



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:30 AM BST

PDB ID : 3SWW
Title : Crystal structure of human dpp-iv in complex with sa-(+)-3-(aminomethyl)-4-(2,4-dichlorophenyl)-6-(2-methoxyphenyl)-2-methyl-5h-pyrrolo[3,4-b]pyridin-7(6h)-one
Authors : Klei, H.E.
Deposited on : 2011-07-14
Resolution : 2.00 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 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 : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

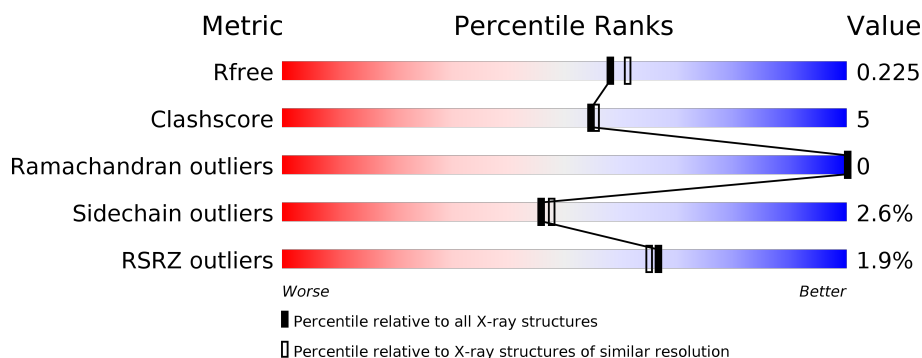
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	753	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	753	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2191	-	-	-	X
3	NAG	B	2191	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12465 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5896	3796	958	1116	26			
1	B	727	Total	C	N	O	S	0	0	0
			5892	3792	956	1118	26			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLU	-	expression tag	UNP P27487
A	38	PHE	-	expression tag	UNP P27487
A	767	PRO	-	expression tag	UNP P27487
A	768	LEU	-	expression tag	UNP P27487
A	769	GLU	-	expression tag	UNP P27487
A	770	GLN	-	expression tag	UNP P27487
A	771	LYS	-	expression tag	UNP P27487
A	772	LEU	-	expression tag	UNP P27487
A	773	ILE	-	expression tag	UNP P27487
A	774	SER	-	expression tag	UNP P27487
A	775	GLU	-	expression tag	UNP P27487
A	776	GLU	-	expression tag	UNP P27487
A	777	ASP	-	expression tag	UNP P27487
A	778	LEU	-	expression tag	UNP P27487
A	779	ASN	-	expression tag	UNP P27487
A	780	SER	-	expression tag	UNP P27487
A	781	ALA	-	expression tag	UNP P27487
A	782	VAL	-	expression tag	UNP P27487
A	783	ASP	-	expression tag	UNP P27487
A	784	HIS	-	expression tag	UNP P27487
A	785	HIS	-	expression tag	UNP P27487
A	786	HIS	-	expression tag	UNP P27487
A	787	HIS	-	expression tag	UNP P27487
A	788	HIS	-	expression tag	UNP P27487
A	789	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLU	-	expression tag	UNP P27487
B	38	PHE	-	expression tag	UNP P27487
B	767	PRO	-	expression tag	UNP P27487
B	768	LEU	-	expression tag	UNP P27487
B	769	GLU	-	expression tag	UNP P27487
B	770	GLN	-	expression tag	UNP P27487
B	771	LYS	-	expression tag	UNP P27487
B	772	LEU	-	expression tag	UNP P27487
B	773	ILE	-	expression tag	UNP P27487
B	774	SER	-	expression tag	UNP P27487
B	775	GLU	-	expression tag	UNP P27487
B	776	GLU	-	expression tag	UNP P27487
B	777	ASP	-	expression tag	UNP P27487
B	778	LEU	-	expression tag	UNP P27487
B	779	ASN	-	expression tag	UNP P27487
B	780	SER	-	expression tag	UNP P27487
B	781	ALA	-	expression tag	UNP P27487
B	782	VAL	-	expression tag	UNP P27487
B	783	ASP	-	expression tag	UNP P27487
B	784	HIS	-	expression tag	UNP P27487
B	785	HIS	-	expression tag	UNP P27487
B	786	HIS	-	expression tag	UNP P27487
B	787	HIS	-	expression tag	UNP P27487
B	788	HIS	-	expression tag	UNP P27487
B	789	HIS	-	expression tag	UNP P27487

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



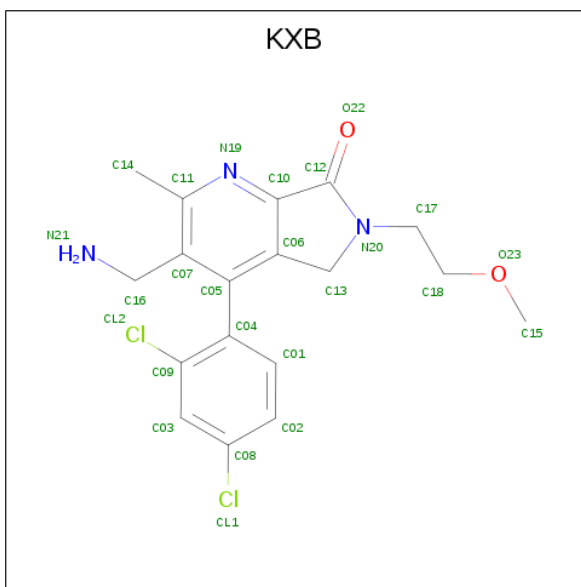
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 3-(aminomethyl)-4-(2,4-dichlorophenyl)-6-(2-methoxyethyl)-2-methyl-5,6-dihydro-7H-pyrrolo[3,4-b]pyridin-7-one (three-letter code: KXB) (formula: C₁₈H₁₉Cl₂N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	2	3	2		
4	B	1	Total	C	Cl	N	O	0	0
			25	18	2	3	2		

