Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 12:09 PM JST

PDB ID	:	8HUE
Title	:	Crystal structure of FGF2-M2 mutant - D28E/C78I/C96I/S137P
Authors	:	Jung, Y.E.; Cha, S.S.; An, Y.J.
Deposited on	:	2022-12-23
Resolution	:	1.48 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:

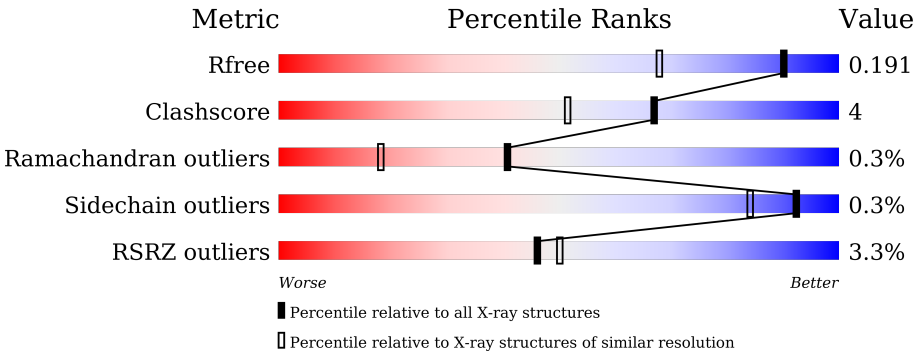
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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

Mol	Chain	Length	Quality of chain
1	A	147	3% 81% 10% • 8%
1	B	147	% 83% • • 12%
1	C	147	5% 81% 7% 12%
2	D	2	100%
2	E	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6820 atoms, of which 3202 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.

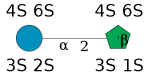
- Molecule 1 is a protein called Fibroblast growth factor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	135	Total	C	H	N	O	S	0	0	0
			2153	689	1080	195	185	4			
1	B	129	Total	C	H	N	O	S	0	0	0
			2079	658	1048	188	181	4			
1	C	130	Total	C	H	N	O	S	0	0	0
			2090	666	1046	190	184	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP P09038
A	28	GLU	ASP	engineered mutation	UNP P09038
A	78	ILE	CYS	engineered mutation	UNP P09038
A	96	ILE	CYS	engineered mutation	UNP P09038
A	137	PRO	SER	engineered mutation	UNP P09038
B	9	MET	-	initiating methionine	UNP P09038
B	28	GLU	ASP	engineered mutation	UNP P09038
B	78	ILE	CYS	engineered mutation	UNP P09038
B	96	ILE	CYS	engineered mutation	UNP P09038
B	137	PRO	SER	engineered mutation	UNP P09038
C	9	MET	-	initiating methionine	UNP P09038
C	28	GLU	ASP	engineered mutation	UNP P09038
C	78	ILE	CYS	engineered mutation	UNP P09038
C	96	ILE	CYS	engineered mutation	UNP P09038
C	137	PRO	SER	engineered mutation	UNP P09038

- Molecule 2 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	2	Total	C	H	O	S	0	0	0
			69	12	14	35	8			
2	E	2	Total	C	H	O	S	0	0	0
			69	12	14	35	8			

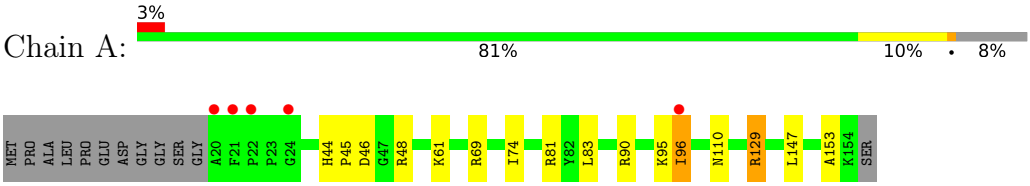
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	135	Total	O	0	0
			135	135		
3	C	133	Total	O	0	0
			133	133		

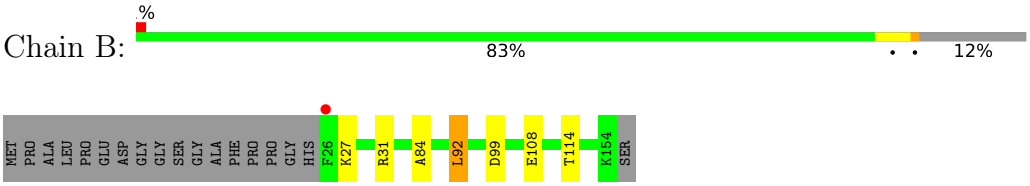
3 Residue-property plots (i)

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.

