Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2024 – 12:36 AM EDT

PDB ID	:	7UBR
Title	:	Integrin alpha IIB beta3 complex with GR144053
Authors	:	Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on	:	2022-03-15
Resolution	:	2.05 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:

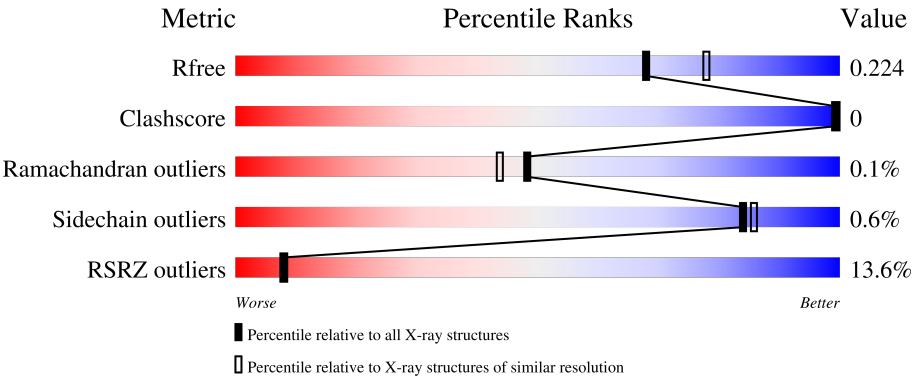
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	454	2% 98%
1	C	454	4% 98%
2	B	472	12% 98%
2	D	472	14% 99%
3	E	221	32% 97%

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Mol	Chain	Length	Quality of chain
3	H	221	29% 97%
4	F	214	24% 100%
4	L	214	16% 99%
5	G	5	60% 40%
6	I	2	100%
6	K	2	100%
7	J	4	50% 50%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22310 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3499	2226	601	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	5	0
			3625	2257	618	716	34			
2	D	471	Total	C	N	O	S	0	1	0
			3633	2261	622	716	34			

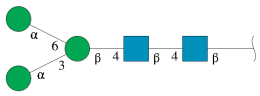
- Molecule 3 is a protein called 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

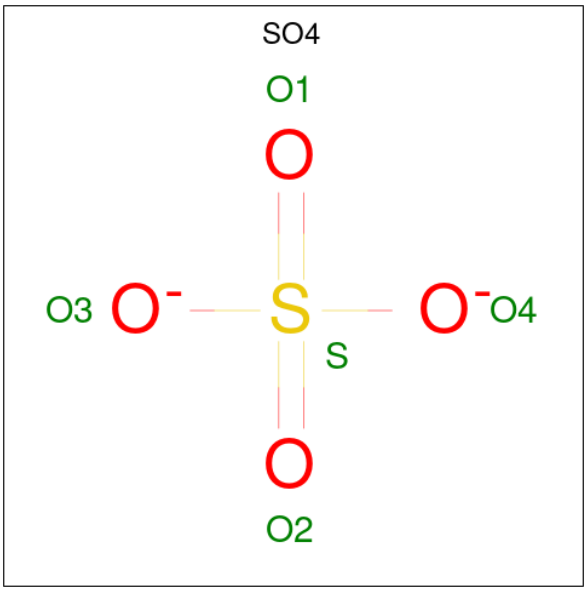
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

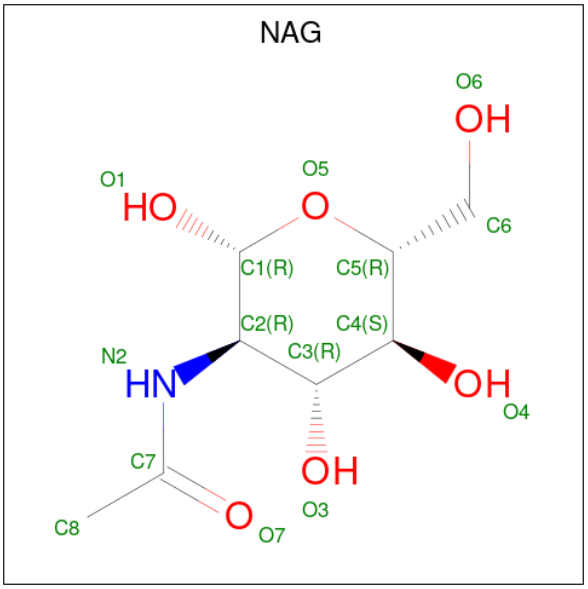
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total Ca 4 4	0	0
9	C	4	Total Ca 4 4	0	0

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

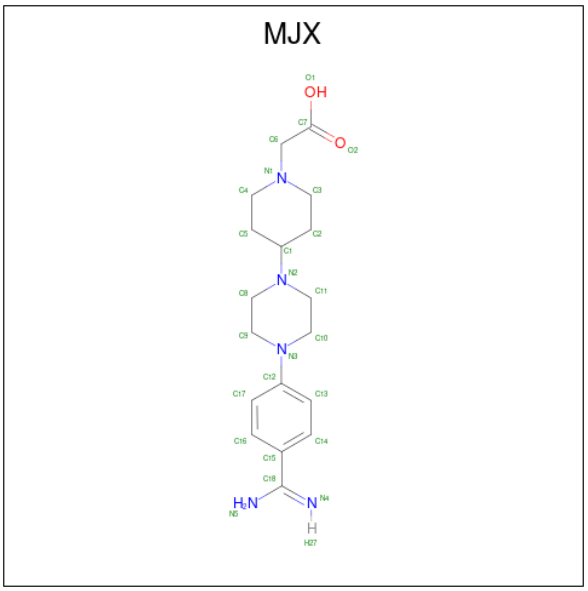
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	3	Total Mn 3 3	0	0
10	D	3	Total Mn 3 3	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is {4-[4-(4-carbamimidoylphenyl)piperazin-1-yl]piperidin-1-yl}acetic acid (three-letter code: MJX) (formula: $C_{18}H_{27}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C N O 25 18 5 2	0	0
12	D	1	Total C N O 25 18 5 2	0	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total Cl 1 1	0	0
13	D	1	Total Cl 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	428	Total O 428 428	0	0
14	B	257	Total O 257 257	0	0
14	C	214	Total O 214 214	0	0
14	D	176	Total O 176 176	0	0
14	E	16	Total O 16 16	0	0

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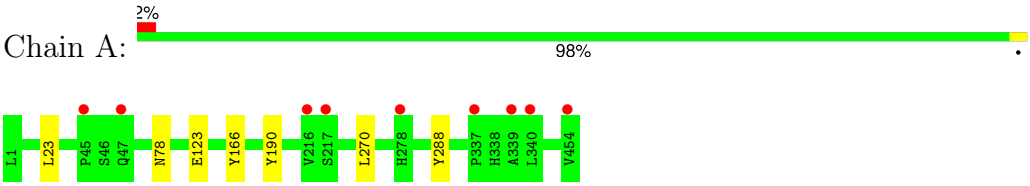
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	12	Total O 12 12	0	0
14	H	34	Total O 34 34	0	0
14	L	46	Total O 46 46	0	0

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.

