Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 04:10 am GMT

PDB ID	:	1GMN
Title	:	CRYSTAL STRUCTURES OF NK1-HEPARIN COMPLEXES REVEAL THE BASIS FOR NK1 ACTIVITY AND ENABLE ENGINEERING OF POTENT AGONISTS OF THE MET RECEPTOR
Authors	:	Lietha, D.; Chirgadze, D.Y.; Mulloy, B.; Blundell, T.L.; Gherardi, E.
Deposited on	:	2001-09-19
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

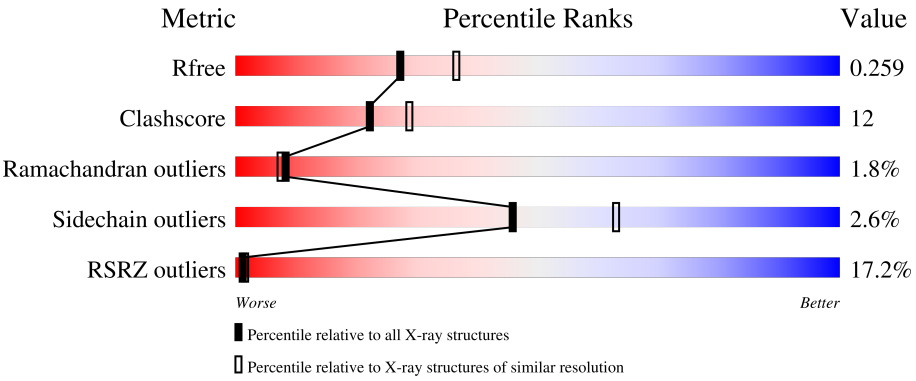
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	183	16% 70% 23% · 7%
1	B	183	10% 50% 12% · 38%
2	C	5	80% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2353 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.

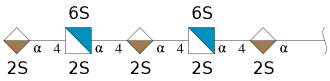
- Molecule 1 is a protein called HEPATOCYTE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	1
			1301	828	229	233	11			
1	B	114	Total	C	N	O	S	0	0	1
			869	549	148	164	8			

There are 4 discrepancies between the modelled and reference sequences:

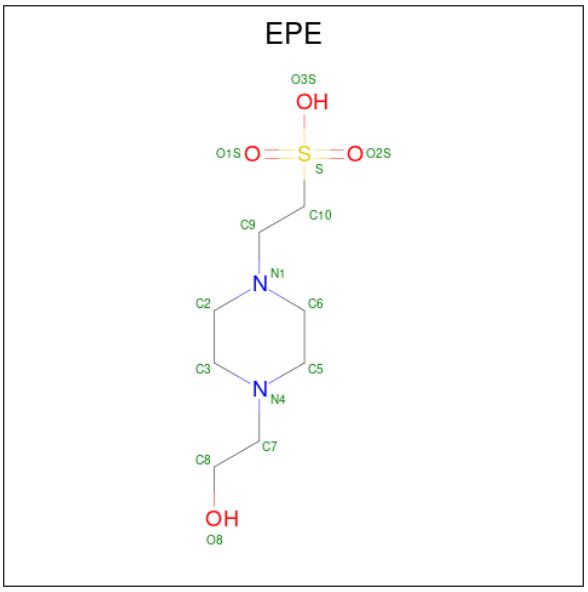
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	ALA	engineered mutation	UNP P14210
A	72	ASP	ASN	engineered mutation	UNP P14210
B	29	VAL	ALA	engineered mutation	UNP P14210
B	72	ASP	ASN	engineered mutation	UNP P14210

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	S	3	0	0
			86	30	2	47	7			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is water.

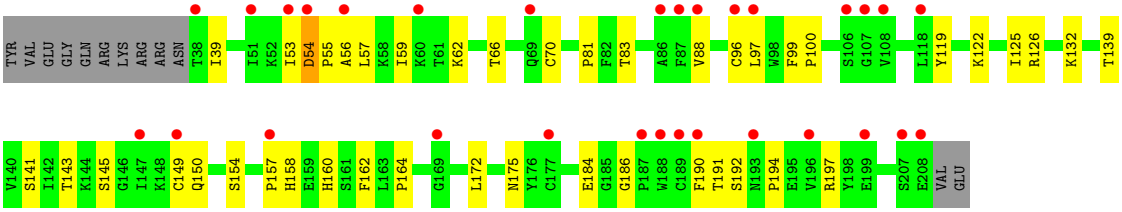
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	35	Total O 35 35	0	0

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.