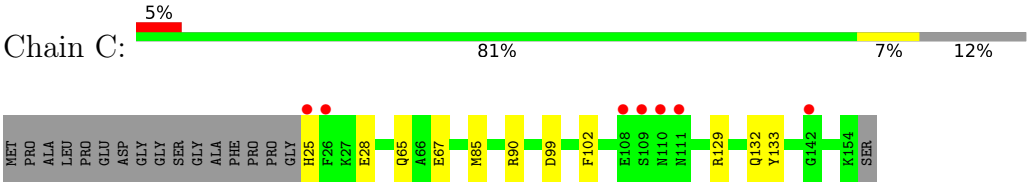
• Molecule 1: Fibroblast growth factor 2



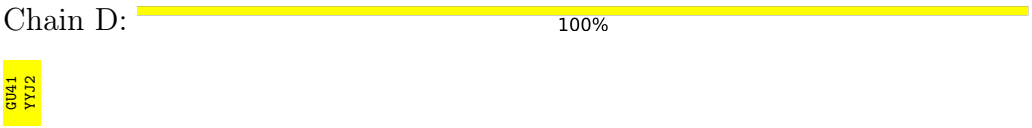
• Molecule 1: Fibroblast growth factor 2



• Molecule 1: Fibroblast growth factor 2



• Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose



• Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.38Å 54.45Å 71.97Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	45.48 – 1.48 45.48 – 1.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.48-1.48) 98.0 (45.48-1.48)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, R_{free}	0.179 , 0.196 0.174 , 0.191	Depositor DCC
R_{free} test set	1999 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6820	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% 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: YYJ, GU4

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	0.65	0/1100	0.91	5/1481 (0.3%)
1	B	0.71	0/1053	0.87	1/1414 (0.1%)
1	C	0.68	1/1068 (0.1%)	0.87	2/1435 (0.1%)
All	All	0.68	1/3221 (0.0%)	0.88	8/4330 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	MET	CB-CG	5.07	1.67	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	90	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	96	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	B	99	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	99	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	90	ARG	CB-CA-C	-5.33	99.73	110.40
1	C	85	MET	CG-SD-CE	-5.18	91.91	100.20
1	A	129	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1073	1080	1070	12	0
1	B	1031	1048	1040	4	0
1	C	1044	1046	1038	9	0
2	D	55	14	6	0	0
2	E	55	14	6	1	0
3	A	92	0	0	2	0
3	B	135	0	0	1	1
3	C	133	0	0	3	1
All	All	3618	3202	3160	25	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLN:OE1	3:C:201:HOH:O	1.87	0.93
1:C:132:GLN:HG2	3:C:307:HOH:O	1.90	0.71
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.55	0.71
1:C:129:ARG:NH1	2:E:2:YYJ:O1S3	2.30	0.65
1:C:25:HIS:NE2	1:C:28:GLU:HG2	2.18	0.59
1:C:28:GLU:HB2	3:C:266:HOH:O	2.05	0.56
1:C:67:GLU:HG3	1:C:102:PHE:CD1	2.41	0.55
1:A:129:ARG:HG2	1:A:129:ARG:NH1	2.21	0.55
1:A:110:ASN:HD21	1:A:147:LEU:HD13	1.72	0.54
1:A:61:LYS:NZ	1:A:153:ALA:O	2.33	0.54
1:C:67:GLU:HG3	1:C:102:PHE:CE1	2.45	0.51
1:B:31:ARG:NH1	3:B:205:HOH:O	2.44	0.51
1:A:44:HIS:ND1	1:A:45:PRO:HD2	2.26	0.50
1:C:90:ARG:HG3	1:C:133:TYR:CZ	2.48	0.49
1:A:81:ARG:HD3	1:A:95:LYS:HA	1.96	0.48
1:B:92:LEU:C	1:B:92:LEU:HD12	2.35	0.47
1:B:84:ALA:HB3	1:B:92:LEU:HD12	1.97	0.47
1:A:74:ILE:HD12	1:A:83:LEU:HD23	1.97	0.46
1:A:46:ASP:CG	1:A:48:ARG:HE	2.20	0.45
1:B:108:GLU:HG3	1:B:114:THR:HG23	1.99	0.45
1:A:46:ASP:OD2	1:A:48:ARG:NE	2.44	0.44
1:C:25:HIS:CD2	1:C:28:GLU:H	2.37	0.43
1:A:69:ARG:NH2	3:A:201:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG21	1:A:96:ILE:HD13	1.77	0.41
1:A:96:ILE:HG12	3:A:284:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:269:HOH:O	3:C:315:HOH:O[1_455]	2.17	0.03