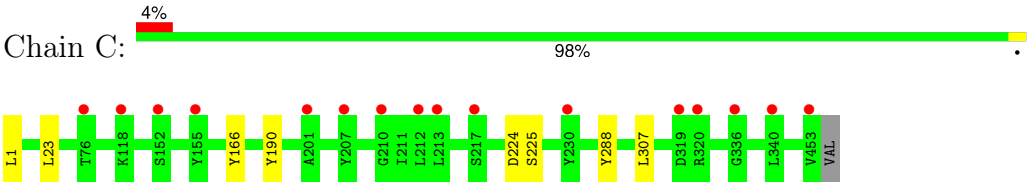
• Molecule 1: Integrin alpha-IIb

Chain A:



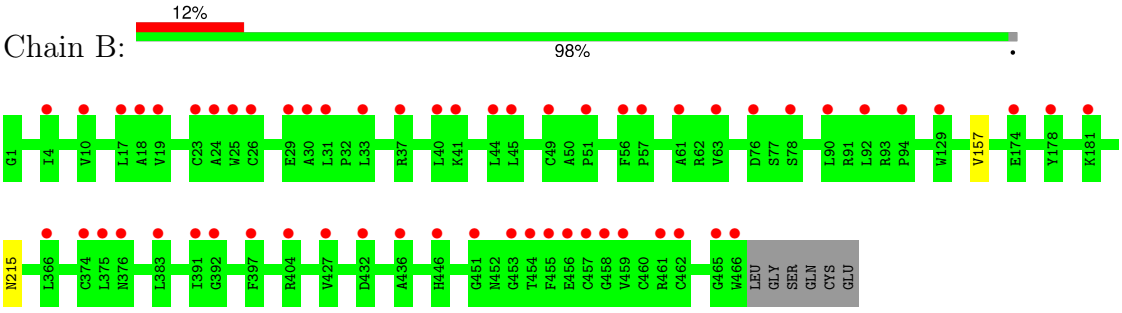
• Molecule 1: Integrin alpha-IIb

Chain C:



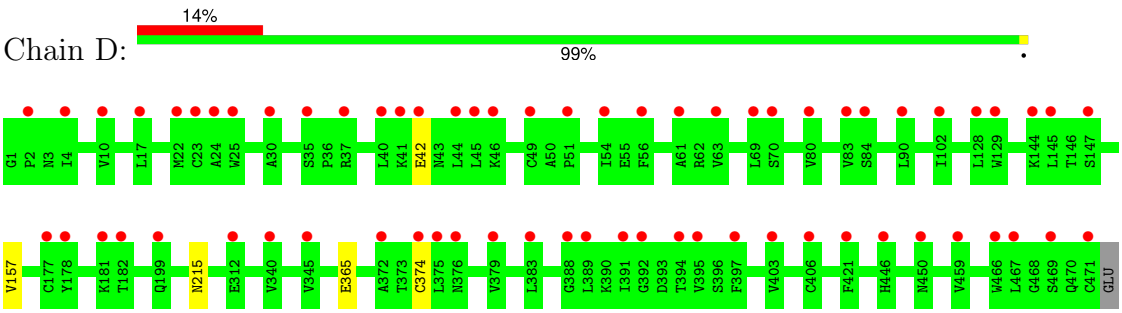
• Molecule 2: Isoform Beta-3C of Integrin beta-3

Chain B:



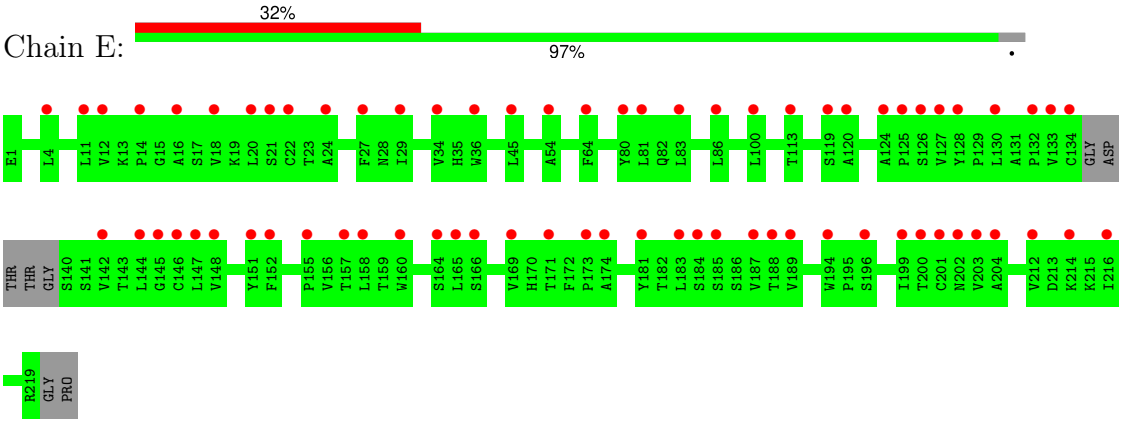
• Molecule 2: Isoform Beta-3C of Integrin beta-3

Chain D:



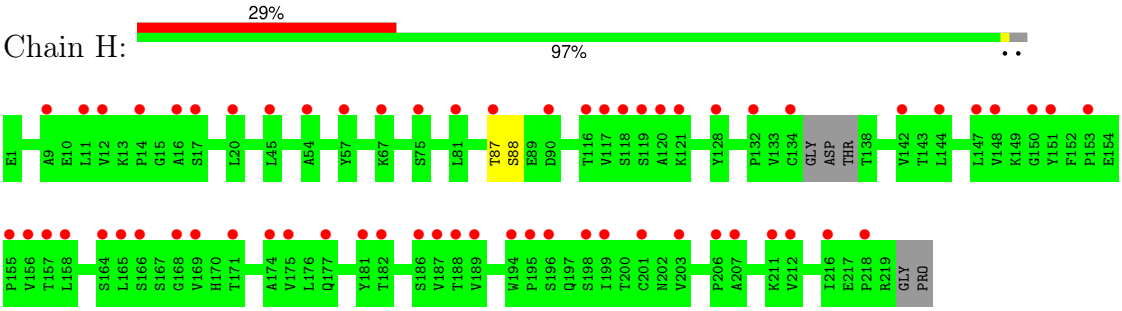
• Molecule 3: 10E5 Fab heavy chain

Chain E:



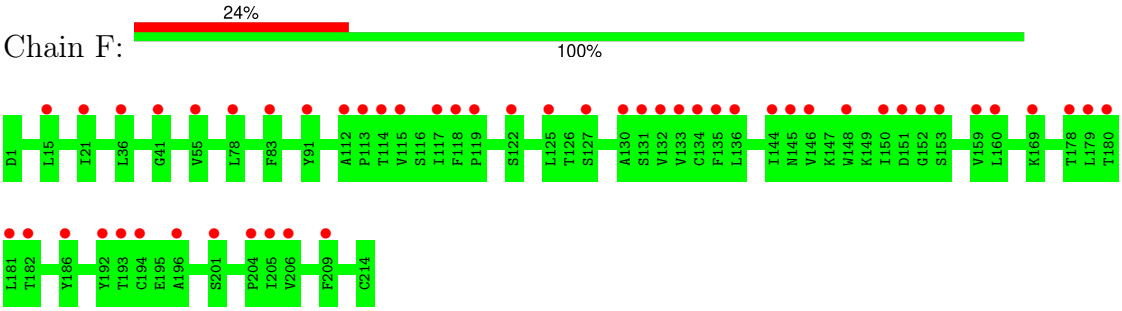
• Molecule 3: 10E5 Fab heavy chain

Chain H:



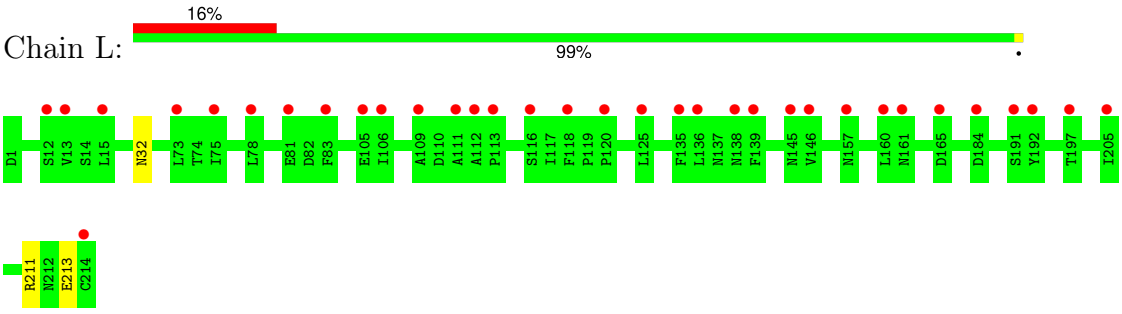
• Molecule 4: 10E5 Fab light chain

Chain F:



• Molecule 4: 10E5 Fab light chain

Chain L:

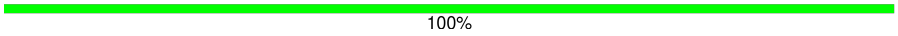


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

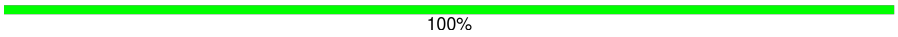
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain K:



• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	257.89Å 144.40Å 104.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.05 49.26 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.26-2.05) 97.0 (49.26-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.209 , 0.223 0.210 , 0.224	Depositor DCC
R_{free} test set	243112 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22310	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: SO4, MJX, NAG, CA, BMA, MAN, MN, CL

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	0.22	0/3608	0.41	0/4918
1	C	0.21	0/3605	0.39	0/4912
2	B	0.22	0/3695	0.39	0/5010
2	D	0.21	0/3701	0.38	0/5018
3	E	0.21	0/1673	0.37	0/2290
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.22	0/1673	0.37	0/2269
All	All	0.21	0/21312	0.38	0/28991

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	3499	0	3345	1	0
1	C	3502	0	3334	3	0
2	B	3625	0	3541	0	0
2	D	3633	0	3546	1	0
3	E	1631	0	1590	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	1	0
4	F	1637	0	1553	0	0
4	L	1637	0	1553	2	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	25	0	0	0	0
8	B	5	0	0	0	0
8	C	20	0	0	0	0
8	D	5	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	25	0	0	0	0
12	D	25	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	A	428	0	0	0	2
14	B	257	0	0	0	0
14	C	214	0	0	2	1
14	D	176	0	0	0	1
14	E	16	0	0	0	0
14	F	12	0	0	0	0
14	H	34	0	0	0	0
14	L	46	0	0	0	0
All	All	22310	0	20233	7	2

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 0.

All (7) 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:1:LEU:N	14:C:607:HOH:O	2.44	0.50
4:L:211:ARG:O	4:L:213:GLU:N	2.46	0.45
1:A:78:ASN:O	4:L:32:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:LEU:N	14:C:614:HOH:O	2.53	0.42
2:D:42:GLU:OE2	2:D:42:GLU:N	2.50	0.41
1:C:224:ASP:OD1	1:C:225:SER:N	2.49	0.40
3:H:87:THR:HG22	3:H:88:SER:N	2.35	0.40

All (2) 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)
14:A:894:HOH:O	14:D:2101:HOH:O[1_554]	2.08	0.12
14:A:935:HOH:O	14:C:784:HOH:O[1_554]	2.14	0.06

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	456/454 (100%)	439 (96%)	16 (4%)	1 (0%)	44 38
1	C	455/454 (100%)	435 (96%)	20 (4%)	0	100 100
2	B	469/472 (99%)	455 (97%)	13 (3%)	1 (0%)	44 38
2	D	470/472 (100%)	453 (96%)	15 (3%)	2 (0%)	30 23
3	E	210/221 (95%)	193 (92%)	17 (8%)	0	100 100
3	H	212/221 (96%)	197 (93%)	15 (7%)	0	100 100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100 100
4	L	212/214 (99%)	201 (95%)	11 (5%)	0	100 100
All	All	2696/2722 (99%)	2572 (95%)	120 (4%)	4 (0%)	48 44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	374	CYS
1	A	123	GLU
2	D	157	VAL
2	B	157	VAL

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	366/362 (101%)	361 (99%)	5 (1%)	62 63
1	C	365/362 (101%)	360 (99%)	5 (1%)	62 63
2	B	417/417 (100%)	416 (100%)	1 (0%)	92 93
2	D	417/417 (100%)	415 (100%)	2 (0%)	86 88
3	E	186/190 (98%)	186 (100%)	0	100 100
3	H	187/190 (98%)	187 (100%)	0	100 100
4	F	188/188 (100%)	188 (100%)	0	100 100
4	L	188/188 (100%)	188 (100%)	0	100 100
All	All	2314/2314 (100%)	2301 (99%)	13 (1%)	84 86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
1	C	307	LEU
2	D	215	ASN

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Mol	Chain	Res	Type
2	D	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

13 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	$\#\|Z\| > 2$
5	NAG	G	1	5,2	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.73	0	15,15,17	0.66	0
5	MAN	G	4	5	11,11,12	0.74	0	15,15,17	1.00	2 (13%)
5	MAN	G	5	5	11,11,12	0.85	0	15,15,17	1.13	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.20	0	17,19,21	0.38	0
6	NAG	I	2	6	14,14,15	0.23	0	17,19,21	0.50	0
7	NAG	J	1	7,2	14,14,15	0.18	0	17,19,21	0.48	0
7	NAG	J	2	7	14,14,15	0.15	0	17,19,21	0.49	0
7	BMA	J	3	7	11,11,12	1.20	2 (18%)	15,15,17	0.96	1 (6%)
7	MAN	J	4	7	11,11,12	0.88	0	15,15,17	1.06	1 (6%)
6	NAG	K	1	6,2	14,14,15	0.43	0	17,19,21	0.46	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	3	BMA	O5-C1	-2.87	1.38	1.43
7	J	3	BMA	C4-C5	2.16	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	4	MAN	C1-O5-C5	2.93	116.12	112.19
5	G	4	MAN	C1-O5-C5	2.52	115.56	112.19
7	J	3	BMA	C3-C4-C5	2.24	114.30	110.23
5	G	5	MAN	C1-O5-C5	2.09	114.99	112.19
5	G	5	MAN	O2-C2-C3	-2.01	105.98	110.15
5	G	4	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

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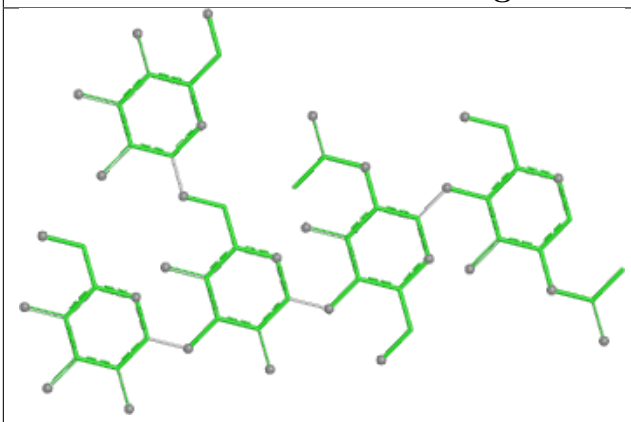
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	K	1	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

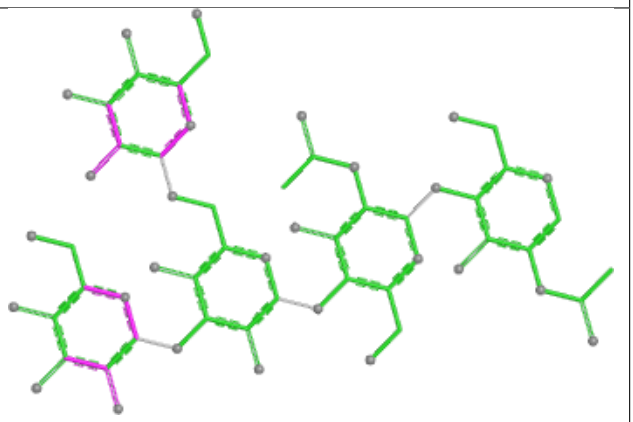
No monomer is involved in short contacts.