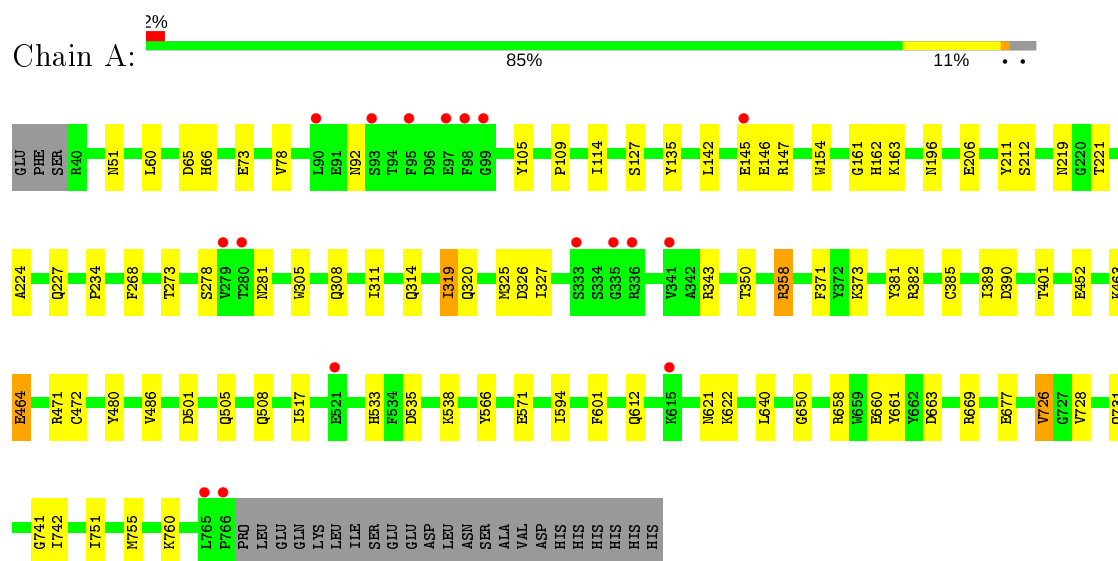
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	213	Total	O	0	0
			213	213		

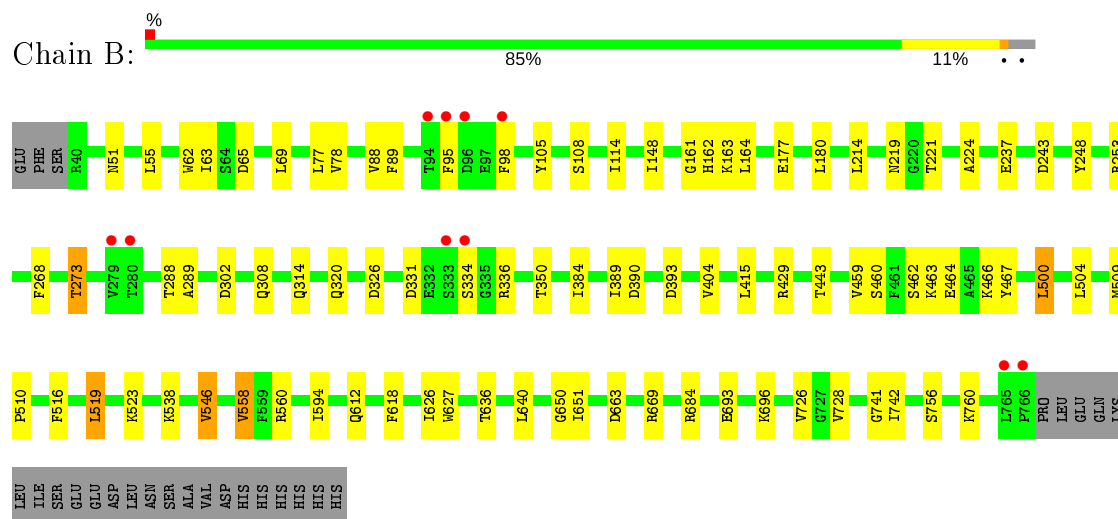
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



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

Chain C:  100%

HA01
HA02

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

Chain D:  50% 50%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.53Å 67.93Å 423.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.16 – 2.00 47.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.8 (47.16-2.00) 84.8 (47.16-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.00Å)	Xtriage
Refinement program	PHENIX dev_613	Depositor
R, R_{free}	0.197 , 0.234 0.188 , 0.225	Depositor DCC
R_{free} test set	5541 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12465	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: KXB, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/6068	0.54	0/8266
1	B	0.38	0/6064	0.55	0/8259
All	All	0.38	0/12132	0.54	0/16525

There are no bond length outliers.

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	5896	0	5536	66	0
1	B	5892	0	5514	54	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	70	0	65	5	0
3	B	70	0	65	1	0
4	A	25	0	19	0	0
4	B	25	0	19	0	0
5	A	218	0	0	8	0
5	B	213	0	0	10	0
All	All	12465	0	11268	121	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 5.