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	133/147 (90%)	131 (98%)	2 (2%)	0	100 100
1	B	127/147 (86%)	125 (98%)	1 (1%)	1 (1%)	19 4
1	C	128/147 (87%)	125 (98%)	3 (2%)	0	100 100
All	All	388/441 (88%)	381 (98%)	6 (2%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	LYS

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	110/123 (89%)	110 (100%)	0	100 100
1	B	107/123 (87%)	106 (99%)	1 (1%)	78 59
1	C	108/123 (88%)	108 (100%)	0	100 100
All	All	325/369 (88%)	324 (100%)	1 (0%)	92 84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	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)

4 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	$\#\|Z\| > 2$
2	GU4	D	1	2	27,27,28	1.72	6 (22%)	29,43,45	1.76	4 (13%)
2	YYJ	D	2	2	27,28,28	1.33	4 (14%)	28,46,46	2.31	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GU4	E	1	2	27,27,28	1.62	5 (18%)	29,43,45	2.89	8 (27%)
2	YYJ	E	2	2	27,28,28	1.73	5 (18%)	28,46,46	0.95	1 (3%)

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
2	GU4	D	1	2	-	5/21/38/41	0/1/1/1
2	YYJ	D	2	2	-	5/23/42/42	0/1/1/1
2	GU4	E	1	2	-	11/21/38/41	0/1/1/1
2	YYJ	E	2	2	-	4/23/42/42	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	YYJ	O2S6-S6	4.56	1.64	1.45
2	E	1	GU4	O22-S6	4.53	1.64	1.45
2	E	1	GU4	O27-S3	4.51	1.64	1.45
2	E	2	YYJ	O3S3-S3	4.49	1.64	1.45
2	D	1	GU4	O22-S6	4.35	1.63	1.45
2	D	1	GU4	O26-S4	4.30	1.63	1.45
2	D	2	YYJ	O2S3-S3	3.90	1.61	1.45
2	E	2	YYJ	O3S1-S1	3.67	1.61	1.45
2	D	1	GU4	O2-C2	-3.29	1.42	1.47
2	D	2	YYJ	O1-C1	-3.00	1.40	1.45
2	D	1	GU4	O12-S2	2.92	1.57	1.45
2	E	1	GU4	O2-C2	-2.85	1.42	1.47
2	E	1	GU4	O24-S4	2.42	1.65	1.50
2	E	2	YYJ	O1S4-S4	2.38	1.65	1.50
2	D	2	YYJ	O1S4-S4	2.30	1.64	1.50
2	E	2	YYJ	O2-C2	2.25	1.44	1.40
2	D	2	YYJ	O1S6-S6	2.21	1.64	1.50
2	D	1	GU4	O4-C4	-2.18	1.41	1.46
2	D	1	GU4	O29-S3	2.07	1.63	1.50
2	E	1	GU4	O10-S2	2.06	1.63	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	YYJ	O3S3-S3-O2S3	-7.78	81.01	112.22
2	E	1	GU4	O24-S4-O25	-7.73	81.62	108.49
2	E	1	GU4	O10-S2-O11	-7.52	82.37	108.49
2	D	2	YYJ	O1S3-S3-O3S3	6.04	129.50	108.49
2	D	1	GU4	O10-S2-O12	-5.73	88.56	108.49
2	E	1	GU4	O24-S4-O26	-5.65	88.84	108.49
2	E	1	GU4	O2-C2-C3	5.01	112.20	106.65
2	D	2	YYJ	O1S3-S3-O2S3	-4.49	92.88	108.49
2	E	1	GU4	O10-S2-O12	-4.42	93.13	108.49
2	E	1	GU4	C4-O4-S4	4.22	127.04	118.88
2	D	1	GU4	O10-S2-O11	3.97	122.29	108.49
2	D	1	GU4	O12-S2-O11	-3.66	97.54	112.22
2	D	2	YYJ	O5-C5-C4	2.98	108.47	103.49
2	E	1	GU4	O12-S2-O11	2.68	122.99	112.22
2	E	2	YYJ	O1-S1-O3S1	2.66	114.94	106.88
2	E	1	GU4	O26-S4-O25	2.51	122.29	112.22
2	D	1	GU4	O24-S4-O26	2.24	116.29	108.49

