50	111.29
4	J	2	NAG	C1-O5-C5	2.88	116.05	112.19
3	I	2	NAG	C1-C2-N2	2.74	114.75	110.43
4	J	1	NAG	C2-N2-C7	2.72	126.55	122.90
3	I	2	NAG	C1-O5-C5	2.61	115.69	112.19
3	I	2	NAG	O5-C1-C2	-2.25	107.80	111.29
4	J	1	NAG	C3-C4-C5	2.21	114.25	110.23
4	J	1	NAG	C1-C2-N2	2.19	113.88	110.43

There are no chirality outliers.

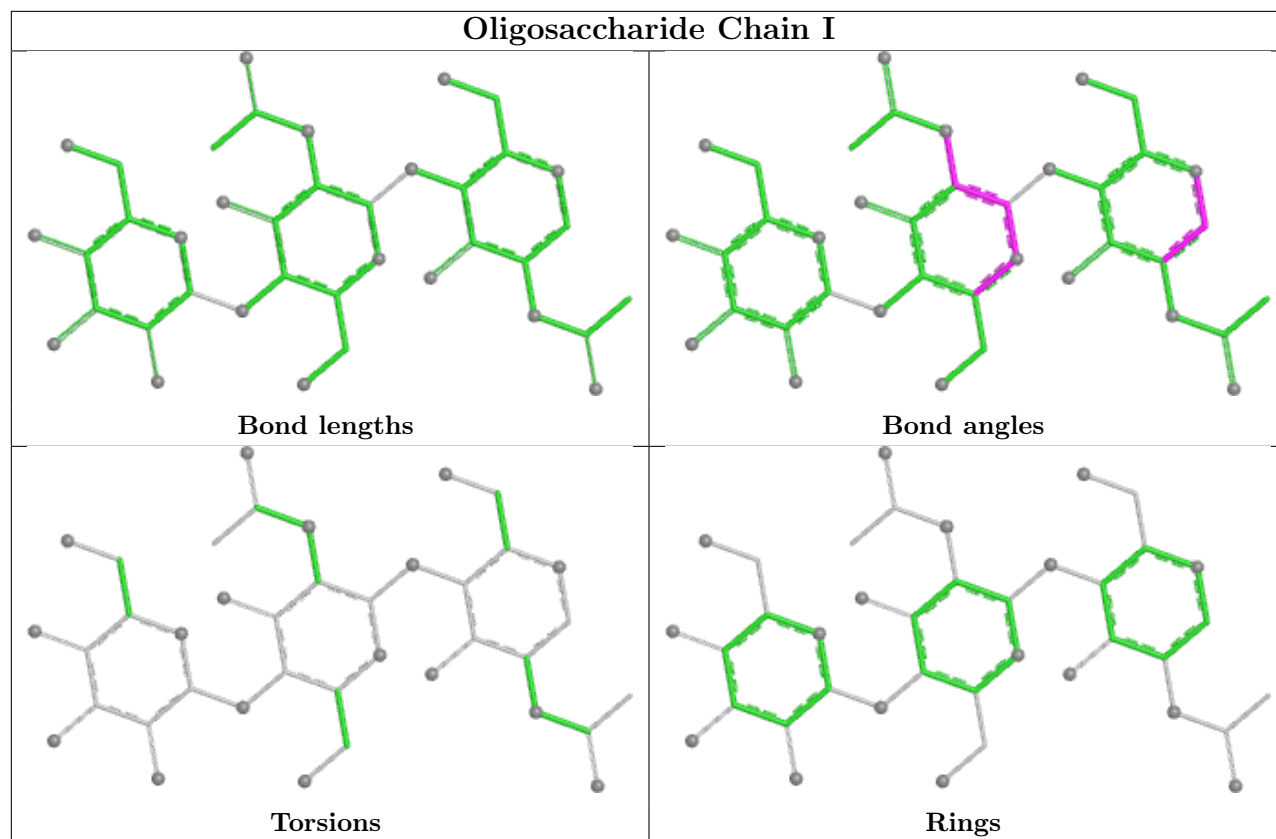
All (2) torsion outliers are listed below:

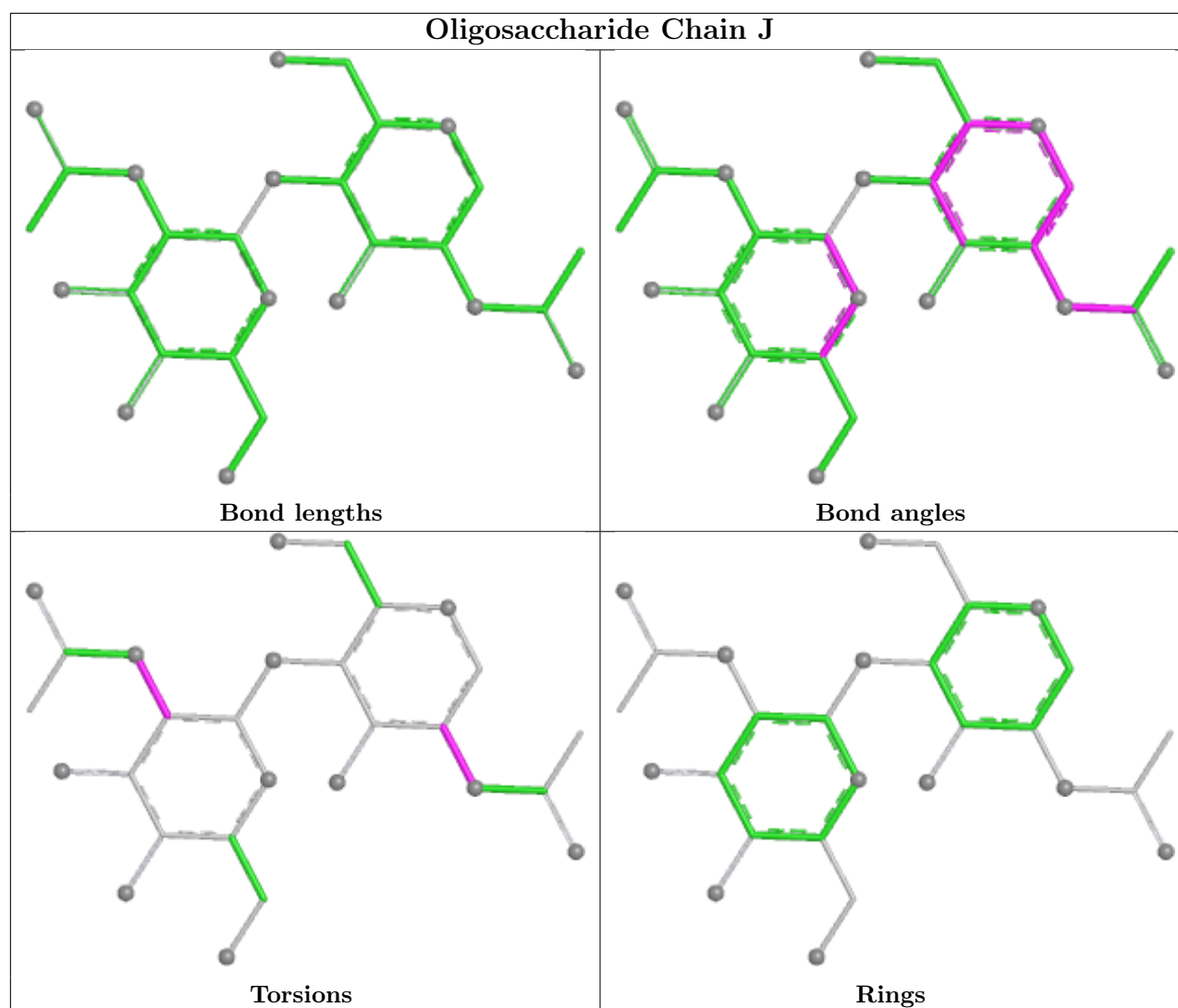
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7

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	H	601	2	14,14,15	0.40	0	17,19,21	1.21	2 (11%)
5	NAG	F	602	2	14,14,15	0.31	0	17,19,21	0.42	0
5	NAG	E	601	2	14,14,15	0.35	0	17,19,21	0.60	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	601	2	14,14,15	0.34	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
5	NAG	H	601	2	-	2/6/23/26	0/1/1/1
5	NAG	F	602	2	-	0/6/23/26	0/1/1/1
5	NAG	E	601	2	-	0/6/23/26	0/1/1/1
5	NAG	F	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	3.84	116.48	110.43
