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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 12:58 AM JST

PDB ID	:	6KD5
Title	:	Crystal structure of the extracellular domain of MSPL/TMPRSS13 in complex with dec-RVKR-cmk inhibitor
Authors	:	Ohno, A.; Maita, N.; Okumura, Y.; Nikawa, T.
Deposited on	:	2019-06-30
Resolution	:	2.60 Å(reported)

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

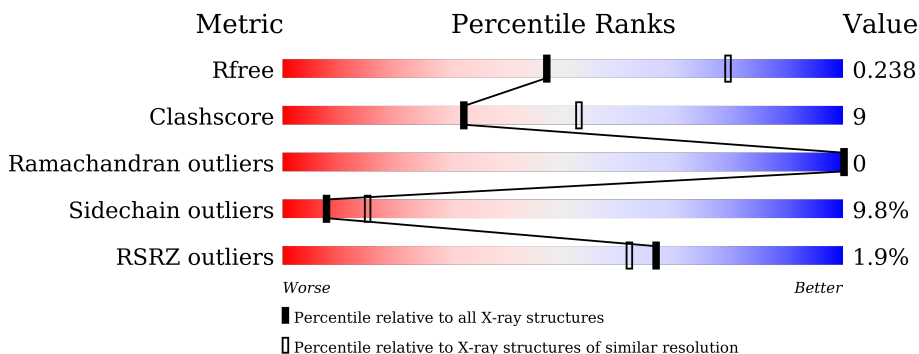|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		9.8%
RSRZ outliers		1.9%

Worse ← → Better

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	156	3% — 61% / 21% / • / 16%
2	B	261	% — 70% / 18% / • / 9%
3	C	6	83% / 17%
4	D	2	50% / 50%
5	E	2	100%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3130 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 Transmembrane protease serine 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	1047	644	191	202	10	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ASP	-	expression tag	UNP Q9BYE2
A	171	TYR	-	expression tag	UNP Q9BYE2
A	172	LYS	-	expression tag	UNP Q9BYE2
A	173	ASP	-	expression tag	UNP Q9BYE2
A	174	HIS	-	expression tag	UNP Q9BYE2
A	175	ASP	-	expression tag	UNP Q9BYE2
A	176	GLY	-	expression tag	UNP Q9BYE2
A	177	ASP	-	expression tag	UNP Q9BYE2
A	178	TYR	-	expression tag	UNP Q9BYE2
A	179	LYS	-	expression tag	UNP Q9BYE2
A	180	ASP	-	expression tag	UNP Q9BYE2
A	181	HIS	-	expression tag	UNP Q9BYE2
A	182	ASP	-	expression tag	UNP Q9BYE2
A	183	ILE	-	expression tag	UNP Q9BYE2
A	184	ASP	-	expression tag	UNP Q9BYE2
A	185	TYR	-	expression tag	UNP Q9BYE2
A	186	LYS	-	expression tag	UNP Q9BYE2
A	187	ASP	-	expression tag	UNP Q9BYE2
A	188	ASP	-	expression tag	UNP Q9BYE2
A	189	ASP	-	expression tag	UNP Q9BYE2
A	190	ASP	-	expression tag	UNP Q9BYE2
A	191	LYS	-	expression tag	UNP Q9BYE2

- Molecule 2 is a protein called Transmembrane protease serine 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total 1864	C 1181	N 318	O 351	S 14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	VAL	LEU	variant	UNP Q9BYE2

- Molecule 3 is a protein called DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKE TONE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total 50	C 34	N 11	O 5	0	0	1

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	A	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	B	1	Total 5	O 4	S 1	0	0
6	C	1	Total 5	O 4	S 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Ca 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total 28	O 28	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	53	Total 53	O 53	0	0

3 Residue-property plots ⓘ

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.
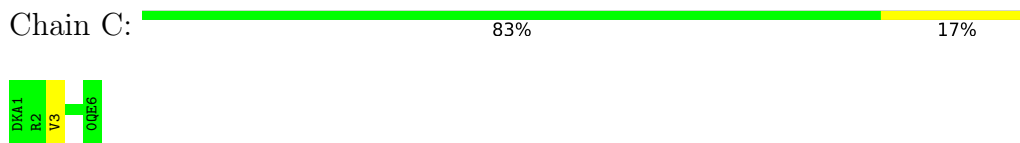
• Molecule 1: Transmembrane protease serine 13