All (121) 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:B:162:HIS:HB3	5:B:800:HOH:O	1.58	1.00
1:A:508:GLN:HE21	1:A:533:HIS:CE1	1.85	0.95
1:A:319:ILE:HD12	1:A:319:ILE:H	1.32	0.93
1:A:508:GLN:HE21	1:A:533:HIS:HE1	1.15	0.92
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.80	0.81
1:B:462:SER:OG	5:B:802:HOH:O	1.97	0.81
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.63	0.81
1:A:135:TYR:HD1	1:A:142:LEU:HD12	1.49	0.77
1:B:108:SER:HB2	5:B:800:HOH:O	1.86	0.75
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.87	0.74
1:A:660:GLU:HG2	5:A:904:HOH:O	1.86	0.74
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.56	0.70
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.73	0.70
1:A:147:ARG:HE	3:A:1501:NAG:H83	1.57	0.69
1:A:219:ASN:HB2	1:A:308:GLN:OE1	1.92	0.69
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.78	0.66
1:B:95:PHE:HB3	1:B:98:PHE:HB2	1.79	0.65
1:A:508:GLN:NE2	1:A:533:HIS:HE1	1.92	0.65
1:A:281:ASN:ND2	3:A:2811:NAG:C1	2.60	0.65
1:A:471:ARG:HD2	1:A:480:TYR:CE2	2.32	0.64
1:A:145:GLU:HG2	1:A:146:GLU:HG2	1.80	0.64
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.34	0.63
1:B:519:LEU:HB3	3:B:5201:NAG:H82	1.80	0.63
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.79	0.63
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.79	0.63
1:A:281:ASN:HD21	3:A:2811:NAG:C1	2.13	0.62
1:A:109:PRO:HD2	1:A:161:GLY:O	2.01	0.61
1:B:161:GLY:O	5:B:800:HOH:O	2.16	0.60
1:A:358:ARG:NH1	5:A:930:HOH:O	2.34	0.60
1:A:319:ILE:HD12	1:A:319:ILE:N	2.13	0.59
1:A:471:ARG:HD2	1:A:480:TYR:HE2	1.66	0.59
1:A:358:ARG:NH1	1:A:358:ARG:HB3	2.17	0.58
1:A:389:ILE:O	1:A:390:ASP:HB2	2.03	0.58
1:B:466:LYS:N	5:B:802:HOH:O	2.35	0.58
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.86	0.58
1:B:63:ILE:HD13	1:B:69:LEU:HG	1.84	0.58
1:A:658:ARG:CZ	5:A:975:HOH:O	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG23	5:B:809:HOH:O	2.02	0.58
1:A:221:THR:O	1:A:273:THR:HB	2.06	0.56
1:B:558:VAL:HG22	1:B:560:ARG:NH1	2.21	0.56
1:B:693:GLU:HG2	1:B:726:VAL:HG21	1.86	0.56
1:B:55:LEU:HD23	1:B:500:LEU:HD12	1.89	0.55
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.06	0.55
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.89	0.55
1:A:65:ASP:OD1	1:A:463:LYS:O	2.26	0.54
1:B:65:ASP:OD1	1:B:463:LYS:O	2.26	0.53
1:A:319:ILE:H	1:A:319:ILE:CD1	2.08	0.53
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.90	0.53
1:B:538:LYS:O	1:B:618:PHE:HA	2.09	0.53
1:A:501:ASP:O	1:A:505:GLN:HG3	2.08	0.53
1:B:516:PHE:CZ	1:B:523:LYS:HE2	2.44	0.53
1:A:281:ASN:HD21	3:A:2811:NAG:C2	2.21	0.52
1:A:314:GLN:HG3	1:A:325:MET:HG3	1.90	0.52
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.91	0.52
1:A:135:TYR:CD1	1:A:142:LEU:HD12	2.39	0.52
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.67	0.52
1:B:558:VAL:HG22	1:B:560:ARG:CZ	2.40	0.51
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.27	0.51
1:B:288:THR:HG22	1:B:289:ALA:O	2.10	0.51
1:A:163:LYS:HZ3	1:A:273:THR:HG22	1.75	0.51
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.94	0.50
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.46	0.50
1:B:389:ILE:O	1:B:390:ASP:HB2	2.11	0.50
1:A:463:LYS:O	1:A:464:GLU:HB2	2.11	0.49
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.94	0.49
1:B:415:LEU:HD23	1:B:415:LEU:C	2.34	0.49
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.94	0.48
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.94	0.48
1:B:756:SER:O	1:B:760:LYS:HG3	2.13	0.48
1:B:243:ASP:HB3	5:B:913:HOH:O	2.13	0.47
1:B:148:ILE:HD11	1:B:164:LEU:HD13	1.97	0.47
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.50	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.49	0.46
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.95	0.46
1:B:626:ILE:O	1:B:650:GLY:HA2	2.15	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.51	0.46
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.78	0.46
1:B:384:ILE:HG13	1:B:404:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.31	0.46
1:B:463:LYS:O	1:B:464:GLU:HB2	2.16	0.46
1:B:253:ARG:NH1	5:B:907:HOH:O	2.36	0.46
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.99	0.45
1:B:65:ASP:OD1	1:B:466:LYS:HB2	2.16	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.45
1:A:658:ARG:NH2	5:A:975:HOH:O	2.50	0.45
1:A:751:ILE:O	1:A:755:MET:HG3	2.17	0.45
1:A:66:HIS:HB2	5:A:895:HOH:O	2.17	0.44
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.98	0.44
1:A:382:ARG:NH2	5:A:830:HOH:O	2.50	0.44
1:B:467:TYR:N	5:B:802:HOH:O	2.15	0.44
1:A:535:ASP:HB3	1:A:538:LYS:HG3	1.98	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.52	0.44
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.99	0.44
1:A:73:GLU:OE1	1:A:92:ASN:ND2	2.50	0.44
1:A:281:ASN:HD21	3:A:2811:NAG:C7	2.31	0.43
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.43
1:B:429:ARG:NE	5:B:859:HOH:O	2.40	0.43
1:B:546:VAL:HG11	1:B:626:ILE:HD11	2.00	0.43
1:A:145:GLU:CG	1:A:146:GLU:HG2	2.48	0.43
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.19	0.43
1:A:327:ILE:HB	1:A:343:ARG:HD3	2.01	0.43
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.54	0.43
1:A:594:ILE:HG23	1:A:594:ILE:O	2.18	0.43
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.49	0.42
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.54	0.42
1:A:726:VAL:HG13	1:A:726:VAL:O	2.18	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.42
1:A:571:GLU:CD	1:A:760:LYS:HD3	2.39	0.42
1:A:658:ARG:NE	5:A:975:HOH:O	2.52	0.42
1:B:594:ILE:O	1:B:594:ILE:HG23	2.20	0.42
2:D:1:NAG:H61	2:D:2:NAG:H82	2.00	0.42
1:B:221:THR:O	1:B:273:THR:HG22	2.20	0.42
1:B:459:VAL:HG22	1:B:460:SER:N	2.35	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.54	0.41
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.56	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.41
1:B:78:VAL:HG23	1:B:89:PHE:HB2	2.02	0.41
1:A:486:VAL:HG13	5:A:900:HOH:O	2.21	0.41
2:C:1:NAG:H61	2:C:2:NAG:C7	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD12	1:A:60:LEU:C	2.42	0.41
1:A:658:ARG:HD3	1:A:661:TYR:CZ	2.55	0.41

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	725/753 (96%)	694 (96%)	31 (4%)	0	100	100
1	B	725/753 (96%)	698 (96%)	27 (4%)	0	100	100
All	All	1450/1506 (96%)	1392 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	631/677 (93%)	612 (97%)	19 (3%)	41	41
1	B	629/677 (93%)	615 (98%)	14 (2%)	52	55
All	All	1260/1354 (93%)	1227 (97%)	33 (3%)	46	48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	78	VAL
1	A	162	HIS
1	A	278	SER
1	A	319	ILE
1	A	326	ASP
1	A	350	THR
1	A	358	ARG
1	A	373	LYS
1	A	385	CYS
1	A	452	GLU
1	A	464	GLU
1	A	472	CYS
1	A	566	TYR
1	A	621	ASN
1	A	622	LYS
1	A	677	GLU
1	A	726	VAL
1	A	731	GLN
1	B	51	ASN
1	B	214	LEU
1	B	273	THR
1	B	326	ASP
1	B	336	ARG
1	B	350	THR
1	B	393	ASP
1	B	500	LEU
1	B	519	LEU
1	B	546	VAL
1	B	558	VAL
1	B	612	GLN
1	B	663	ASP
1	B	684	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	247	GLN
1	A	281	ASN
1	A	388	GLN
1	A	506	ASN
1	A	533	HIS

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Mol	Chain	Res	Type
1	A	586	GLN
1	A	592	HIS
1	A	748	HIS
1	A	757	HIS
1	B	103	ASN
1	B	123	GLN
1	B	169	ASN
1	B	383	HIS
1	B	586	GLN
1	B	612	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 ⓘ

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	NAG	C	1	1,2	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.06	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.53	0	17,19,21	0.99	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	1.12	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	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(°)
2	C	2	NAG	C1-O5-C5	3.35	116.73	112.19
2	D	2	NAG	C1-O5-C5	2.61	115.73	112.19
2	C	1	NAG	O5-C5-C6	2.52	111.16	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