5	H	601	NAG	C2-N2-C7	2.75	126.59	122.90
5	E	601	NAG	C1-O5-C5	2.20	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	145/155 (93%)	0.81	15 (10%) 12 12	190, 214, 264, 266	0
1	B	134/155 (86%)	0.88	7 (5%) 33 22	181, 205, 234, 242	0
1	C	133/155 (85%)	0.88	11 (8%) 17 14	173, 194, 228, 239	0
1	D	134/155 (86%)	1.03	16 (11%) 9 10	169, 198, 235, 244	0
2	E	332/582 (57%)	0.99	40 (12%) 9 10	205, 262, 285, 289	0
2	F	413/582 (70%)	0.82	33 (7%) 18 14	136, 257, 287, 293	1 (0%)
2	G	352/582 (60%)	1.08	50 (14%) 6 8	187, 262, 284, 288	0
2	H	316/582 (54%)	0.94	36 (11%) 10 11	109, 245, 291, 298	1 (0%)
All	All	1959/2948 (66%)	0.94	208 (10%) 11 12	109, 239, 285, 298	2 (0%)

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	457	TYR	6.4
1	D	134	PRO	5.9
2	F	464	TRP	5.5
2	H	399	ASN	5.1
2	G	398	ASP	4.7
2	G	452	CYS	4.6
2	E	452	CYS	4.2
2	H	324	ASP	4.0
1	C	129	GLU	4.0
2	F	445	ALA	4.0
1	C	57	MET	3.9
2	G	413	PRO	3.9
2	H	413	PRO	3.9
2	G	458	PRO	3.7
2	G	427	PHE	3.6