Chain A:
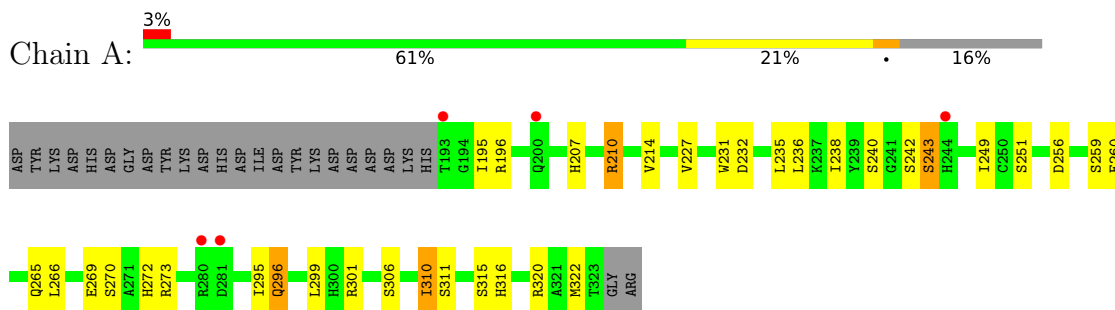
• Molecule 2: Transmembrane protease serine 13

Chain B:
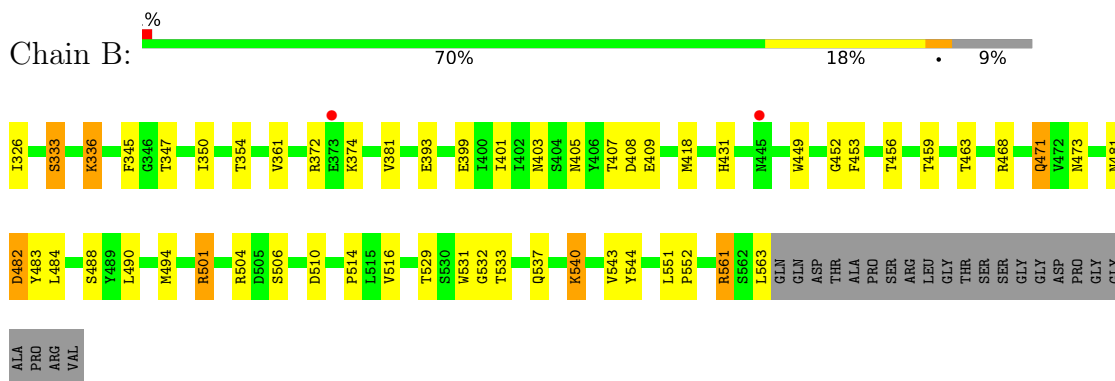
• Molecule 3: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE IN-HIBITOR

Chain C:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain E:

100%

MAG1
MAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.84Å 62.40Å 171.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 2.60 39.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.99-2.60) 99.5 (39.96-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.184 , 0.236 0.191 , 0.238	Depositor DCC
R_{free} test set	1493 reflections (7.83%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.2	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3130	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FUC, DKA, AR7, NAG, 0QE, CA

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	0.63	0/1070	0.70	0/1442
2	B	0.62	0/1912	0.70	0/2601
3	C	0.60	0/26	0.64	0/32
All	All	0.62	0/3008	0.70	0/4075

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	514	PRO	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1047	0	984	21	0
2	B	1864	0	1795	32	1
3	C	50	0	66	1	0
4	D	24	0	22	0	0
5	E	28	0	25	0	0
6	A	15	0	0	1	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
7	A	1	0	0	0	0
8	A	28	0	0	2	0
8	B	53	0	0	1	0
All	All	3130	0	2892	52	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 9.

The worst 5 of 52 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:B:533:THR:HB	2:B:540:LYS:HG2	1.47	0.97
1:A:196:ARG:HG3	2:B:561:ARG:HH11	1.32	0.94
2:B:399:GLU:OE1	2:B:561:ARG:CZ	2.36	0.73
1:A:227:VAL:HG22	1:A:266:LEU:HD11	1.69	0.73
1:A:251:SER:HA	1:A:310:ILE:HD12	1.73	0.71

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)
2:B:408:ASP:OD2	2:B:501:ARG:NH2[4_455]	1.98	0.22