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

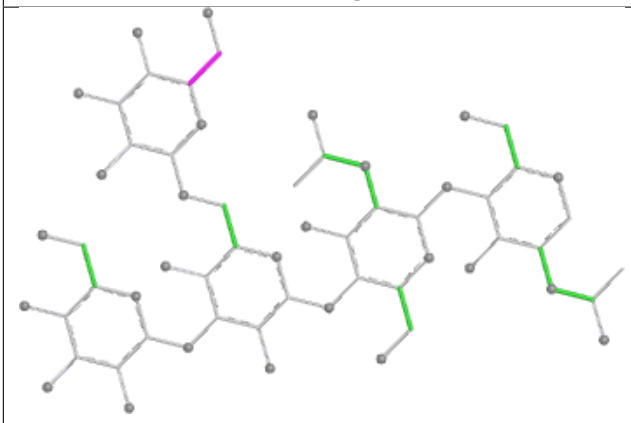
Oligosaccharide Chain G



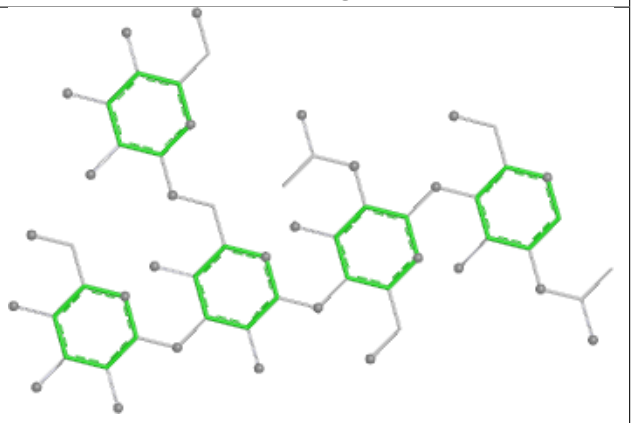
Bond lengths



Bond angles

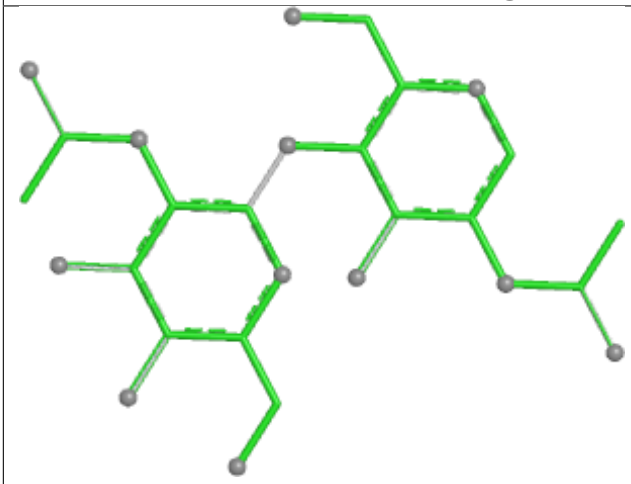


Torsions

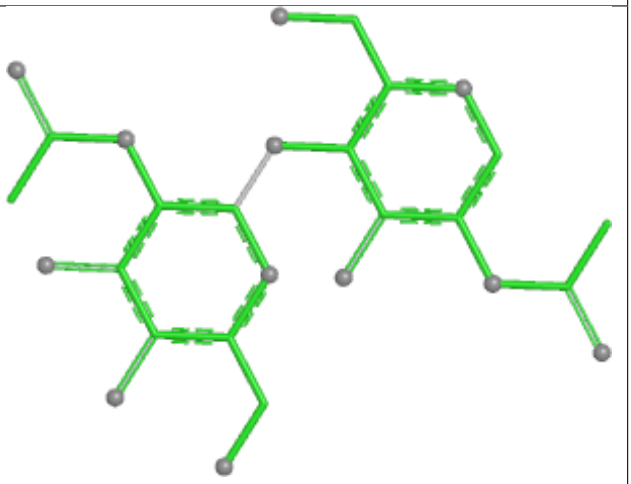


Rings

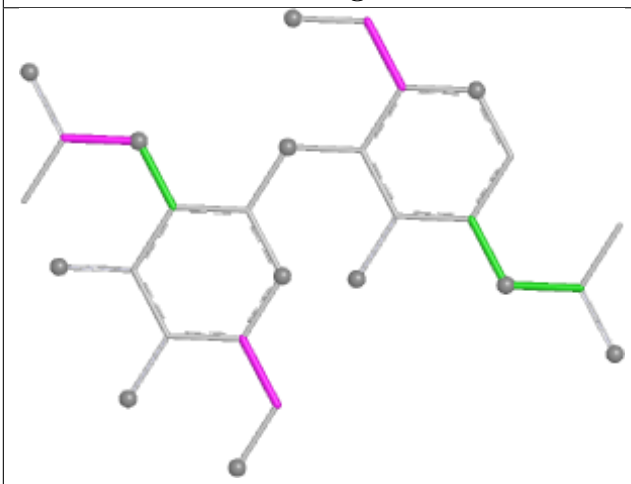
Oligosaccharide Chain I



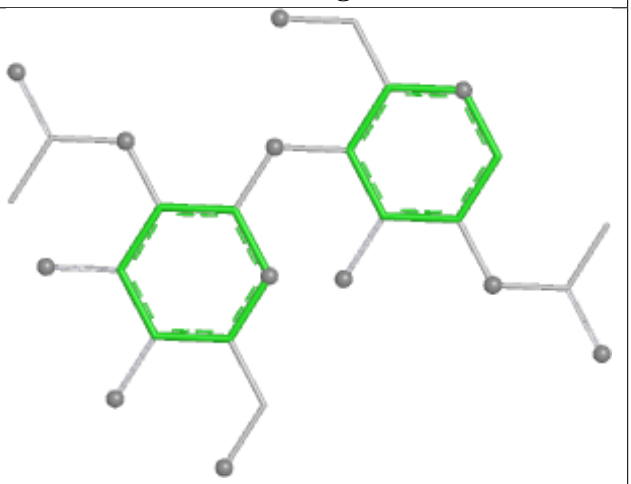
Bond lengths



Bond angles

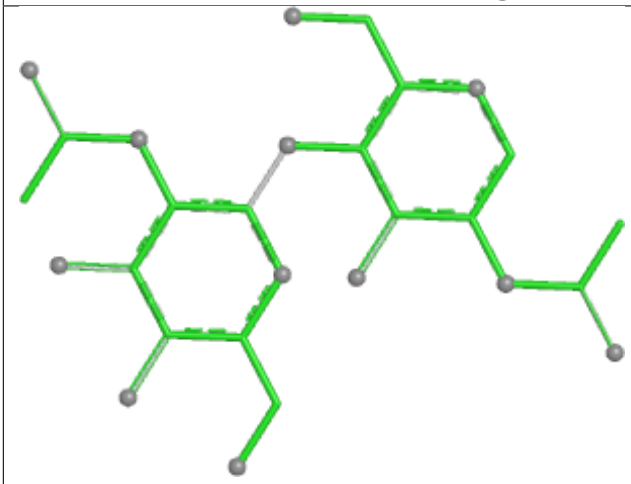


Torsions

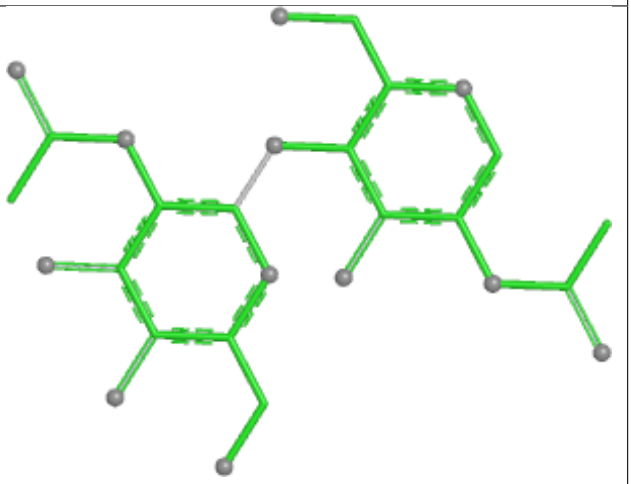


Rings

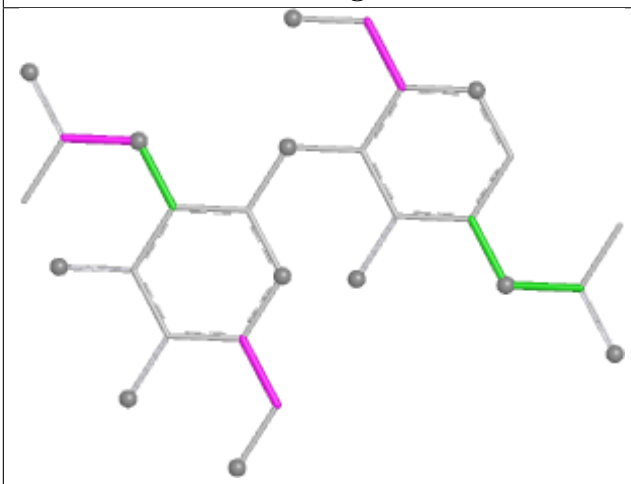
Oligosaccharide Chain K



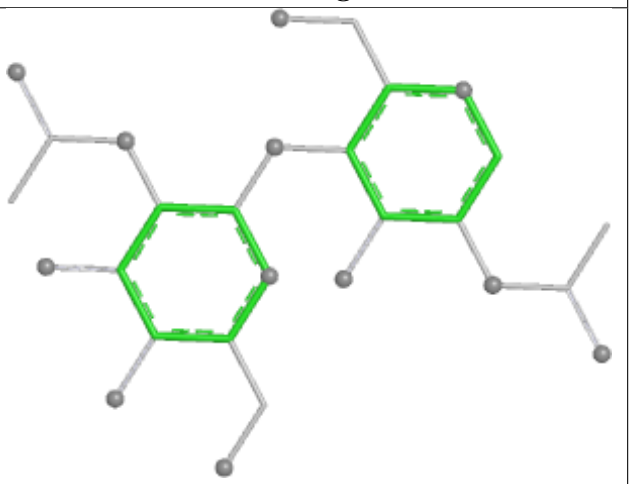
Bond lengths



Bond angles

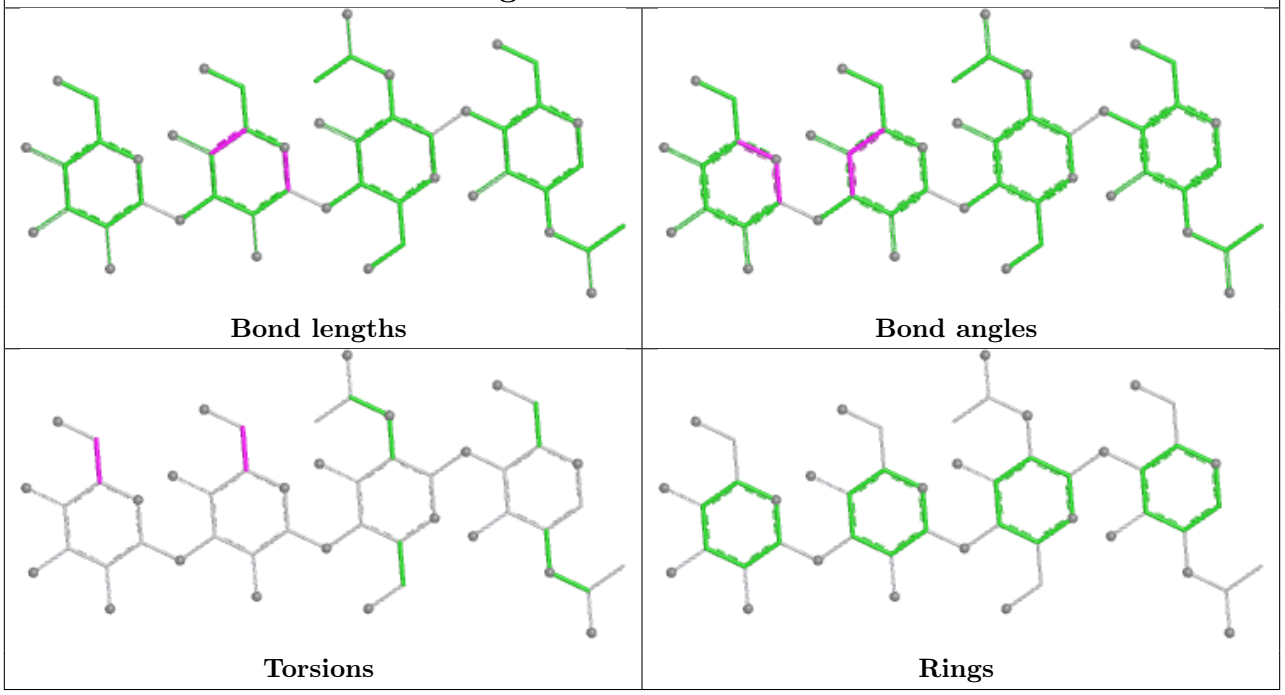


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	SO4	A	507	-	4,4,4	0.25	0	6,6,6	0.10	0
8	SO4	A	508	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	A	509	-	4,4,4	0.25	0	6,6,6	0.07	0
8	SO4	D	2007	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.08	0
11	NAG	B	2004	2	14,14,15	0.28	0	17,19,21	0.62	0
8	SO4	B	2006	-	4,4,4	0.24	0	6,6,6	0.11	0
11	NAG	D	2004	2	14,14,15	0.23	0	17,19,21	0.38	0
12	MJX	D	2006	10	27,27,27	0.98	0	33,37,37	1.07	2 (6%)
12	MJX	B	2005	10	27,27,27	0.95	0	33,37,37	1.04	0
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	509	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.07	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
12	MJX	D	2006	10	-	4/16/36/36	0/3/3/3
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	MJX	B	2005	10	-	3/16/36/36	0/3/3/3
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	2006	MJX	C6-N1-C3	2.21	114.58	111.14
12	D	2006	MJX	C2-C1-C5	-2.09	106.45	111.17