2	H	340	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	400	GLY	3.5
2	F	253	PRO	3.5
1	C	134	PRO	3.5
2	H	443	ALA	3.5
2	E	524	CYS	3.4
2	G	456	GLY	3.4
2	G	340	ALA	3.4
2	G	486	LYS	3.4
2	H	394	GLN	3.4
2	E	512	VAL	3.4
2	E	458	PRO	3.3
2	H	333	SER	3.3
1	A	3	ASP	3.2
2	E	304	SER	3.2
2	F	259	GLN	3.2
2	H	307	ARG	3.2
2	F	118	PHE	3.2
2	G	502	ASN	3.2
2	F	448	SER	3.1
2	H	400	GLY	3.1
2	E	305	THR	3.1
2	F	399	ASN	3.1
1	D	38	LEU	3.1
1	A	129	GLU	3.1
1	A	63	VAL	3.0
1	A	62	THR	3.0
1	B	88	GLN	3.0
2	G	504	SER	3.0
2	H	317	VAL	2.9
2	E	256	THR	2.9
2	F	255	THR	2.9
2	E	443	ALA	2.9
2	G	464	TRP	2.9
2	E	500	THR	2.9
2	E	498	SER	2.9
2	F	331	SER	2.9
2	E	460	PRO	2.9
2	H	348	GLY	2.8
2	H	269	TRP	2.8
1	C	92	SER	2.8
2	H	441	VAL	2.8
2	G	443	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	342	VAL	2.8
2	G	223	GLU	2.8
2	E	391	PRO	2.8
1	A	-7	LEU	2.8
1	D	42	GLU	2.7
2	G	409	HIS	2.7
2	E	337	SER	2.7
1	D	14	ASP	2.7
2	F	469	ASP	2.7
2	H	243[A]	ARG	2.7
1	A	119	ILE	2.7
2	E	392	CYS	2.7
2	H	351	ASN	2.7
2	G	440	GLN	2.6
2	E	526	THR	2.6
1	D	129	GLU	2.6