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	GU4	C2-O2-S2-O10
2	D	2	YYJ	C2-C3-O3-S3
2	E	1	GU4	O5-C5-C6-O6
2	E	1	GU4	C4-C5-C6-O6
2	E	1	GU4	C6-O6-S6-O21
2	E	1	GU4	C4-O4-S4-O26
2	E	1	GU4	C4-O4-S4-O24
2	E	1	GU4	C6-O6-S6-O23
2	E	1	GU4	C6-O6-S6-O22
2	E	2	YYJ	C1-O1-S1-O3S1
2	D	1	GU4	O5-C5-C6-O6
2	D	1	GU4	C3-O3-S3-O28
2	D	1	GU4	C3-O3-S3-O27
2	D	2	YYJ	C3-O3-S3-O3S3
2	E	1	GU4	C3-O3-S3-O27
2	E	1	GU4	C2-O2-S2-O12
2	D	2	YYJ	C5-C4-O4-S4
2	E	2	YYJ	C1-O1-S1-O2S1
2	E	2	YYJ	C1-O1-S1-O1S1
2	D	1	GU4	C3-O3-S3-O29
2	E	1	GU4	C3-O3-S3-O28

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Mol	Chain	Res	Type	Atoms
2	E	1	GU4	C3-O3-S3-O29
2	D	2	YYJ	C3-C4-O4-S4
2	D	2	YYJ	C4-O4-S4-O1S4
2	E	2	YYJ	C2-C1-O1-S1

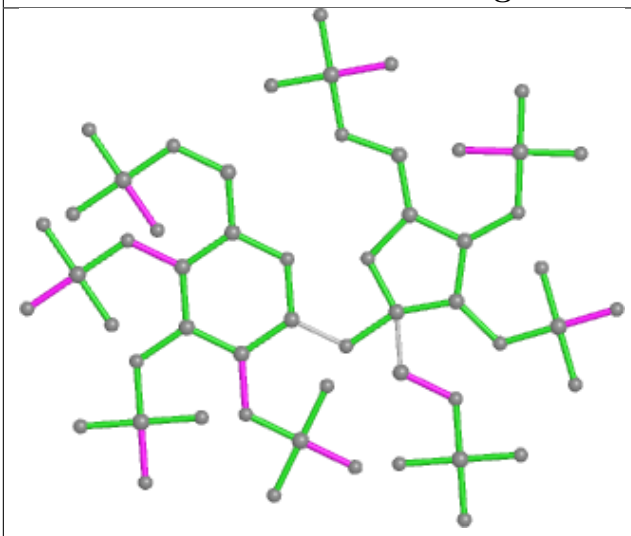
There are no ring outliers.

1 monomer is involved in 1 short contact:

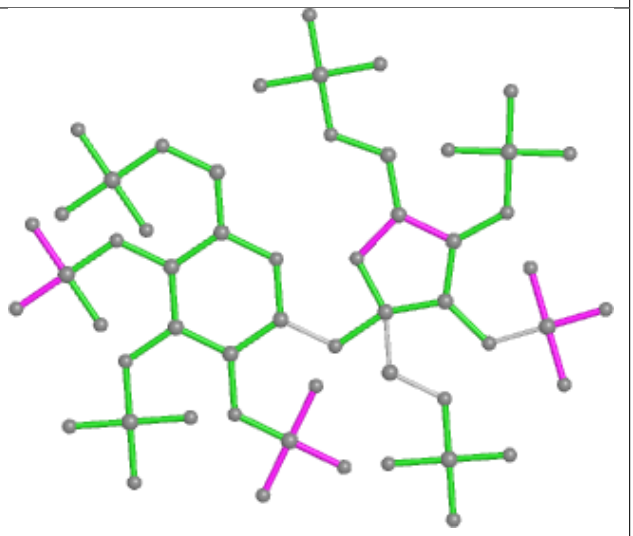
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	YYJ	1	0