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	MJX	C14-C15-C18-N5
12	B	2005	MJX	C16-C15-C18-N5
11	D	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
12	D	2006	MJX	C14-C15-C18-N4
12	D	2006	MJX	C16-C15-C18-N5
12	B	2005	MJX	C7-C6-N1-C4
12	D	2006	MJX	C7-C6-N1-C4
12	D	2006	MJX	C13-C12-N3-C9

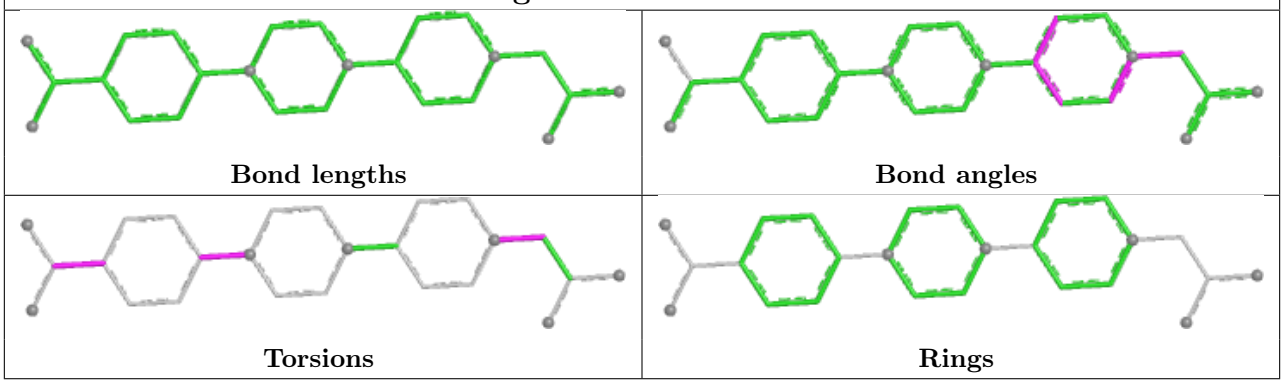
There are no ring outliers.

No monomer is involved in short contacts.

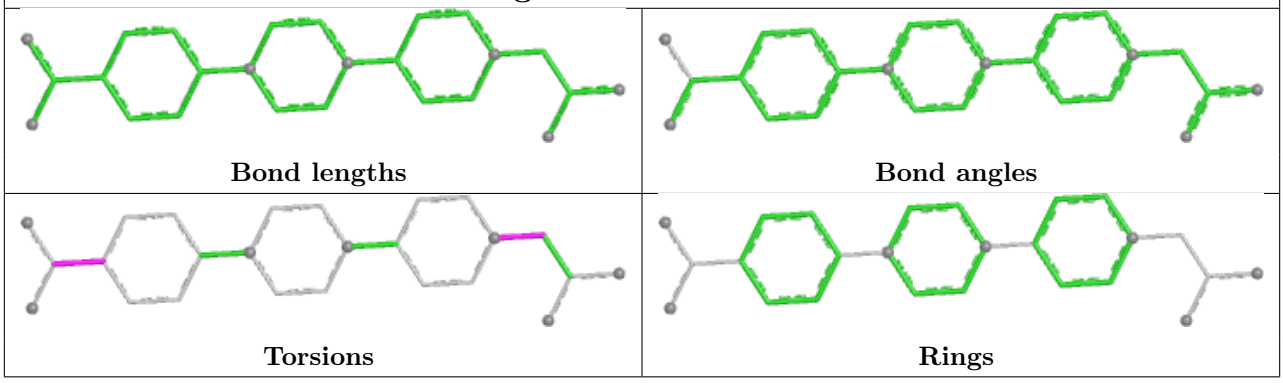
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for 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 then 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.

Ligand MJX D 2006



Ligand MJX B 2005



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	454/454 (100%)	0.02	9 (1%) 64 68	22, 40, 64, 104	4 (0%)
1	C	453/454 (99%)	0.59	16 (3%) 47 49	26, 55, 80, 109	4 (0%)
2	B	466/472 (98%)	0.73	58 (12%) 9 9	18, 63, 136, 158	5 (1%)
2	D	471/472 (99%)	1.07	66 (14%) 7 7	38, 71, 123, 143	1 (0%)
3	E	214/221 (96%)	1.85	71 (33%) 1 0	66, 115, 163, 188	0
3	H	216/221 (97%)	1.56	63 (29%) 1 1	47, 92, 138, 159	0
4	F	214/214 (100%)	1.56	51 (23%) 2 1	68, 114, 163, 186	0
4	L	214/214 (100%)	1.27	34 (15%) 6 5	53, 80, 104, 140	0
All	All	2702/2722 (99%)	0.91	368 (13%) 8 8	18, 68, 142, 188	14 (0%)

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	446[A]	HIS	6.6
3	E	147	LEU	6.1
3	E	165	LEU	6.0
4	F	130	ALA	5.3
3	E	203	VAL	5.3
3	E	212	VAL	4.9
4	F	135	PHE	4.8
1	A	454	VAL	4.8
4	F	181	LEU	4.6
3	E	201	CYS	4.5
3	E	160	TRP	4.2
1	A	217	SER	4.2
2	D	391	ILE	4.1
4	F	209	PHE	4.1
3	E	199	ILE	4.1
3	H	194	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	54	ALA	3.9
3	H	195	PRO	3.9
3	E	146	CYS	3.9
2	B	17	LEU	3.9
2	B	44	LEU	3.8
3	H	187	VAL	3.8
3	H	189	VAL	3.8
4	F	180	THR	3.7
2	D	375	LEU	3.7
4	L	15	LEU	3.7
4	F	179	LEU	3.7
2	B	458	GLY	3.7
3	E	216	ILE	3.6
4	F	148	TRP	3.6
2	D	145	LEU	3.6
2	B	178	TYR	3.5
3	E	81	LEU	3.5
3	H	120	ALA	3.5
2	B	10	VAL	3.5
3	E	86	LEU	3.5
4	F	136	LEU	3.5
2	D	30	ALA	3.5
4	F	132	VAL	3.5
4	L	75	ILE	3.5
3	E	130	LEU	3.5
3	H	142	VAL	3.4
2	B	4	ILE	3.4
3	H	199	ILE	3.4
3	E	158	LEU	3.4
2	B	446	HIS	3.4
2	D	45	LEU	3.3
3	E	12	VAL	3.3
3	H	171	THR	3.3
4	F	160	LEU	3.3
2	B	129	TRP	3.3
3	E	184	SER	3.3
4	F	192	TYR	3.3
2	D	144	LYS	3.3
2	D	4	ILE	3.2
3	E	127	VAL	3.2
3	H	181	TYR	3.2
2	D	22	MET	3.2