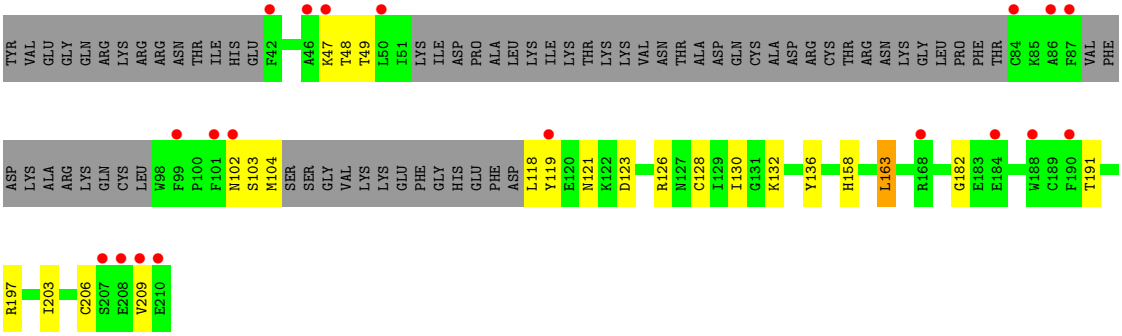
• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain A:



• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain B:



• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.56Å 86.56Å 117.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.30 20.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (21.00-2.30) 99.6 (20.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.279 0.254 , 0.259	Depositor DCC
R_{free} test set	1040 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2353	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: IDS, EPE, SGN

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	0.41	1/1335 (0.1%)	0.57	0/1803
1	B	0.41	0/891	0.58	0/1203
All	All	0.41	1/2226 (0.0%)	0.58	0/3006

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	GLU	CB-CG	-5.13	1.42	1.52

There are no bond angle outliers.

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	1301	0	1242	37	0
1	B	869	0	791	15	0
2	C	86	0	27	1	0
3	A	15	0	17	0	0
3	B	15	0	17	0	0
4	A	32	0	0	1	0
4	B	35	0	0	0	0
All	All	2353	0	2094	51	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 12.