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	129/156 (83%)	121 (94%)	8 (6%)	0	100	100
2	B	236/261 (90%)	219 (93%)	17 (7%)	0	100	100
3	C	2/6 (33%)	2 (100%)	0	0	100	100
All	All	367/423 (87%)	342 (93%)	25 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	119/143 (83%)	106 (89%)	13 (11%)	6	11
2	B	203/219 (93%)	184 (91%)	19 (9%)	8	17
3	C	3/3 (100%)	3 (100%)	0	100	100
All	All	325/365 (89%)	293 (90%)	32 (10%)	8	15

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	516	VAL
2	B	537	GLN
1	A	322	MET
1	A	320	ARG
2	B	540	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	307	GLN
2	B	344	HIS
2	B	473	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	AR7	C	5	3,2	10,10,11	0.58	0	9,11,13	0.68	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
3	AR7	C	5	3,2	-	<mark>2/9/9/11</mark>	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	AR7	O-C-CA-N
3	C	5	AR7	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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	#$|Z| > 2$
4	NAG	D	1	1,4	14,14,15	0.50	0	17,19,21	1.14	1 (5%)
4	FUC	D	2	4	10,10,11	0.40	0	14,14,16	0.77	0
5	NAG	E	1	5,2	14,14,15	0.40	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	14,14,15	0.31	0	17,19,21	0.75	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
5	NAG	E	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1	NAG	C1-O5-C5	2.84	116.04	112.19
4	D	1	NAG	C3-C4-C5	-2.68	105.46	110.24
5	E	2	NAG	O5-C1-C2	-2.06	108.03	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain D