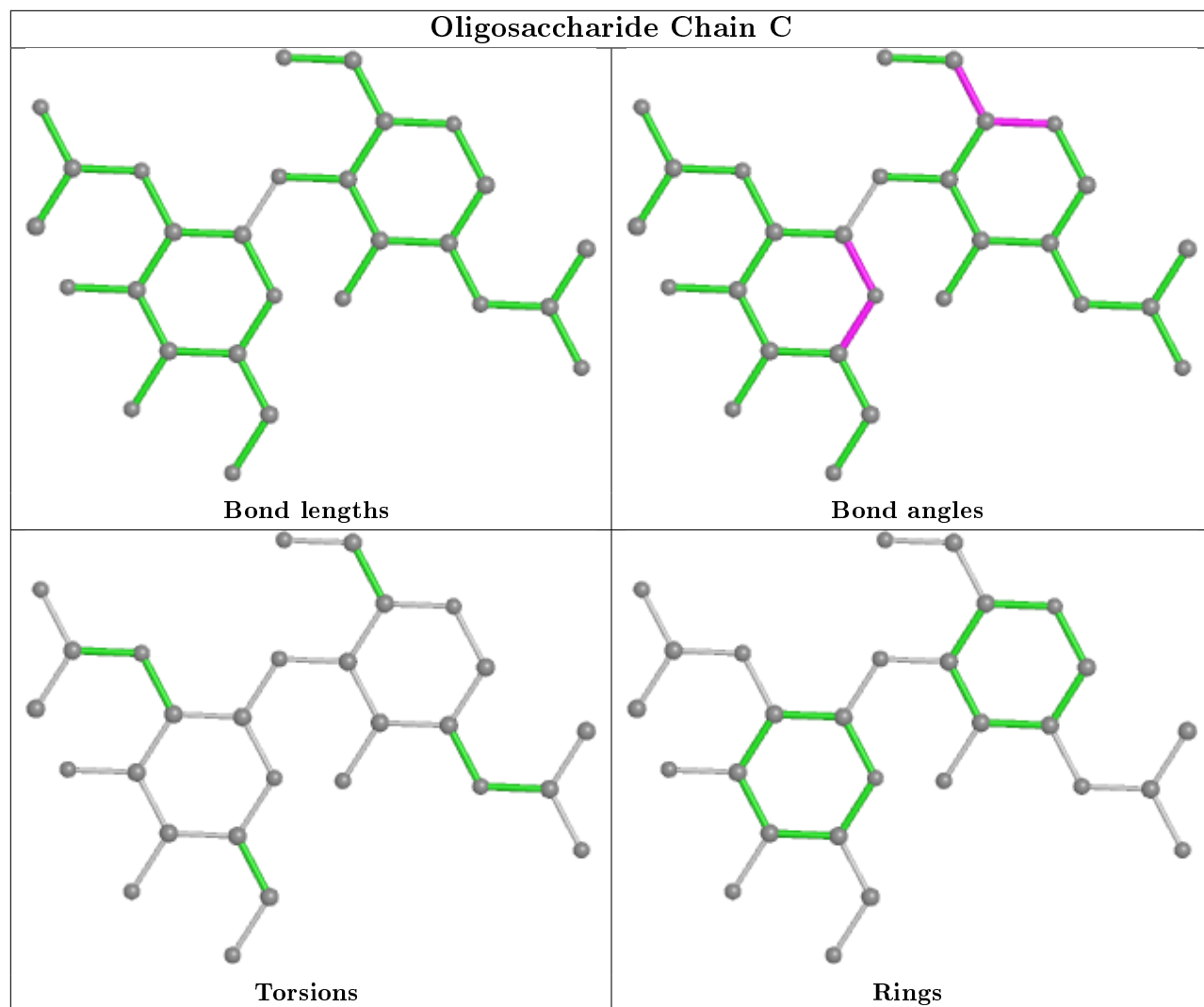
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

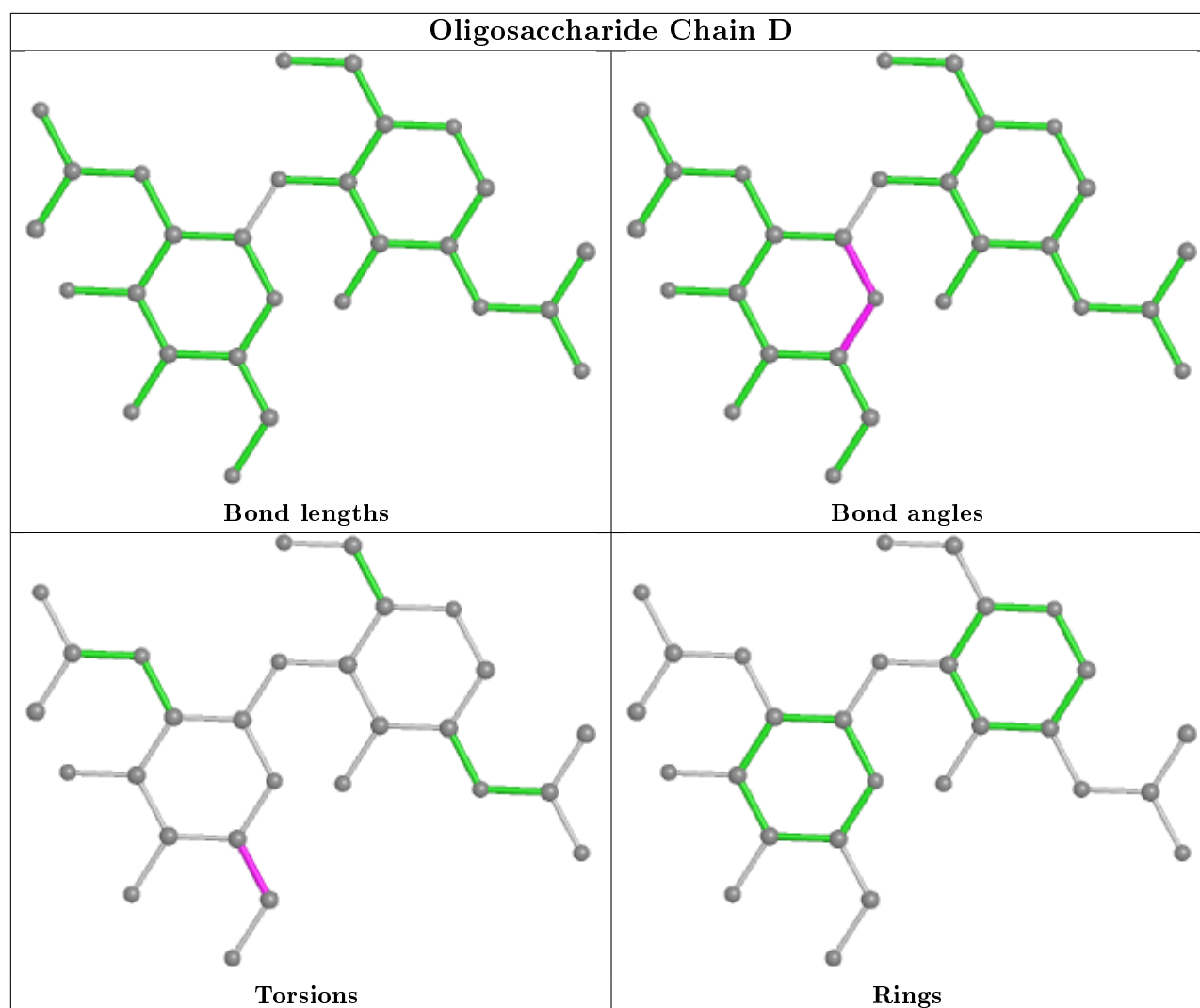
There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	D	2	NAG	1	0
2	D	1	NAG	1	0
2	C	1	NAG	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 ⓘ