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

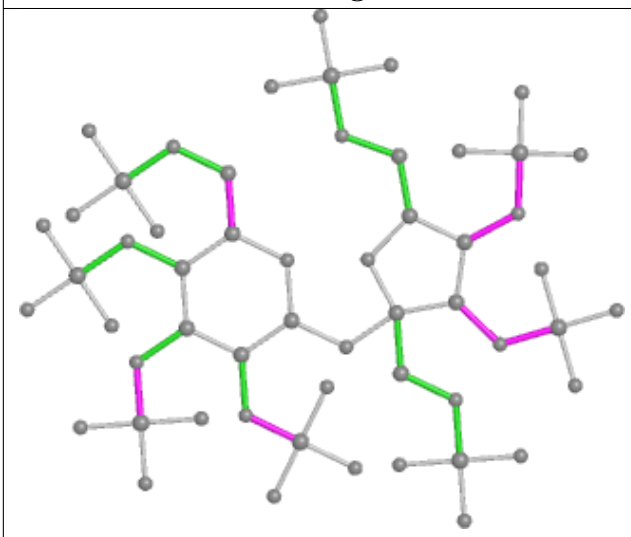
Oligosaccharide Chain D



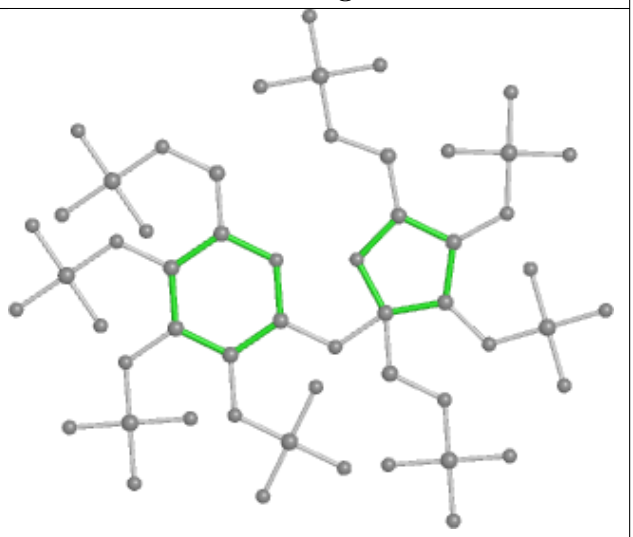
Bond lengths



Bond angles

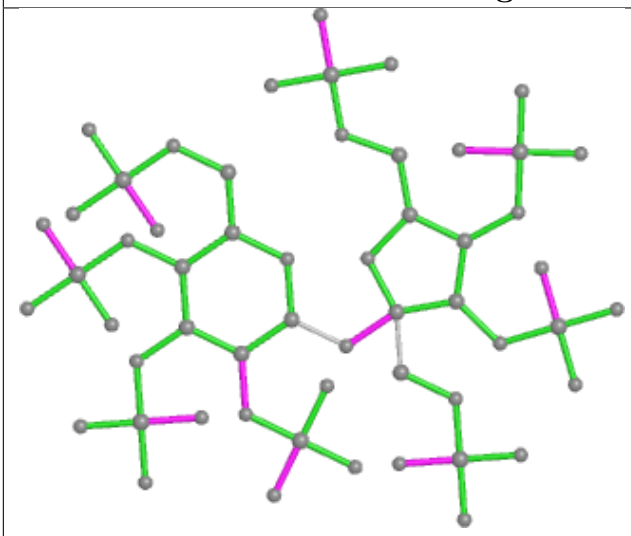


Torsions

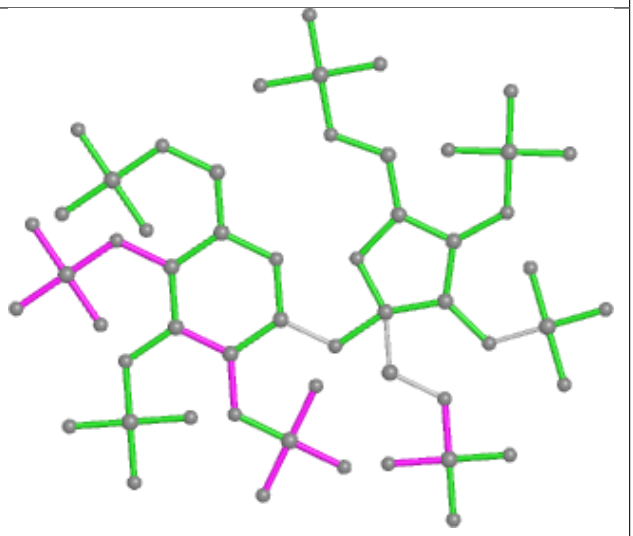


Rings

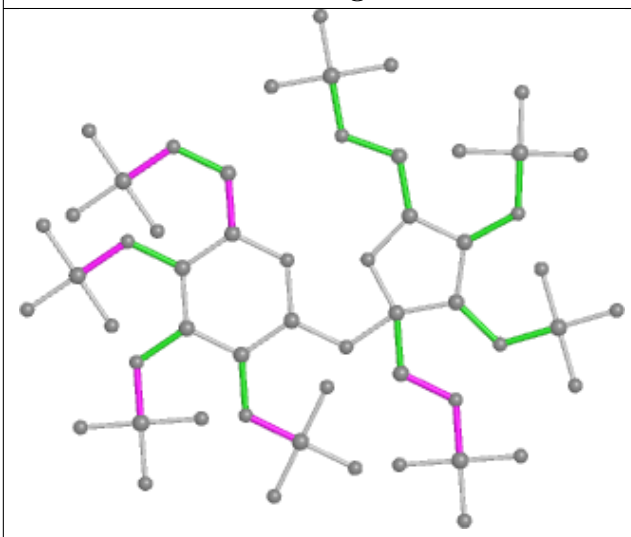
Oligosaccharide Chain E



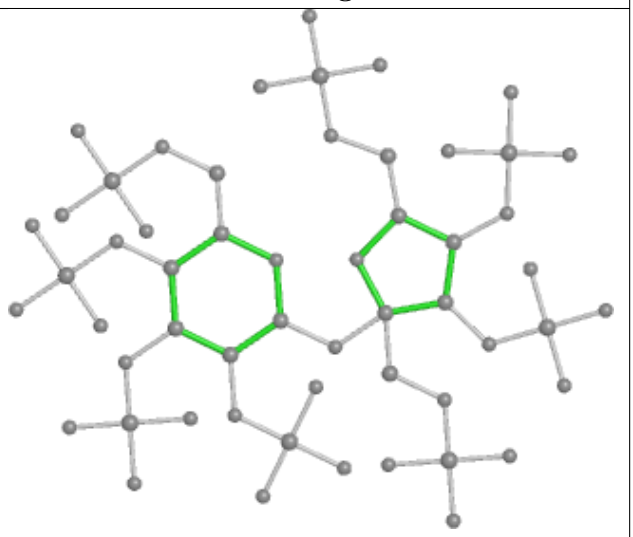
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	135/147 (91%)	0.04	5 (3%) 41 45	8, 17, 30, 37	0
1	B	129/147 (87%)	-0.07	1 (0%) 86 88	6, 12, 22, 38	0
1	C	130/147 (88%)	-0.01	7 (5%) 25 28	8, 14, 32, 40	0
All	All	394/441 (89%)	-0.01	13 (3%) 46 50	6, 15, 29, 40	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	PHE	6.6
1	A	96	ILE	4.6
1	A	20	ALA	3.0
1	C	25	HIS	2.9
1	C	110	ASN	2.8
1	C	111	ASN	2.7
1	A	22	PRO	2.5
1	A	24	GLY	2.4
1	C	142	GLY	2.4
1	C	109	SER	2.3
1	A	21	PHE	2.1
1	C	26	PHE	2.1
1	C	108	GLU	2.1