All (51) 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:A:158:HIS:CD2	1:A:197:ARG:HA	2.13	0.84
1:B:128:CYS:HG	1:B:206:CYS:HG	0.85	0.83
1:A:154:SER:HB3	4:A:402:HOH:O	1.84	0.77
1:A:88:VAL:HG23	1:A:99:PHE:HE2	1.54	0.73
1:A:160:HIS:HD2	1:A:162:PHE:H	1.35	0.73
1:A:70:CYS:SG	1:A:96:CYS:HB2	2.30	0.72
1:A:158:HIS:NE2	1:A:197:ARG:HA	2.04	0.71
1:A:126:ARG:HH22	1:B:209:VAL:HG22	1.56	0.71
1:A:70:CYS:HG	1:A:96:CYS:HB2	1.57	0.70
1:A:160:HIS:CD2	1:A:162:PHE:H	2.10	0.69
1:A:122:LYS:HE2	1:A:139:THR:HG21	1.75	0.68
1:A:59:ILE:HD12	1:A:99:PHE:HD1	1.58	0.67
1:A:96:CYS:C	1:A:97:LEU:HD12	2.18	0.64
1:B:163:LEU:HD23	1:B:163:LEU:N	2.14	0.63
1:A:57:LEU:HD13	1:A:100:PRO:HG3	1.83	0.61
1:A:70:CYS:HG	1:A:96:CYS:CB	2.13	0.60
1:A:57:LEU:HD13	1:A:100:PRO:CG	2.32	0.59
1:B:48:THR:HG22	1:B:49:THR:H	1.67	0.59
1:A:70:CYS:SG	1:A:96:CYS:SG	3.01	0.58
1:B:136:TYR:CZ	1:B:203:ILE:HD13	2.39	0.58
1:A:141:SER:HB2	1:A:175:ASN:ND2	2.19	0.58
1:A:157:PRO:HG2	1:A:158:HIS:ND1	2.20	0.56
1:B:48:THR:HG22	1:B:49:THR:N	2.22	0.55
1:A:160:HIS:CD2	1:A:162:PHE:HB2	2.43	0.54
1:A:160:HIS:HD2	1:A:162:PHE:N	2.04	0.54
1:B:102:ASN:C	1:B:104:MET:H	2.11	0.53
1:A:160:HIS:HD2	1:A:162:PHE:HB2	1.73	0.53
1:B:158:HIS:CE1	1:B:197:ARG:HA	2.45	0.52
1:B:102:ASN:O	1:B:104:MET:N	2.44	0.50
1:A:70:CYS:SG	1:A:96:CYS:CB	3.00	0.50
1:A:53:ILE:O	1:A:54:ASP:HB3	2.13	0.49
1:A:62:LYS:HE2	2:C:5:IDS:O2S	2.13	0.48
1:B:121:ASN:ND2	1:B:123:ASP:HB2	2.30	0.47
1:A:192:SER:O	1:A:194:PRO:HD3	2.15	0.46
1:A:70:CYS:HB3	1:A:96:CYS:SG	2.56	0.46
1:B:102:ASN:C	1:B:104:MET:N	2.69	0.45
1:A:88:VAL:CG2	1:A:99:PHE:HE2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HG3	1:A:172:LEU:O	2.16	0.45
1:B:163:LEU:N	1:B:163:LEU:CD2	2.80	0.44
1:A:143:THR:C	1:A:145:SER:H	2.21	0.44
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.83	0.43
1:A:160:HIS:CD2	1:A:162:PHE:N	2.83	0.43
1:A:97:LEU:HD12	1:A:97:LEU:N	2.34	0.43
1:A:132:LYS:O	1:A:186:GLY:HA2	2.19	0.42
1:B:126:ARG:HH12	1:B:130:ILE:HD12	1.85	0.42
1:A:39:ILE:HD11	1:A:119:TYR:CE2	2.55	0.41
1:A:149:CYS:HB2	1:A:175:ASN:HD22	1.85	0.41
1:B:132:LYS:HD3	1:B:182:GLY:O	2.20	0.41
1:B:118:LEU:HD12	1:B:119:TYR:N	2.36	0.41
1:A:125:ILE:O	1:A:126:ARG:C	2.60	0.40
1:A:150:GLN:N	1:A:190:PHE:O	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	169/183 (92%)	152 (90%)	14 (8%)	3 (2%)	8 7
1	B	106/183 (58%)	97 (92%)	7 (7%)	2 (2%)	8 7
All	All	275/366 (75%)	249 (90%)	21 (8%)	5 (2%)	8 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PRO
1	A	56	ALA
1	B	103	SER
1	B	47	LYS

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Mol	Chain	Res	Type
1	A	81	PRO

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	136/165 (82%)	132 (97%)	4 (3%)	42 58
1	B	93/165 (56%)	91 (98%)	2 (2%)	52 69
All	All	229/330 (69%)	223 (97%)	6 (3%)	46 63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	66	THR
1	A	83	THR
1	A	191	THR
1	B	163	LEU
1	B	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	A	175	ASN
1	B	158	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	IDS	C	1	2	17,17,17	1.59	4 (23%)	20,26,26	3.80	6 (30%)
2	SGN	C	2	2	18,19,20	1.21	2 (11%)	22,29,31	1.81	6 (27%)
2	IDS	C	3	2	16,16,17	1.39	3 (18%)	17,24,26	2.57	6 (35%)
2	SGN	C	4	2	18,19,20	1.48	3 (16%)	22,29,31	2.10	6 (27%)
2	IDS	C	5	2	15,15,17	1.64	4 (26%)	15,22,26	2.45	3 (20%)