12 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	NAG	A	2191	1	14,14,15	0.66	0	17,19,21	1.31	1 (5%)
3	NAG	B	1501	1	14,14,15	0.63	0	17,19,21	0.85	1 (5%)
3	NAG	B	921	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	851	1	14,14,15	0.72	0	17,19,21	1.20	1 (5%)
3	NAG	B	5201	1	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
3	NAG	A	5201	1	14,14,15	0.38	0	17,19,21	1.68	3 (17%)
3	NAG	A	851	1	14,14,15	0.65	0	17,19,21	0.94	0
3	NAG	B	2191	1	14,14,15	0.59	0	17,19,21	1.02	1 (5%)
3	NAG	A	1501	1	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
4	KXB	A	1	-	27,27,27	1.16	3 (11%)	33,39,39	1.22	5 (15%)
3	NAG	A	2811	-	14,14,15	0.55	0	17,19,21	0.92	0
4	KXB	B	2	-	27,27,27	1.35	5 (18%)	33,39,39	1.14	3 (9%)

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	A	2191	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	921	1	-	2/6/23/26	0/1/1/1
3	NAG	B	851	1	-	0/6/23/26	0/1/1/1
3	NAG	B	5201	1	-	4/6/23/26	0/1/1/1
3	NAG	A	5201	1	-	0/6/23/26	0/1/1/1
3	NAG	A	851	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2191	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
4	KXB	A	1	-	-	3/9/22/22	0/3/3/3
3	NAG	A	2811	-	-	2/6/23/26	0/1/1/1
4	KXB	B	2	-	-	4/9/22/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	KXB	C12-N20	3.90	1.42	1.36
4	B	2	KXB	C04-C05	-3.02	1.46	1.50
4	A	1	KXB	C17-C18	2.98	1.60	1.50
4	B	2	KXB	C11-N19	2.79	1.38	1.34
4	B	2	KXB	C17-C18	2.56	1.58	1.50
4	A	1	KXB	C11-N19	2.20	1.37	1.34
4	A	1	KXB	C12-N20	2.14	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	KXB	C08-CL1	-2.04	1.70	1.74

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5201	NAG	C1-O5-C5	5.01	118.98	112.19
3	A	2191	NAG	C1-O5-C5	4.17	117.85	112.19
3	B	921	NAG	C1-O5-C5	3.12	116.42	112.19
3	B	2191	NAG	C1-O5-C5	3.04	116.31	112.19
3	B	851	NAG	C1-O5-C5	2.90	116.12	112.19
3	A	5201	NAG	C3-C4-C5	2.88	115.38	110.24
3	B	5201	NAG	C1-O5-C5	2.87	116.08	112.19
4	B	2	KXB	C05-C06-C10	-2.63	118.95	120.10
3	B	1501	NAG	C4-C3-C2	2.56	114.78	111.02
3	A	1501	NAG	O5-C5-C6	2.55	111.20	107.20
4	A	1	KXB	C05-C07-C11	2.33	119.45	117.69
3	B	921	NAG	C2-N2-C7	-2.33	119.59	122.90
3	A	1501	NAG	C1-O5-C5	2.30	115.31	112.19
4	A	1	KXB	C09-C03-C08	-2.28	116.16	118.71
4	A	1	KXB	C14-C11-N19	-2.26	112.99	116.49
3	A	5201	NAG	C6-C5-C4	-2.25	107.74	113.00
4	A	1	KXB	C05-C04-C09	-2.18	119.85	122.32
4	B	2	KXB	C14-C11-N19	-2.17	113.13	116.49
4	A	1	KXB	C10-N19-C11	-2.10	114.26	117.61
4	B	2	KXB	C05-C07-C11	2.03	119.22	117.69

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	921	NAG	C8-C7-N2-C2
3	B	921	NAG	O7-C7-N2-C2
3	B	1501	NAG	O5-C5-C6-O6
3	B	1501	NAG	C4-C5-C6-O6
3	B	2191	NAG	C8-C7-N2-C2
3	A	2811	NAG	C4-C5-C6-O6
3	B	5201	NAG	C8-C7-N2-C2
3	B	2191	NAG	O7-C7-N2-C2
3	A	2811	NAG	O5-C5-C6-O6
3	B	5201	NAG	O7-C7-N2-C2
4	A	1	KXB	C17-C18-O23-C15
4	B	2	KXB	C17-C18-O23-C15