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

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

6.3 Carbohydrates (i)

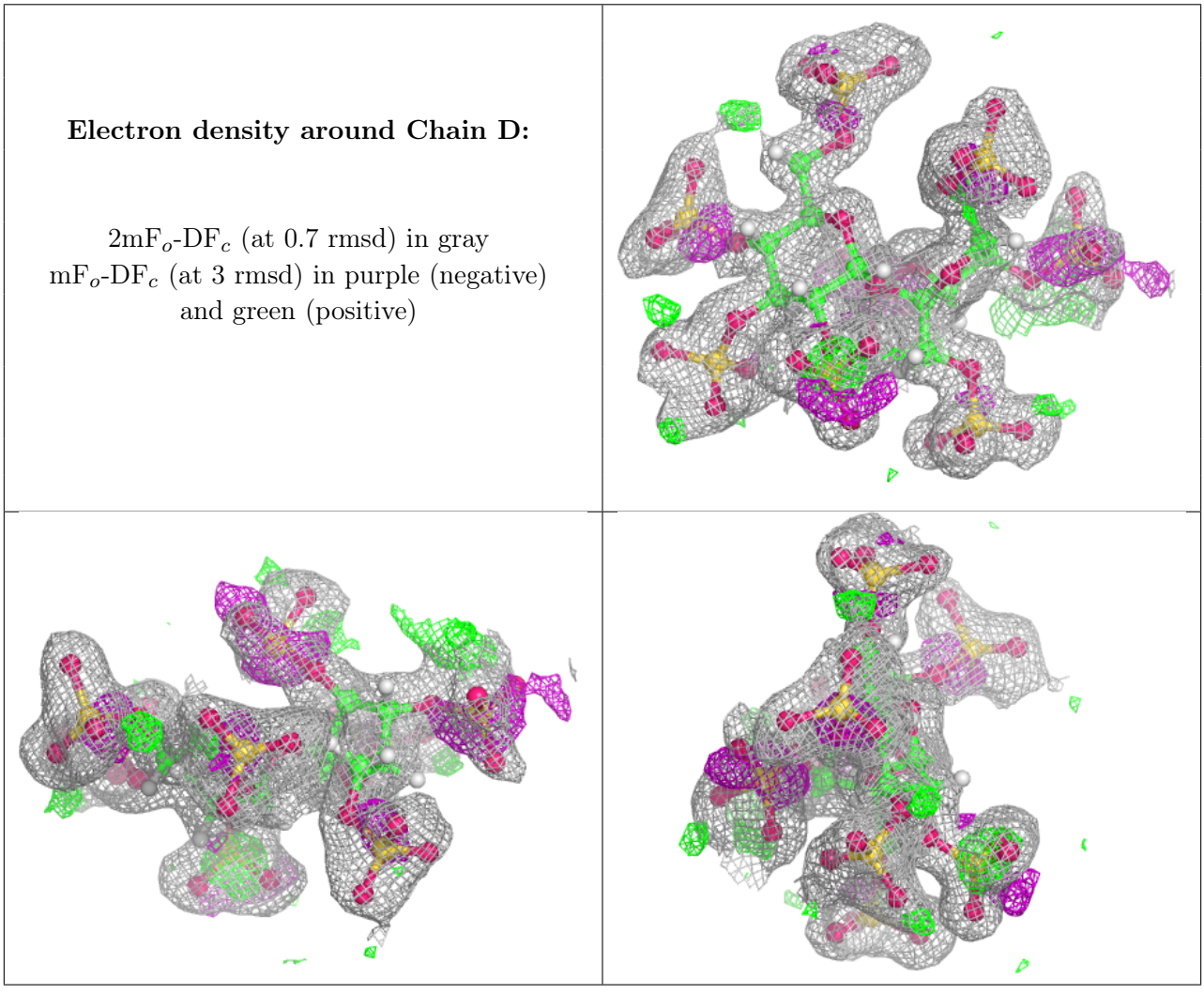
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	GU4	D	1	27/28	0.88	0.11	19,26,36,42	0
2	GU4	E	1	27/28	0.88	0.19	31,41,50,54	0
2	YYJ	E	2	28/28	0.91	0.16	23,39,49,53	0
2	YYJ	D	2	28/28	0.93	0.12	14,27,41,48	0