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Mol	Chain	Res	Type	RSRZ
3	E	189	VAL	3.2
3	E	128	TYR	3.2
1	A	45	PRO	3.2
4	L	165	ASP	3.2
2	B	466	TRP	3.2
3	E	148	VAL	3.2
3	E	152	PHE	3.2
3	H	206	PRO	3.2
2	D	471	CYS	3.2
3	E	204	ALA	3.2
4	F	131	SER	3.1
2	D	389	LEU	3.1
2	B	181	LYS	3.1
3	H	168	GLY	3.1
3	H	216	ILE	3.1
4	F	159	VAL	3.1
4	F	186	TYR	3.1
2	D	10	VAL	3.1
4	L	135	PHE	3.1
3	E	144	LEU	3.1
3	E	145	GLY	3.1
2	B	374	CYS	3.1
2	D	181	LYS	3.1
1	C	453	VAL	3.1
3	H	218	PRO	3.0
4	F	117	ILE	3.0
4	F	134	CYS	3.0
4	F	206	VAL	3.0
2	B	375	LEU	3.0
2	D	40	LEU	3.0
3	E	11	LEU	3.0
3	E	183	LEU	3.0
1	C	217	SER	3.0
2	D	379	VAL	3.0
3	E	187	VAL	3.0
2	D	383	LEU	3.0
3	E	45	LEU	3.0
4	F	125	LEU	3.0
4	L	78	LEU	3.0
2	D	80	VAL	2.9
3	E	34	VAL	2.9
2	D	90	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	29	ILE	2.9
3	H	75	SER	2.9
4	L	145	ASN	2.9
2	B	436	ALA	2.9
2	D	23	CYS	2.9
2	D	178	TYR	2.9
2	B	453	GLY	2.9
3	E	194	TRP	2.9
4	F	152	GLY	2.9
4	F	204	PRO	2.9
2	D	44	LEU	2.9
3	E	20	LEU	2.9
2	D	61	ALA	2.9
2	B	25	TRP	2.8
2	D	129	TRP	2.8
3	E	36	TRP	2.8
4	L	136	LEU	2.8
3	H	144	LEU	2.8
4	L	13	VAL	2.8
2	B	56	PHE	2.8
4	L	111	ALA	2.8
4	L	146	VAL	2.8
4	L	109	ALA	2.8
2	D	388	GLY	2.8
2	D	392	GLY	2.8
2	B	26	CYS	2.8
2	D	2	PRO	2.8
2	B	383	LEU	2.8
3	H	147	LEU	2.8
4	F	21	ILE	2.7
4	F	113	PRO	2.7
1	C	319	ASP	2.7
4	F	133	VAL	2.7
2	B	61	ALA	2.7
3	H	207	ALA	2.7
3	H	134	CYS	2.7
3	E	214	LYS	2.7
2	B	33	LEU	2.7
1	C	152	SER	2.7
4	L	83	PHE	2.7
4	F	122	SER	2.7
3	E	16	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	178	THR	2.7
2	B	57	PRO	2.6
1	C	118	LYS	2.6
1	C	213	LEU	2.6
3	E	83	LEU	2.6
4	L	125	LEU	2.6
2	D	345	VAL	2.6
2	D	51	PRO	2.6
2	B	92	LEU	2.6
3	H	158	LEU	2.6
2	B	18	ALA	2.6
4	F	196	ALA	2.6
4	F	205	ILE	2.6
4	F	145	ASN	2.6
3	H	11	LEU	2.6
3	E	133	VAL	2.6
2	B	432	ASP	2.6
3	H	87	THR	2.6
3	E	64	PHE	2.6
3	E	173	PRO	2.6
4	L	138	ASN	2.6
4	L	157	ASN	2.6
3	H	198	SER	2.6
2	B	90	LEU	2.6
3	E	4	LEU	2.6
4	L	160	LEU	2.6
2	B	451	GLY	2.5
2	D	24	ALA	2.5
3	H	14	PRO	2.5
2	D	69	LEU	2.5
4	L	112	ALA	2.5
3	H	203	VAL	2.5
3	H	212	VAL	2.5
4	F	115	VAL	2.5
4	F	118	PHE	2.5
4	F	119	PRO	2.5
4	L	120	PRO	2.5
4	F	201	SER	2.5
2	B	31	LEU	2.5
2	D	466	TRP	2.5
4	F	15	LEU	2.5
2	D	177	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	182	THR	2.5
2	D	394	THR	2.5
2	D	42	GLU	2.5
1	C	336	GLY	2.5
2	D	17	LEU	2.5
2	B	462	CYS	2.5
1	C	76	THR	2.5
2	D	403	VAL	2.5
3	H	117	VAL	2.5
4	L	105	GLU	2.4
4	L	139	PHE	2.4
4	F	169	LYS	2.4
4	F	114	THR	2.4
2	B	29	GLU	2.4
2	D	395	VAL	2.4
2	B	94	PRO	2.4
3	H	211	LYS	2.4
3	H	17	SER	2.4
3	H	186	SER	2.4
4	L	184	ASP	2.4
3	H	165	LEU	2.4
3	E	22	CYS	2.4
2	D	450	ASN	2.4
2	B	454	THR	2.4
2	D	25	TRP	2.4
3	E	126	SER	2.4
3	H	118	SER	2.4
4	L	191	SER	2.4
2	B	174	GLU	2.4
1	A	339	ALA	2.4
4	F	194	CYS	2.4
3	H	169	VAL	2.4
2	D	84	SER	2.4
3	E	164	SER	2.4
3	H	166	SER	2.4
2	B	455	PHE	2.4
4	L	118	PHE	2.4
2	D	312	GLU	2.3
3	E	24	ALA	2.3
2	D	147	SER	2.3
2	D	459	VAL	2.3
3	E	21	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	421	PHE	2.3
1	C	230	TYR	2.3
3	E	151	TYR	2.3
3	H	128	TYR	2.3
3	E	100	LEU	2.3
2	B	30	ALA	2.3
3	E	200	THR	2.3
3	H	116	THR	2.3
3	H	174	ALA	2.3
4	F	182	THR	2.3
4	L	214	CYS	2.3
3	H	119	SER	2.3
4	L	116	SER	2.3
2	D	199	GLN	2.3
3	E	169	VAL	2.3
4	F	146	VAL	2.3
2	B	456	GLU	2.3
2	B	397	PHE	2.3
1	C	155	TYR	2.3
2	D	54	ILE	2.3
4	F	144	ILE	2.3
3	E	174	ALA	2.3
4	L	12	SER	2.3
2	B	63	VAL	2.3
2	B	427	VAL	2.3
3	H	148	VAL	2.3
4	L	81	GLU	2.3
2	D	376	ASN	2.3
2	D	397	PHE	2.3
1	C	212	LEU	2.3
1	C	340	LEU	2.3
4	F	193	THR	2.3
3	E	166	SER	2.3
1	A	337	PRO	2.2
2	D	374	CYS	2.2
3	E	14	PRO	2.2
3	E	155	PRO	2.2
4	L	113	PRO	2.2
2	B	19	VAL	2.2
3	H	12	VAL	2.2
1	C	210	GLY	2.2
2	B	41	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	391	ILE	2.2
4	L	106	ILE	2.2
2	B	40	LEU	2.2
2	B	366	LEU	2.2
4	F	36	LEU	2.2
3	E	157	THR	2.2
2	B	51	PRO	2.2
3	E	125	PRO	2.2
2	B	49	CYS	2.2
4	F	151	ASP	2.2
3	E	18	VAL	2.2
3	H	121	LYS	2.2
2	B	376	ASN	2.2
2	D	56	PHE	2.2
4	L	73	LEU	2.2
1	C	207	TYR	2.2
2	B	24	ALA	2.2
2	D	70	SER	2.2
3	H	16	ALA	2.2
3	H	54	ALA	2.2
4	F	153	SER	2.2
3	H	153	PRO	2.2
2	D	41	LYS	2.2
1	A	216	VAL	2.2
4	L	205	ILE	2.2
2	D	467	LEU	2.2
3	E	181	TYR	2.2
2	B	78	SER	2.2
3	E	124	ALA	2.2
3	E	132	PRO	2.2
3	H	150	GLY	2.2
3	H	201	CYS	2.2
2	B	459	VAL	2.2
2	D	63	VAL	2.2
3	H	156	VAL	2.2
3	H	177	GLN	2.2
4	F	150	ILE	2.1
3	E	113	THR	2.1
3	E	188	THR	2.1
3	H	182	THR	2.1
3	H	188	THR	2.1
4	L	197	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	119	SER	2.1
2	B	37	ARG	2.1
2	D	372	ALA	2.1
3	E	120	ALA	2.1
4	F	112	ALA	2.1
2	B	465	GLY	2.1
3	E	27	PHE	2.1
3	H	20	LEU	2.1
3	H	67	LYS	2.1
1	C	320	ARG	2.1
3	E	196	SER	2.1
1	C	201	ALA	2.1
3	H	132	PRO	2.1
3	H	151	TYR	2.1
3	H	155	PRO	2.1
1	A	47	GLN	2.1
2	D	49	CYS	2.1
2	D	406	CYS	2.1
3	E	134	CYS	2.1
2	D	340	VAL	2.1
3	E	142	VAL	2.1
4	F	55	VAL	2.1
1	A	340	LEU	2.1
2	B	45	LEU	2.1
2	B	76	ASP	2.1
3	H	81	LEU	2.1
4	F	78	LEU	2.1
2	D	35	SER	2.1
2	D	469	SER	2.1
3	E	185	SER	2.1
3	H	157	THR	2.1
4	F	127	SER	2.1
3	E	202	ASN	2.1
4	F	91	TYR	2.1
4	L	161	ASN	2.1
2	B	23	CYS	2.1
3	H	175	VAL	2.1
2	B	461	ARG	2.1
2	D	37	ARG	2.1
3	H	90	ASP	2.1
2	D	128	LEU	2.1
3	H	45	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	171	THR	2.1
4	F	83	PHE	2.1
3	H	9	ALA	2.0
3	E	80	TYR	2.0
3	H	57	TYR	2.0
2	D	46	LYS	2.0
1	A	278[A]	HIS	2.0
3	H	164	SER	2.0
3	H	196	SER	2.0
2	D	102	ILE	2.0
2	B	392	GLY	2.0
4	F	41	GLY	2.0
2	B	404	ARG	2.0
4	L	192	TYR	2.0
2	B	457	CYS	2.0
2	D	83	VAL	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)