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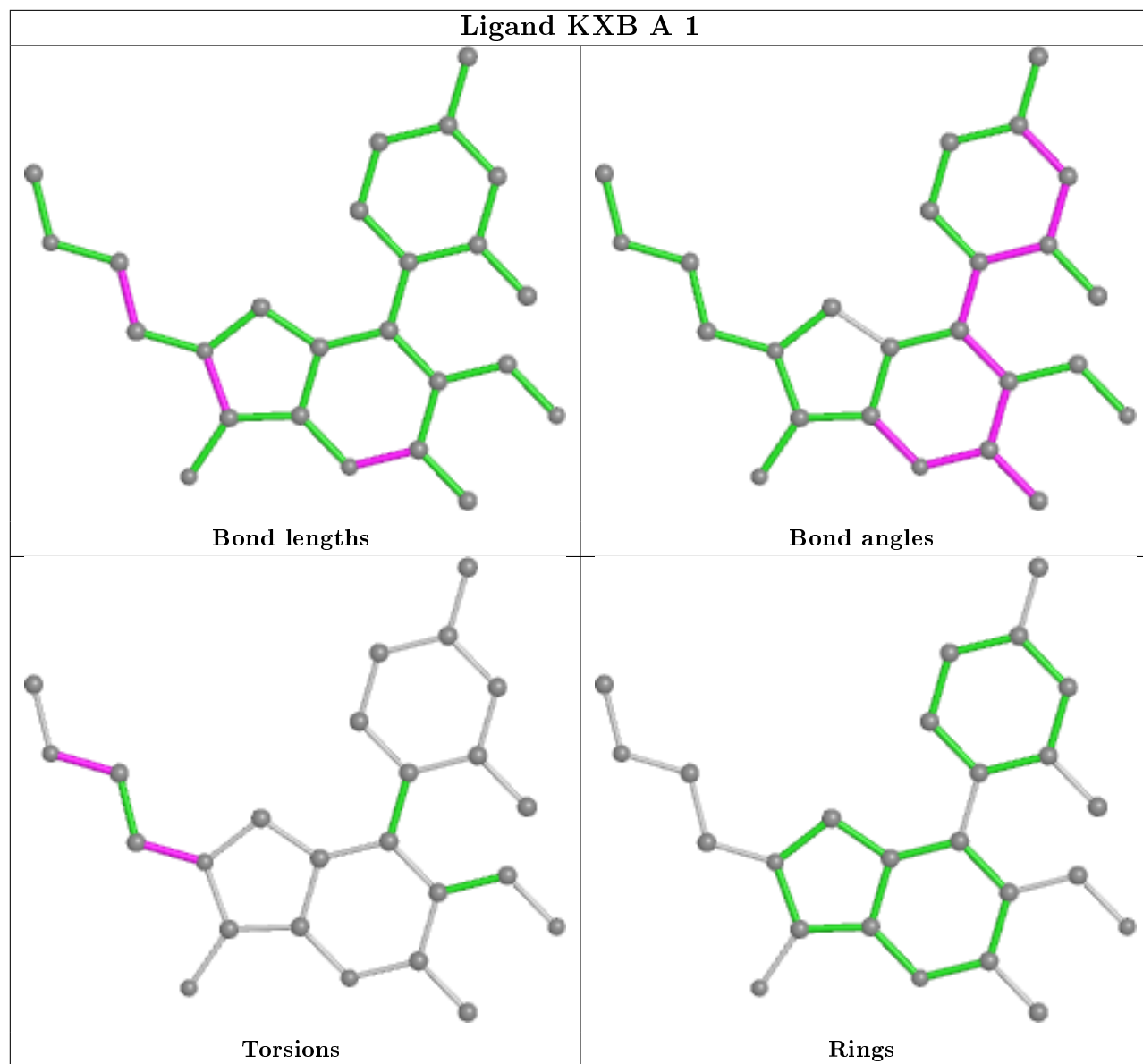
Mol	Chain	Res	Type	Atoms
3	A	2191	NAG	O5-C5-C6-O6
4	A	1	KXB	C18-C17-N20-C12
4	B	2	KXB	C05-C07-C16-N21
3	B	5201	NAG	O5-C5-C6-O6
3	B	5201	NAG	C4-C5-C6-O6
4	B	2	KXB	C18-C17-N20-C12
4	A	1	KXB	C18-C17-N20-C13
4	B	2	KXB	C18-C17-N20-C13

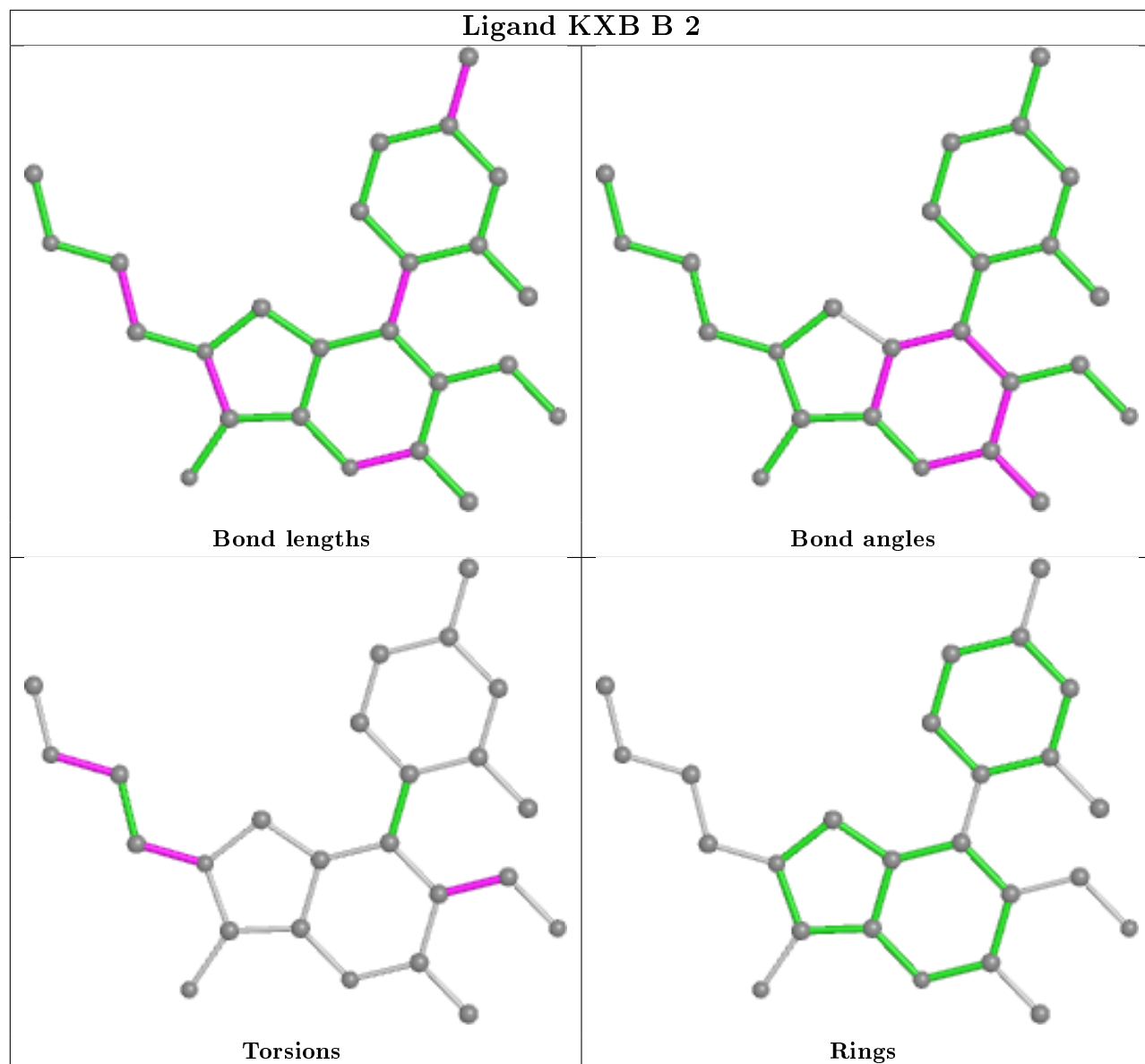
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5201	NAG	1	0
3	A	1501	NAG	1	0
3	A	2811	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	727/753 (96%)	-0.03	17 (2%) 60 59	23, 33, 56, 78	0
1	B	727/753 (96%)	-0.05	10 (1%) 75 74	23, 34, 55, 77	0
All	All	1454/1506 (96%)	-0.04	27 (1%) 66 65	23, 33, 56, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	5.6
1	B	766	PRO	4.1
1	B	765	LEU	3.9
1	A	766	PRO	3.8
1	A	280	THR	3.4
1	B	279	VAL	3.4
1	A	145	GLU	2.9
1	A	95	PHE	2.9
1	B	280	THR	2.7
1	A	97	GLU	2.6
1	A	90	LEU	2.6
1	A	336	ARG	2.6
1	A	341	VAL	2.5
1	A	335	GLY	2.4
1	B	94	THR	2.3
1	B	96	ASP	2.3
1	B	334	SER	2.3
1	B	333	SER	2.3
1	B	98	PHE	2.3
1	A	615	LYS	2.2
1	A	98	PHE	2.2
1	A	93	SER	2.2
1	A	279	VAL	2.1
1	B	95	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	SER	2.1
1	A	99	GLY	2.1
1	A	521	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](#)