2	E	261	PHE	2.6
2	G	225	PHE	2.6
2	G	515	CYS	2.6
1	D	8	HIS	2.6
2	H	401	TYR	2.6
1	B	84	LYS	2.6
2	F	97	ALA	2.6
2	G	372	ARG	2.6
1	D	132	CYS	2.6
2	E	459	LEU	2.6
2	G	453	PHE	2.6
2	E	255	THR	2.5
2	F	93	VAL	2.5
1	D	3	ASP	2.5
2	E	224	LEU	2.5
1	B	16	ALA	2.5
2	G	378	GLN	2.5
1	B	95	ARG	2.5
2	E	515	CYS	2.5
2	E	423	ASP	2.5
2	G	200	ASP	2.5
2	H	502	ASN	2.5
2	H	253	PRO	2.5
2	G	328	TYR	2.5
2	G	514	CYS	2.5
2	E	189	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	85	VAL	2.5
2	H	225	PHE	2.5
2	E	244	LEU	2.5
2	F	135	GLU	2.4
2	F	98	PRO	2.4
1	D	40	ASP	2.4
2	G	353	THR	2.4
2	F	520	LEU	2.4
2	F	400	GLY	2.4
1	B	82	VAL	2.4
2	H	416	TYR	2.4
2	H	341	LEU	2.4
1	A	86	ALA	2.4
1	A	31	PRO	2.4
2	F	424	ASP	2.4
2	E	499	SER	2.4
2	G	256	THR	2.4
2	G	416	TYR	2.4
2	H	393	GLU	2.4
1	A	46	GLY	2.4
2	F	348	GLY	2.4
2	G	396	GLY	2.4
2	F	123	ARG	2.4
2	H	419	HIS	2.3
2	G	491	VAL	2.3
1	C	20	ARG	2.3
1	B	29	ASP	2.3
1	C	131	GLN	2.3
2	G	286	GLU	2.3
2	G	348	GLY	2.3
1	B	90	PRO	2.3
1	C	90	PRO	2.3
1	D	13	SER	2.3
2	G	498	SER	2.3
1	A	123	ASN	2.3