Bond lengths　　　Bond angles

Torsions　　　Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
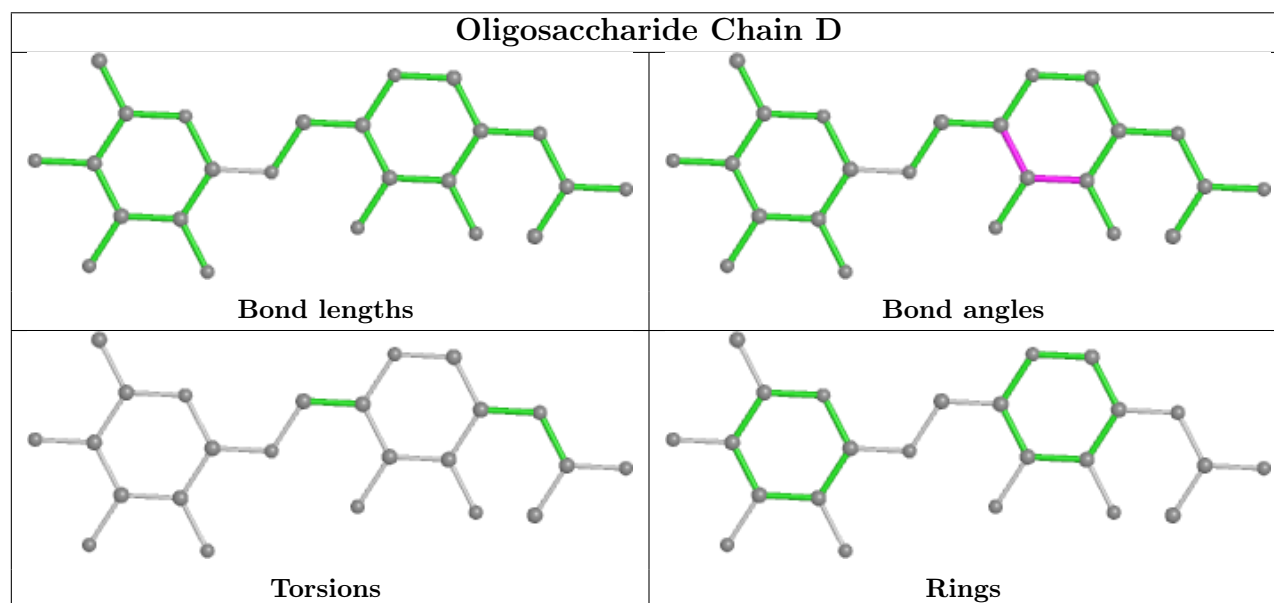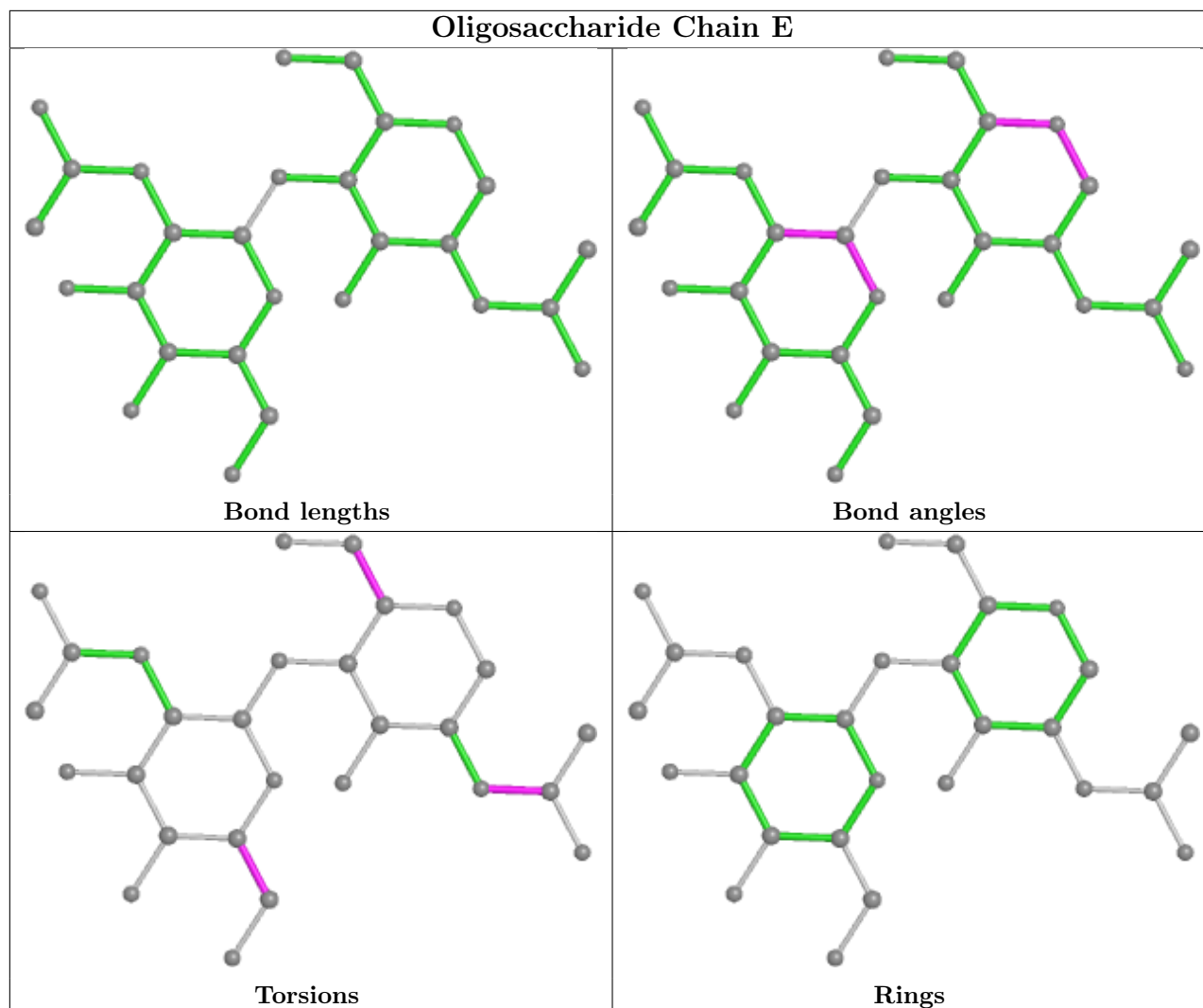
5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	$\#|Z| > 2$
6	SO4	B	601	-	4,4,4	0.37	0	6,6,6	0.05	0
6	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.10	0
6	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.11	0
6	SO4	A	401	-	4,4,4	0.40	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z|>2$	Counts	RMSZ	$\#|Z|>2$
6	SO4	C	101	-	4,4,4	0.37	0	6,6,6	0.09	0
6	SO4	B	603	-	4,4,4	0.34	0	6,6,6	0.04	0
6	SO4	B	602	-	4,4,4	0.35	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	403	SO4	1	0

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.