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	IDS	C	1	2	-	0/9/29/29	0/1/1/1
2	SGN	C	2	2	-	0/11/28/31	0/1/1/1
2	IDS	C	3	2	-	4/9/26/29	0/1/1/1
2	SGN	C	4	2	-	3/11/28/31	0/1/1/1
2	IDS	C	5	2	-	1/9/22/29	1/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	IDS	C1-C2	4.06	1.56	1.52
2	C	4	SGN	S1-N2	3.98	1.64	1.59
2	C	5	IDS	O2-C2	-3.21	1.42	1.47
2	C	3	IDS	O2-C2	-3.21	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	SGN	S1-N2	3.03	1.63	1.59
2	C	1	IDS	O6B-C6	-2.83	1.21	1.30
2	C	1	IDS	C4-C5	2.83	1.58	1.53
2	C	5	IDS	O6B-C6	-2.73	1.21	1.30
2	C	5	IDS	C4-C5	2.72	1.57	1.52
2	C	3	IDS	O6B-C6	-2.68	1.21	1.30
2	C	5	IDS	C1-C2	2.51	1.55	1.51
2	C	3	IDS	C1-C2	2.46	1.55	1.51
2	C	4	SGN	C1-C2	2.34	1.55	1.52
2	C	1	IDS	O2-C2	-2.13	1.42	1.46
2	C	4	SGN	O2S-S1	2.11	1.44	1.42
2	C	2	SGN	C1-C2	2.07	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	IDS	O4-C4-C5	15.20	143.83	109.74
2	C	3	IDS	C2-O2-S	7.99	128.33	117.91
2	C	5	IDS	C2-O2-S	7.79	128.07	117.91
2	C	4	SGN	O4-C4-C5	6.06	124.36	109.30
2	C	1	IDS	C2-O2-S	4.58	127.72	118.88
2	C	2	SGN	O4-C4-C5	4.11	119.50	109.30
2	C	3	IDS	C1-C2-C3	4.10	115.54	109.40
2	C	4	SGN	O4-C4-C3	-3.84	101.46	110.35
2	C	2	SGN	O1S-S1-O2S	-3.66	111.51	120.16
2	C	2	SGN	O4-C4-C3	-3.62	101.98	110.35
2	C	4	SGN	O1S-S1-O2S	-3.54	111.78	120.16
2	C	4	SGN	C1-O5-C5	3.16	116.48	112.19
2	C	1	IDS	O4-C4-C3	-3.13	103.12	110.35
2	C	5	IDS	O6B-C6-C5	3.03	121.67	113.03
2	C	3	IDS	O4-C4-C3	-2.90	103.65	110.35
2	C	1	IDS	O6B-C6-O6A	-2.82	117.69	124.09
2	C	5	IDS	O6B-C6-O6A	-2.78	117.78	124.09
2	C	3	IDS	O6B-C6-O6A	-2.73	117.90	124.09
2	C	2	SGN	O1S-S1-N2	-2.62	104.09	108.87
2	C	2	SGN	C1-O5-C5	2.55	115.64	112.19
2	C	4	SGN	O1S-S1-N2	-2.43	104.44	108.87
2	C	1	IDS	C1-O5-C5	2.31	115.63	112.22
2	C	1	IDS	O6B-C6-C5	2.23	121.82	113.65
2	C	2	SGN	O6-C6-C5	2.13	111.59	107.62
2	C	4	SGN	C4-C3-C2	-2.11	107.92	111.02
2	C	3	IDS	C4-C3-C2	2.07	113.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	IDS	O6B-C6-C5	2.02	121.04	113.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	IDS	C2-O2-S-O1S
2	C	3	IDS	C2-O2-S-O2S
2	C	3	IDS	C2-O2-S-O3S
2	C	4	SGN	C2-N2-S1-O1S
2	C	4	SGN	C2-N2-S1-O3S
2	C	5	IDS	O5-C5-C6-O6A
2	C	4	SGN	C2-N2-S1-O2S
2	C	3	IDS	O5-C5-C6-O6B