2	F	82	GLU	2.3
1	A	1	THR	2.3
1	A	98	GLN	2.3
1	D	39	GLN	2.3
2	H	223	GLU	2.3
2	H	355	SER	2.3
2	F	223	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	324	ASP	2.3
2	E	289	ASN	2.2
2	G	399	ASN	2.2
2	H	236	GLU	2.2
1	C	2	GLN	2.2
2	F	300	MET	2.2
2	F	288	GLU	2.2
1	A	93	CYS	2.2
1	C	4	CYS	2.2
2	G	312	ILE	2.2
2	G	314	PHE	2.2
2	E	464	TRP	2.2
2	E	258	PRO	2.2
1	C	29	ASP	2.2
2	E	445	ALA	2.2
2	F	378	GLN	2.2
2	G	318	SER	2.2
2	H	346	GLU	2.2
2	E	513	LYS	2.2
2	G	250	ASN	2.2
1	D	24	ASP	2.1
1	D	103	ARG	2.1
2	H	327	TYR	2.1
2	F	346	GLU	2.1
2	F	377	PRO	2.1
2	E	473	ASN	2.1
2	E	485	ARG	2.1
2	G	424	ASP	2.1
1	D	44	CYS	2.1
2	E	328	TYR	2.1
2	H	328	TYR	2.1
2	H	286	GLU	2.1
2	G	284	THR	2.1
2	E	201	SER	2.1
2	G	517	TYR	2.1
2	G	460	PRO	2.1
2	G	459	LEU	2.1
2	E	451	SER	2.1
2	F	278	ASN	2.1
2	H	193	ILE	2.1
2	H	373	PHE	2.1
2	F	336	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	78	GLU	2.1
2	E	475	THR	2.1
2	G	442	LEU	2.1
2	G	180	ASP	2.1
2	H	462	TRP	2.1
2	F	187	GLU	2.1
2	G	475	THR	2.1
2	G	199	CYS	2.1
1	D	54	GLN	2.1