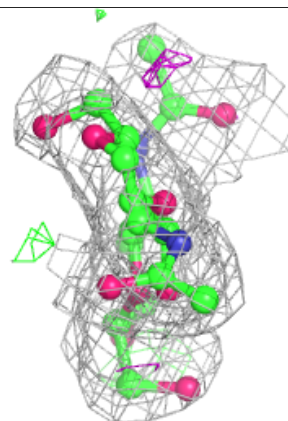
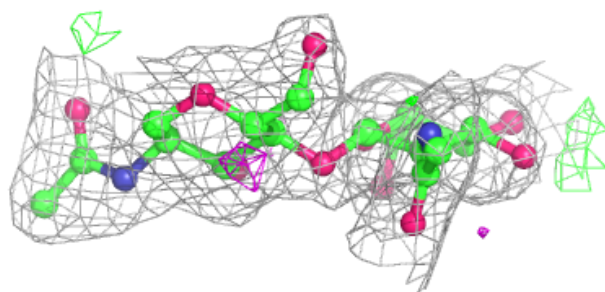
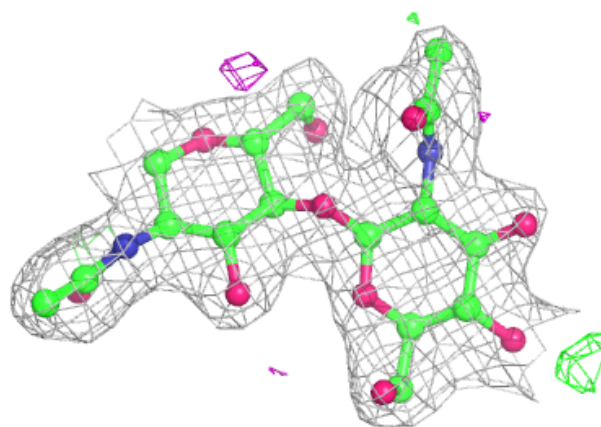
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

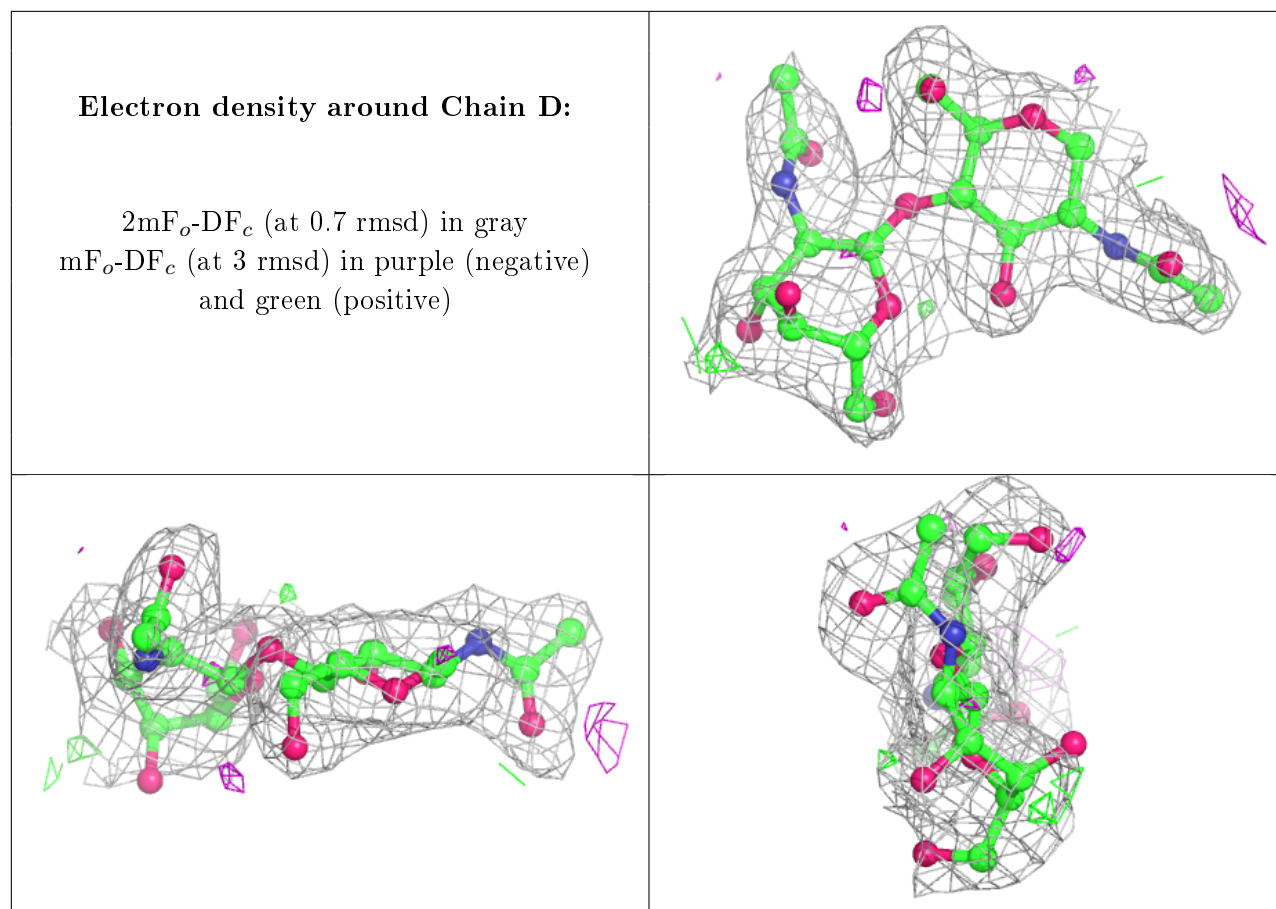
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.76	0.26	54,61,66,66	0
2	NAG	D	2	14/15	0.84	0.33	53,66,72,75	0
2	NAG	C	1	14/15	0.92	0.13	37,45,53,57	0
2	NAG	D	1	14/15	0.93	0.14	37,44,52,56	0