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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(Å²)	Q<0.9
1	A	131/156 (83%)	-0.15	5 (3%)	40	33	21, 35, 69, 97	0
2	B	238/261 (91%)	-0.45	2 (0%)	86	84	18, 28, 56, 94	0
3	C	3/6 (50%)	-0.87	0	100	100	22, 22, 26, 50	0
All	All	372/423 (87%)	-0.35	7 (1%)	66	62	18, 30, 63, 97	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	5.5
1	A	193	THR	4.3
1	A	200	GLN	3.7
1	A	281	ASP	2.7
1	A	244	HIS	2.5

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

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.
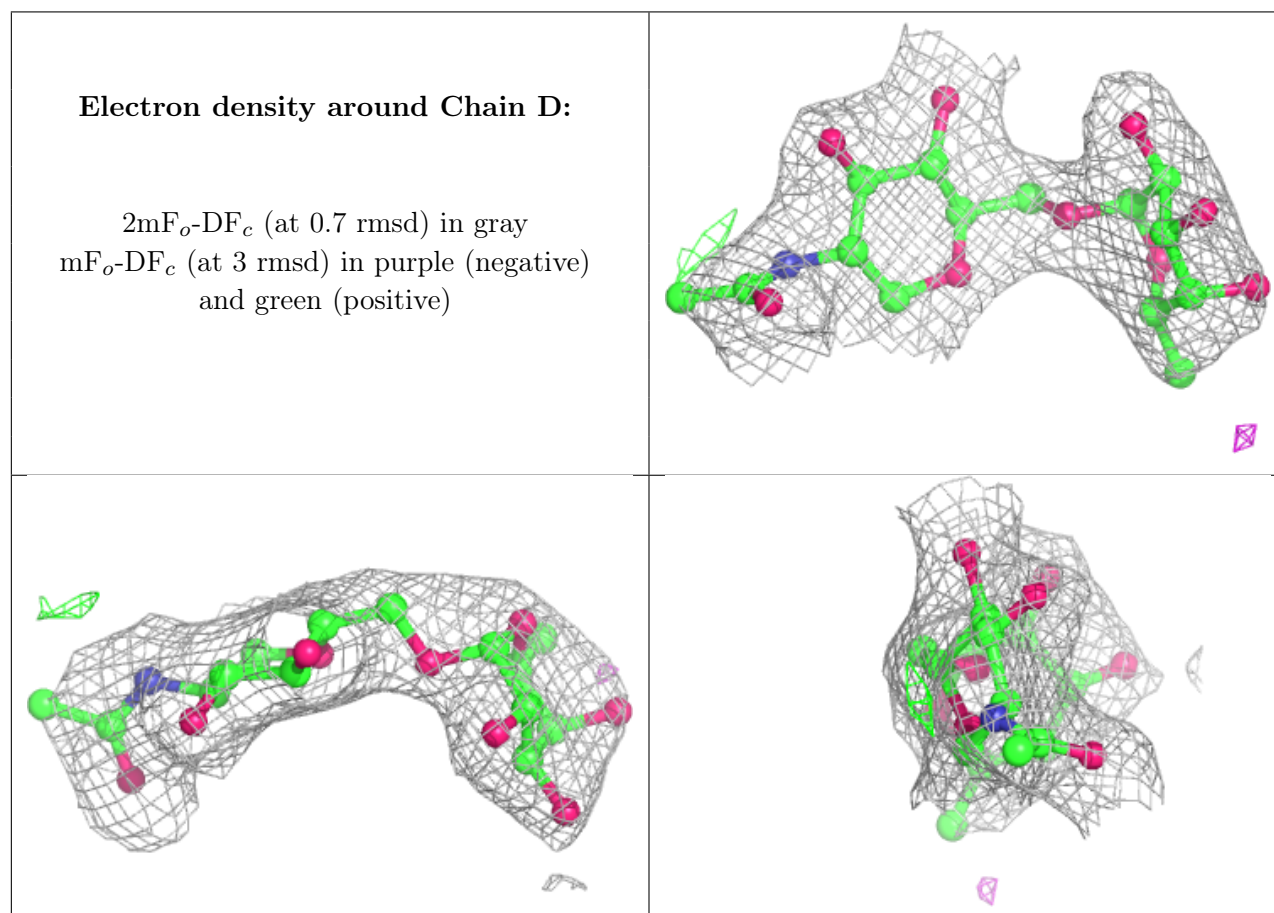
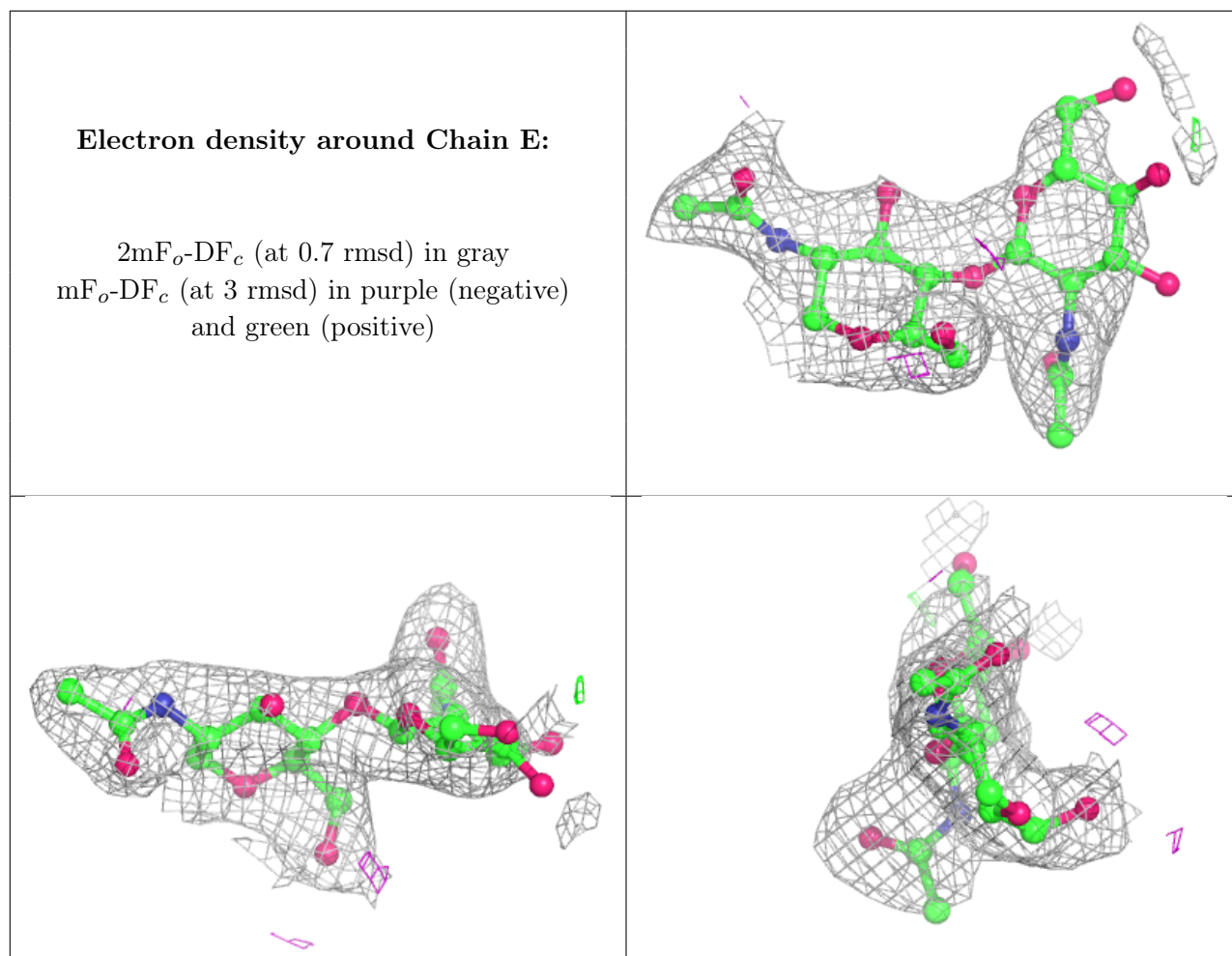| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	AR7	C	5	11/12	0.97	0.14	19,21,25,25	0

6.3   Carbohydrates ⓘ

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	E	2	14/15	0.84	0.32	51,94,111,113	0
5	NAG	E	1	14/15	0.95	0.19	35,41,54,67	0
4	NAG	D	1	14/15	0.95	0.15	40,43,57,58	0
4	FUC	D	2	10/11	0.96	0.25	44,52,52,54	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 (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
6	SO4	A	403	5/5	0.93	0.18	52,60,70,80	0
6	SO4	A	402	5/5	0.95	0.14	54,54,63,63	0
6	SO4	B	603	5/5	0.95	0.34	65,67,72,75	0
6	SO4	A	401	5/5	0.97	0.14	43,45,48,56	0
6	SO4	B	602	5/5	0.98	0.25	49,49,56,68	0
6	SO4	B	601	5/5	0.98	0.20	56,57,61,65	0
6	SO4	C	101	5/5	0.98	0.10	49,50,55,62	0
7	CA	A	404	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.