2	E	484	ASN	2.1
2	G	224	LEU	2.1
1	D	70	GLY	2.0
1	C	40	ASP	2.0
2	H	200	ASP	2.0
2	G	516	ALA	2.0
2	E	232	CYS	2.0
2	F	441	VAL	2.0
2	E	300	MET	2.0
2	F	366[A]	GLU	2.0
2	G	444	GLU	2.0
1	A	-6	VAL	2.0
2	F	440	GLN	2.0
2	H	300	MET	2.0
2	E	444	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

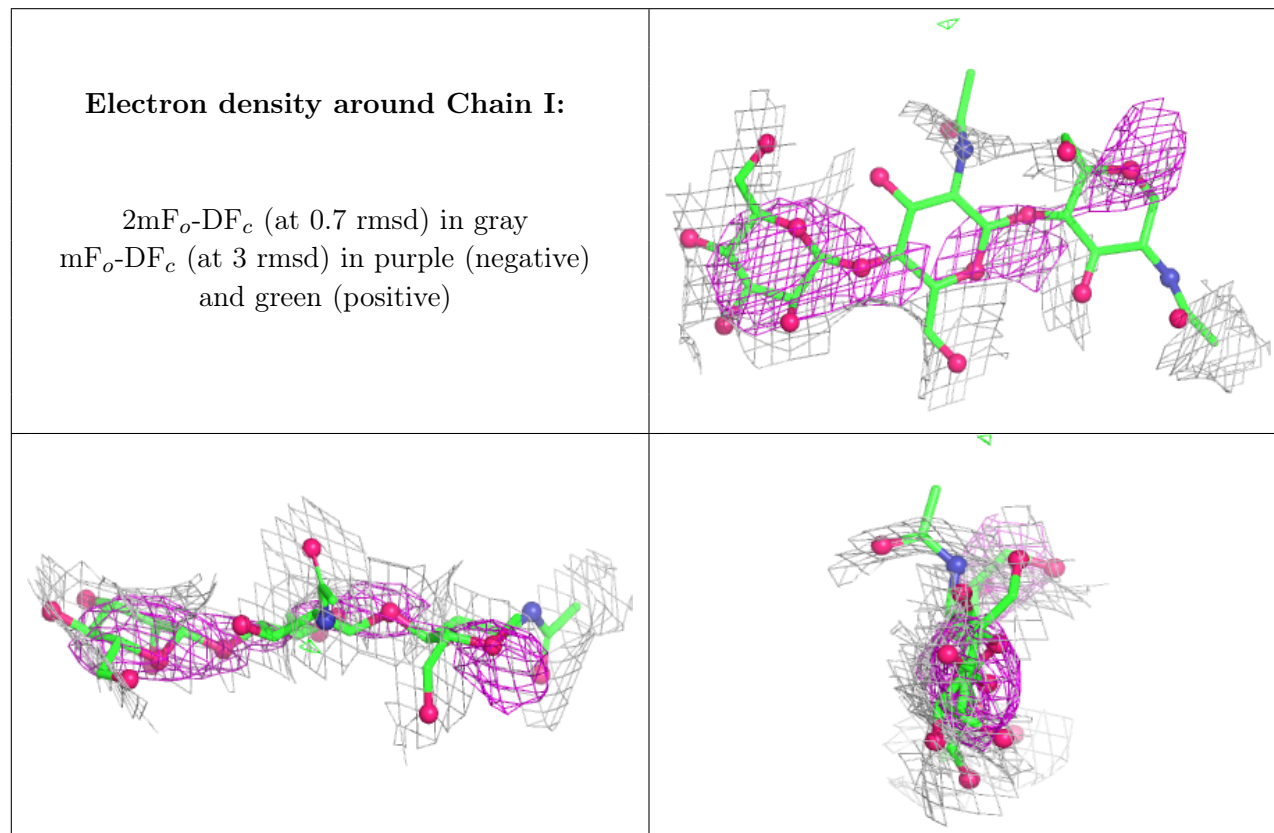
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	I	1	14/15	0.18	0.22	253,254,256,258	0
3	BMA	I	3	11/12	0.28	0.17	265,265,265,265	0
4	NAG	J	2	14/15	0.33	0.16	257,258,258,258	0
3	NAG	I	2	14/15	0.34	0.18	260,261,263,264	0

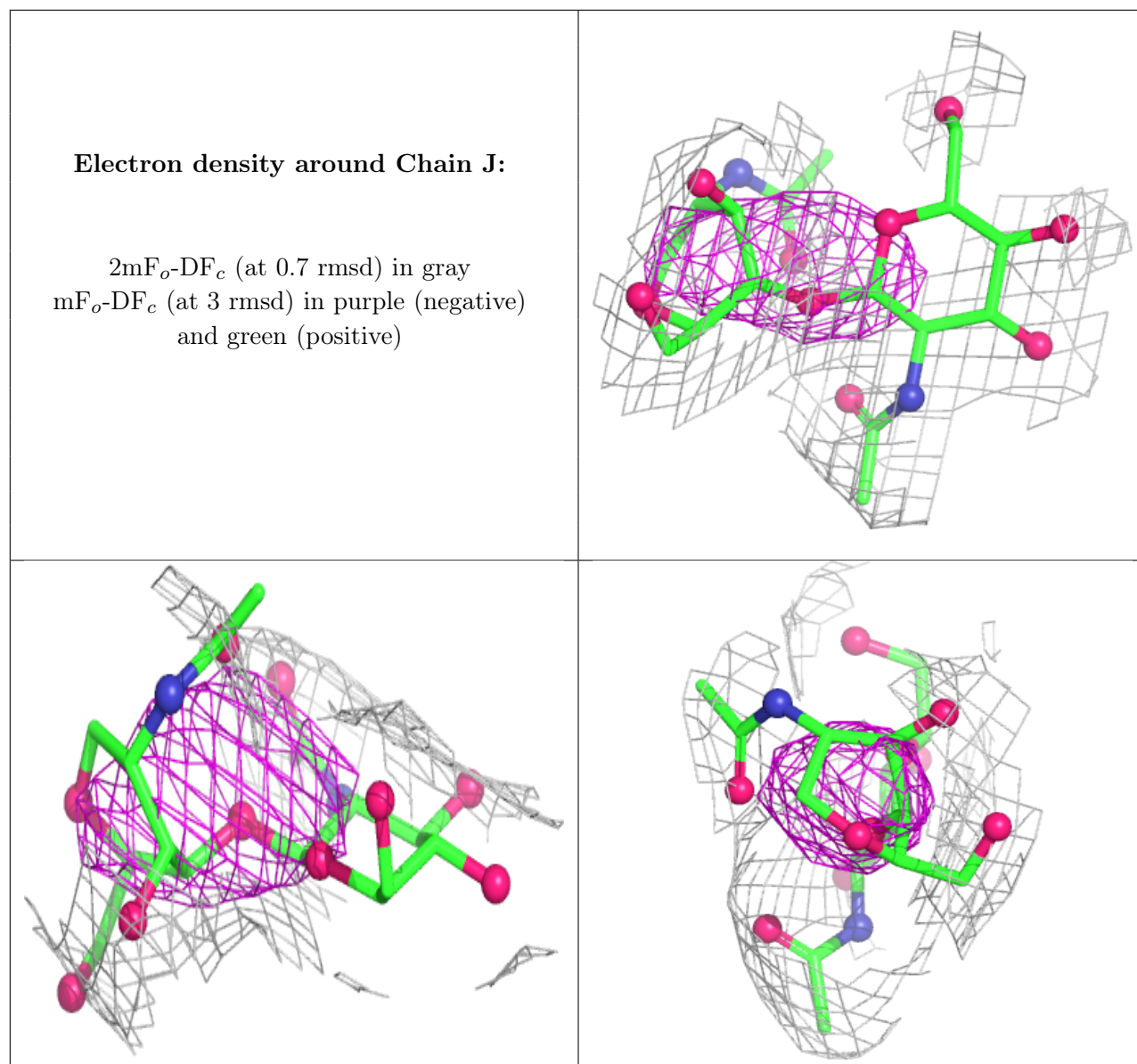
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	J	1	14/15	0.46	0.19	253,254,256,257	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	H	601	14/15	0.24	0.18	232,233,234,234	0
5	NAG	E	601	14/15	0.40	0.17	245,246,246,246	0
5	NAG	F	601	14/15	0.76	0.10	221,222,222,222	0
5	NAG	F	602	14/15	0.85	0.18	236,237,237,237	0

6.5 Other polymers [i](#)

There are no such residues in this entry.