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 C:

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





6.4 Ligands ⓘ

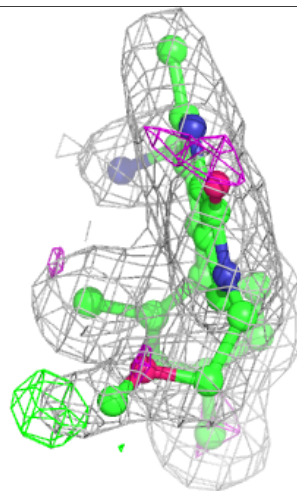
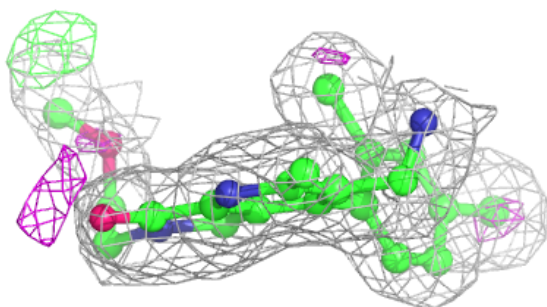
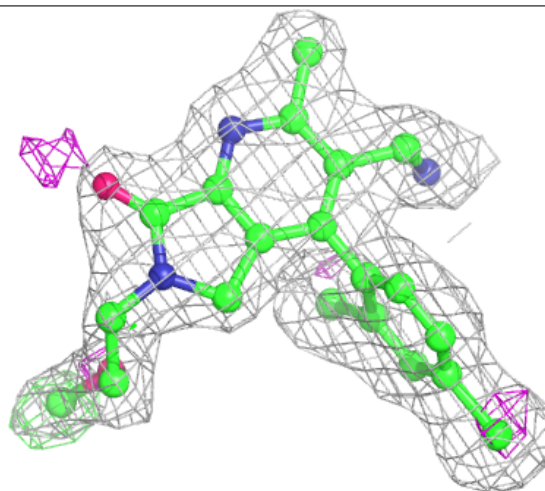
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

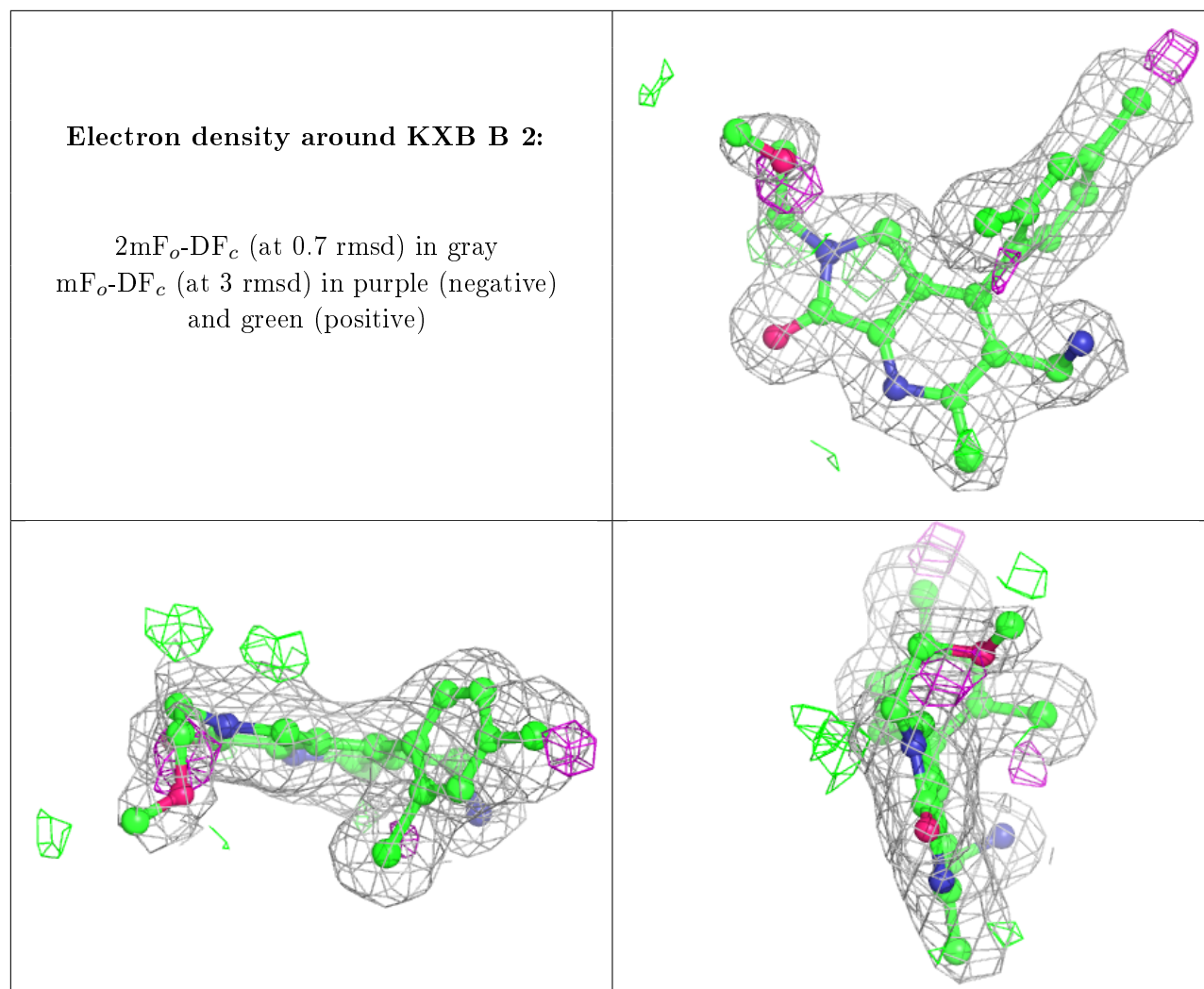
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	2191	14/15	0.62	0.41	58,66,70,70	0
3	NAG	A	2191	14/15	0.71	0.40	49,61,67,68	0
3	NAG	B	5201	14/15	0.72	0.29	49,65,71,71	0
3	NAG	B	1501	14/15	0.78	0.23	40,65,77,82	0
3	NAG	A	5201	14/15	0.82	0.29	47,64,69,69	0
3	NAG	A	2811	14/15	0.85	0.28	61,66,69,73	0
3	NAG	B	921	14/15	0.88	0.24	60,62,66,68	0
3	NAG	A	1501	14/15	0.89	0.21	55,58,62,63	0
4	KXB	A	1	25/25	0.94	0.17	25,31,40,44	0
4	KXB	B	2	25/25	0.94	0.18	23,33,43,50	0
3	NAG	A	851	14/15	0.96	0.08	30,34,36,38	0
3	NAG	B	851	14/15	0.96	0.09	31,35,40,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KXB A 1:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.