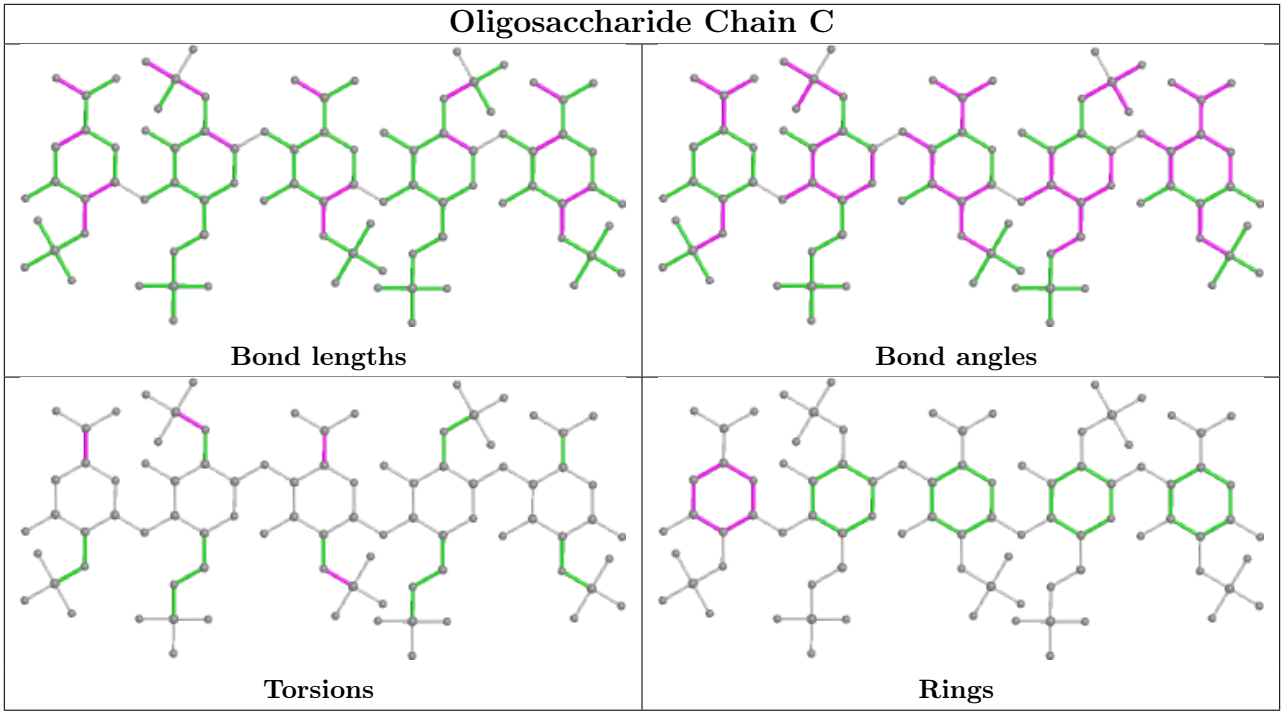
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	IDS	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	IDS	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.



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	EPE	A	306	-	15,15,15	1.29	2 (13%)	18,20,20	0.90	0
3	EPE	B	301	-	15,15,15	1.17	1 (6%)	18,20,20	1.76	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	306	-	-	3/9/19/19	0/1/1/1
3	EPE	B	301	-	-	3/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	EPE	C6-N1	2.32	1.53	1.46
3	B	301	EPE	C6-N1	2.24	1.53	1.46
3	A	306	EPE	C10-S	2.19	1.80	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	EPE	O1S-S-C10	-5.54	100.25	106.92
3	B	301	EPE	O2S-S-C10	3.73	111.41	106.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	EPE	C10-C9-N1-C2
3	B	301	EPE	C10-C9-N1-C6
3	B	301	EPE	N4-C7-C8-O8
3	A	306	EPE	C10-C9-N1-C2
3	A	306	EPE	C10-C9-N1-C6
3	A	306	EPE	N4-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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	171/183 (93%)	1.00	30 (17%)	1	1	35, 56, 77, 94	0
1	B	114/183 (62%)	1.11	19 (16%)	1	2	24, 48, 105, 110	0
All	All	285/366 (77%)	1.05	49 (17%)	1	1	24, 55, 99, 110	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	9.0
1	B	210	GLU	8.3
1	A	53	ILE	6.2
1	B	119	TYR	6.1
1	A	56	ALA	6.0
1	B	208	GLU	4.8
1	B	99	PHE	4.8
1	B	101	PHE	4.7
1	A	196	VAL	4.7
1	A	88	VAL	4.6
1	A	96	CYS	4.3
1	A	188	TRP	4.2
1	A	87	PHE	4.0
1	B	50	LEU	3.8
1	A	51	ILE	3.7
1	B	84	CYS	3.6
1	B	87	PHE	3.6
1	B	47	LYS	3.5
1	A	38	THR	3.4
1	B	168	ARG	3.3
1	A	86	ALA	3.2
1	B	184	GLU	3.2
1	A	189	CYS	3.0
1	A	169	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	2.9
1	A	69	GLN	2.9
1	A	149	CYS	2.8
1	B	86	ALA	2.8
1	A	177	CYS	2.8
1	A	107	GLY	2.8
1	B	190	PHE	2.8
1	A	190	PHE	2.7
1	A	147	ILE	2.7
1	B	46	ALA	2.6
1	B	188	TRP	2.6
1	B	102	ASN	2.5
1	A	54	ASP	2.4
1	A	208	GLU	2.4
1	A	118	LEU	2.4
1	A	207	SER	2.3
1	A	97	LEU	2.3
1	A	157	PRO	2.3
1	A	60	LYS	2.2
1	A	108	VAL	2.2
1	B	42	PHE	2.2
1	A	106	SER	2.2
1	A	187	PRO	2.2
1	B	207	SER	2.2
1	A	193	ASN	2.1