SUGAR-RSR INFOmissingINFO

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, 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
8	SO4	C	502	5/5	0.60	0.20	89,89,89,89	0
8	SO4	A	508	5/5	0.62	0.17	91,91,91,91	0
8	SO4	A	509	5/5	0.70	0.18	73,73,73,73	0
11	NAG	B	2004	14/15	0.70	0.12	101,101,101,101	0
8	SO4	A	507	5/5	0.72	0.15	80,80,80,80	0
11	NAG	D	2004	14/15	0.72	0.14	96,96,96,96	0
8	SO4	C	503	5/5	0.75	0.10	98,98,98,98	0

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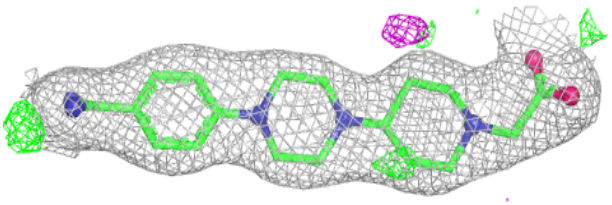
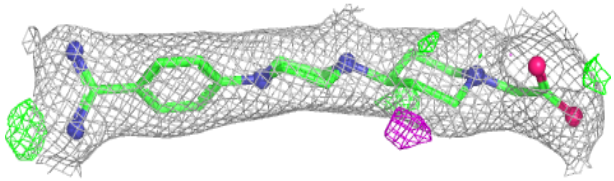
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	C	501	5/5	0.78	0.14	83,83,83,83	0
8	SO4	C	509	5/5	0.81	0.10	90,90,90,90	0
8	SO4	A	501	5/5	0.82	0.14	70,70,70,70	0
8	SO4	L	301	5/5	0.82	0.10	85,85,85,85	0
13	CL	D	2005	1/1	0.83	0.20	84,84,84,84	0
8	SO4	B	2006	5/5	0.93	0.11	45,45,45,45	5
12	MJX	D	2006	25/25	0.94	0.10	51,51,51,51	0
13	CL	C	504	1/1	0.94	0.12	80,80,80,80	0
8	SO4	A	502	5/5	0.94	0.07	60,60,60,60	0
12	MJX	B	2005	25/25	0.95	0.08	39,39,39,39	0
10	MN	B	2002	1/1	0.95	0.17	73,73,73,73	0
8	SO4	D	2007	5/5	0.96	0.09	55,55,55,55	5
9	CA	A	505	1/1	0.97	0.05	34,34,34,34	0
9	CA	C	505	1/1	0.97	0.06	71,71,71,71	0
9	CA	A	504	1/1	0.97	0.04	36,36,36,36	0
9	CA	A	503	1/1	0.98	0.04	44,44,44,44	0
10	MN	D	2002	1/1	0.98	0.05	59,59,59,59	0
9	CA	C	506	1/1	0.98	0.04	60,60,60,60	0
9	CA	C	507	1/1	0.98	0.04	53,53,53,53	0
10	MN	B	2003	1/1	0.99	0.03	34,34,34,34	0
10	MN	D	2001	1/1	0.99	0.03	43,43,43,43	0
9	CA	C	508	1/1	0.99	0.03	53,53,53,53	0
10	MN	D	2003	1/1	0.99	0.03	44,44,44,44	0
9	CA	A	506	1/1	0.99	0.03	36,36,36,36	0
10	MN	B	2001	1/1	1.00	0.03	34,34,34,34	0

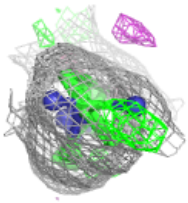
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MJX D 2006:

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

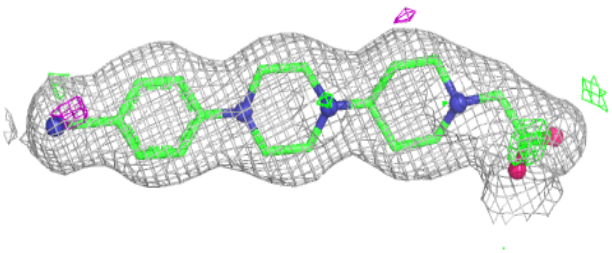


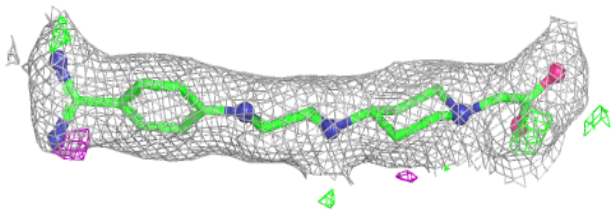


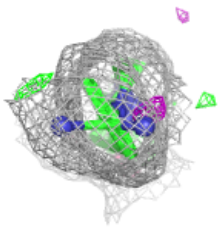


Electron density around MJX B 2005:

$2mF_o$-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 (i)

There are no such residues in this entry.