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

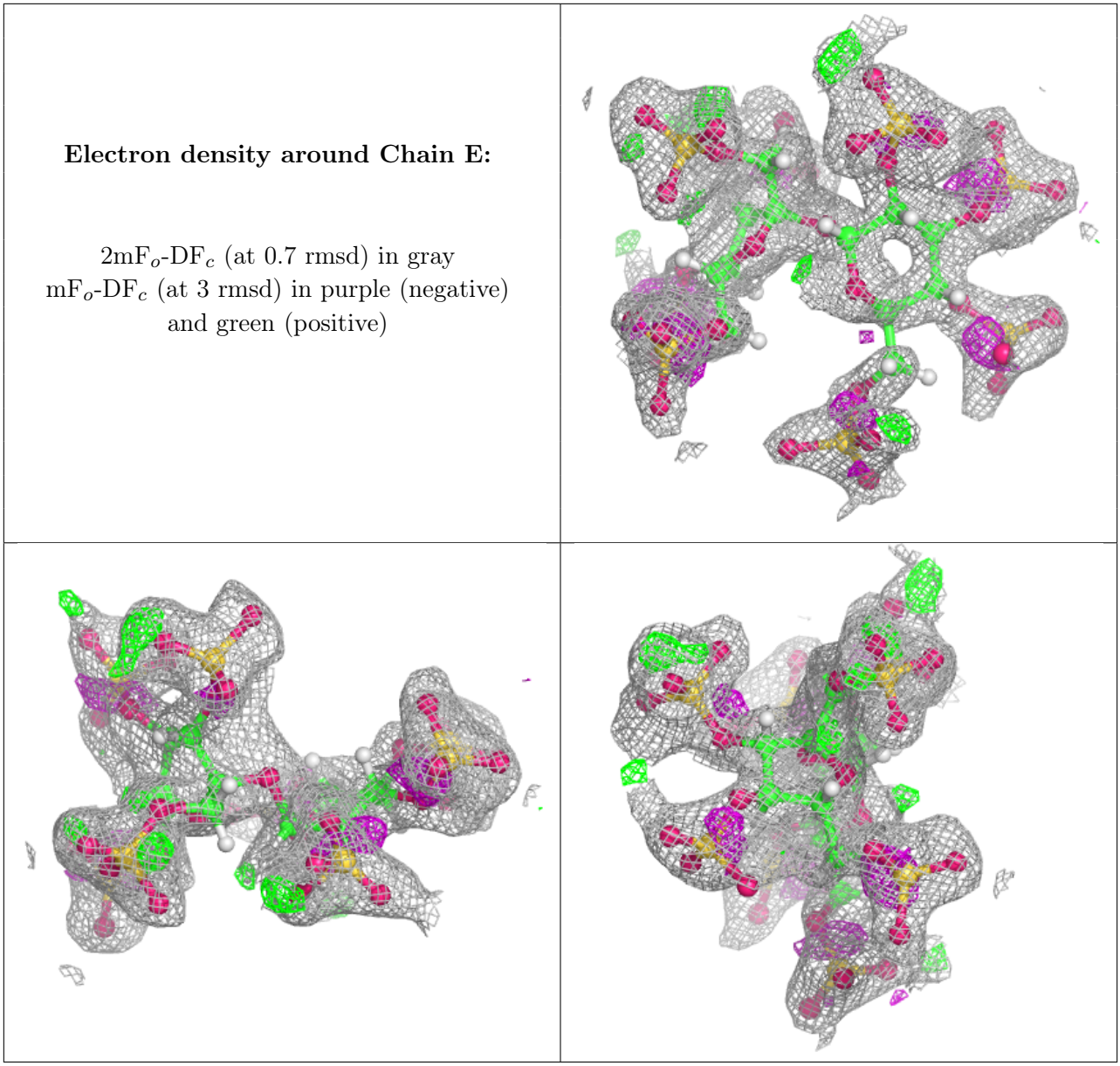
Electron density around Chain D:

$2mF_o$-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 E:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.