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, 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	IDS	C	1	17/17	0.78	0.28	73,94,102,102	3
2	IDS	C	5	15/17	0.82	0.34	95,97,99,100	0
2	IDS	C	3	16/17	0.88	0.22	73,77,85,85	0

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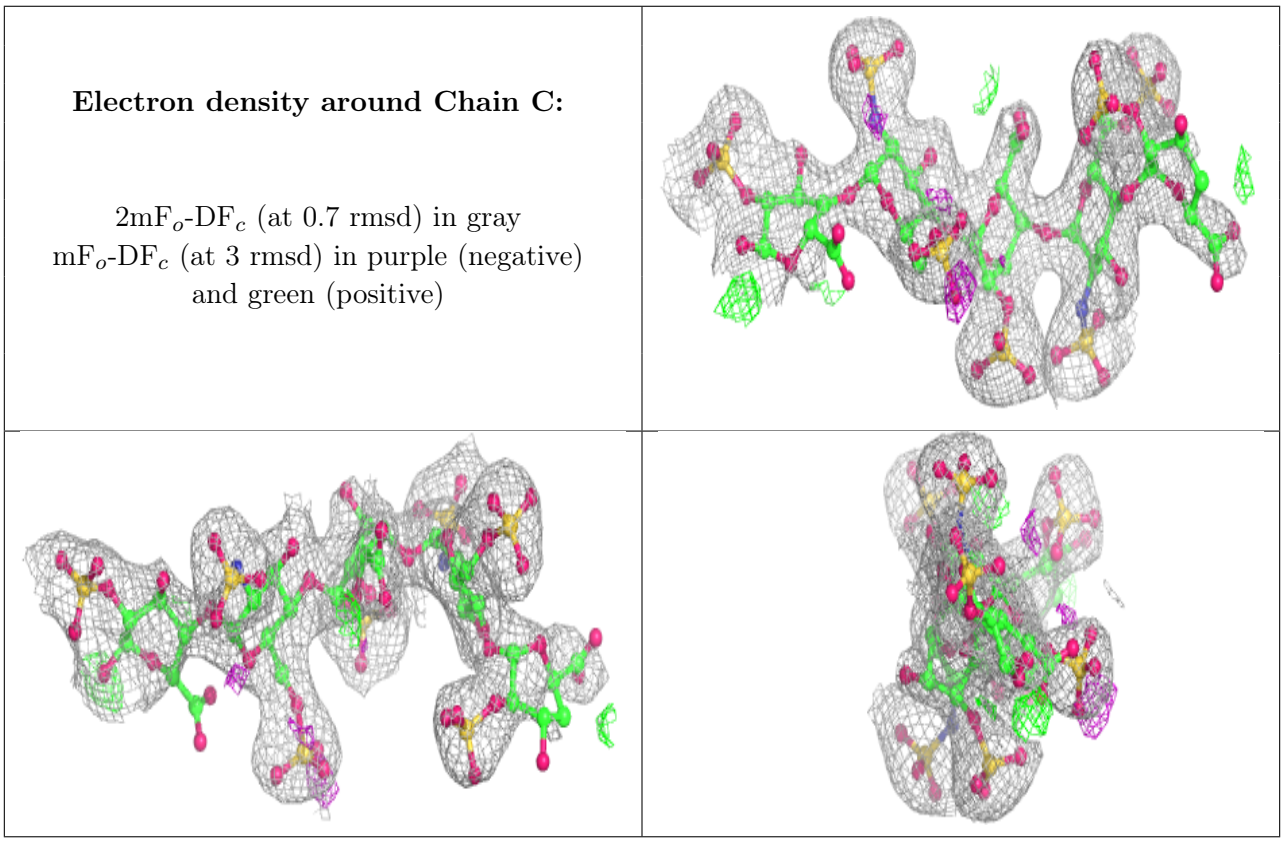
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SGN	C	2	19/20	0.89	0.18	56,67,71,72	0
2	SGN	C	4	19/20	0.91	0.17	84,86,88,93	0

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

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	EPE	A	306	15/15	0.91	0.23	63,64,67,67	0
3	EPE	B	301	15/15	0.94	0.22	30,46,50,50	0

6.5 Other polymers

There are no such residues in this entry.