wwPDB X-ray Structure Validation Summary Report (i)

Aug 10, 2020 – 01:38 PM BST

PDB ID	:	5HDB
Title	:	Integrin alphaIIbbeta3 in complex with Ro-435054
Authors	:	Lin, F.Y.
Deposited on	:	2016-01-05
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

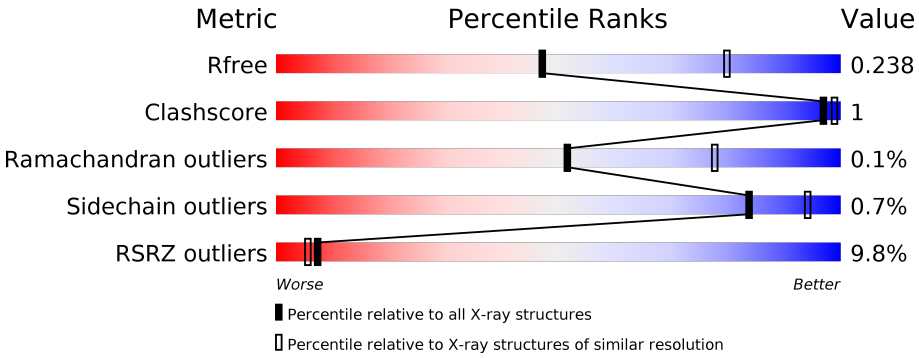
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	97%
1	C	454	2% 96%
2	B	471	10% 96%
2	D	471	8% 97%
3	E	219	36% 95%
3	H	219	9% 97%

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Mol	Chain	Length	Quality of chain
4	F	214	28% 100%
4	L	214	4% 97%
5	G	5	40% 60%
6	I	2	100%
6	K	2	100%
7	J	4	75% 25%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CA	D	503	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 42246 atoms, of which 20351 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	H	N	O	S	0	9	0
			6908	2242	3381	610	667	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6840	2224	3338	604	666	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	24	8	0
			7184	2260	3556	619	715	34			
2	D	471	Total	C	H	N	O	S	28	2	0
			7182	2260	3551	620	716	35			

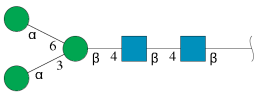
- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	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	H	N	O	0	0	0
			113	34	52	2	25			

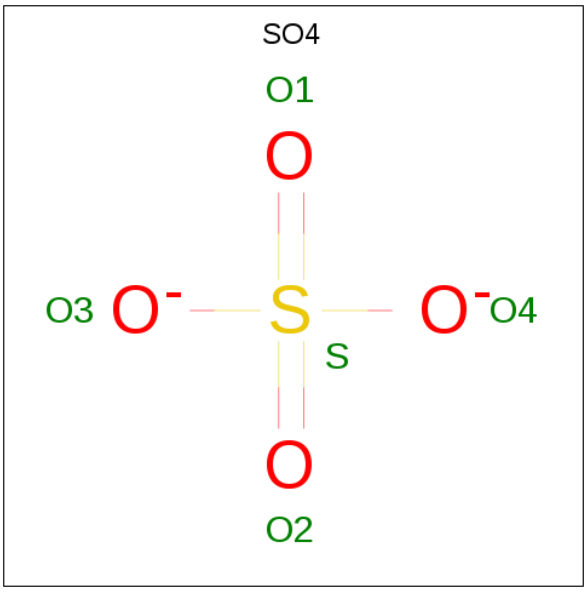
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
6	K	2	Total	C	H	N	O	0	0	0
			53	16	25	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.

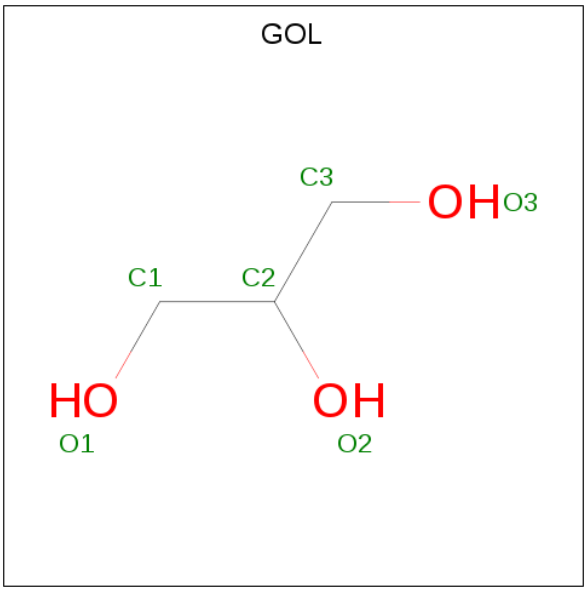
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- 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	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	L	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C H O 14 3 8 3	0	0

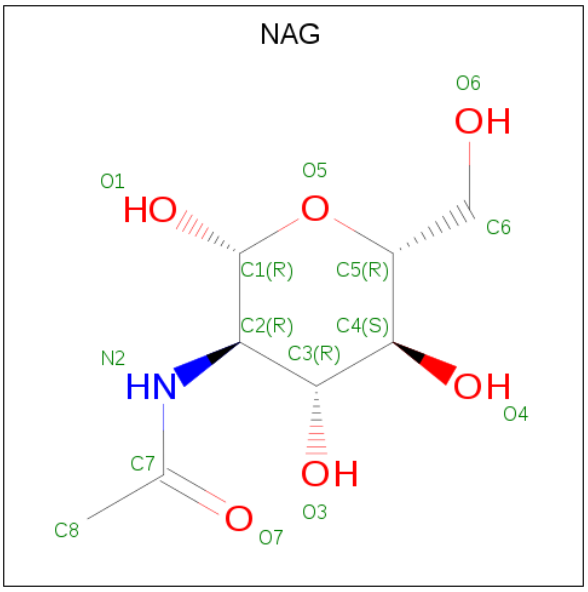
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Ca 1 1	0	0
10	A	4	Total Ca 4 4	0	0
10	D	2	Total Ca 2 2	0	0
10	C	4	Total Ca 4 4	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

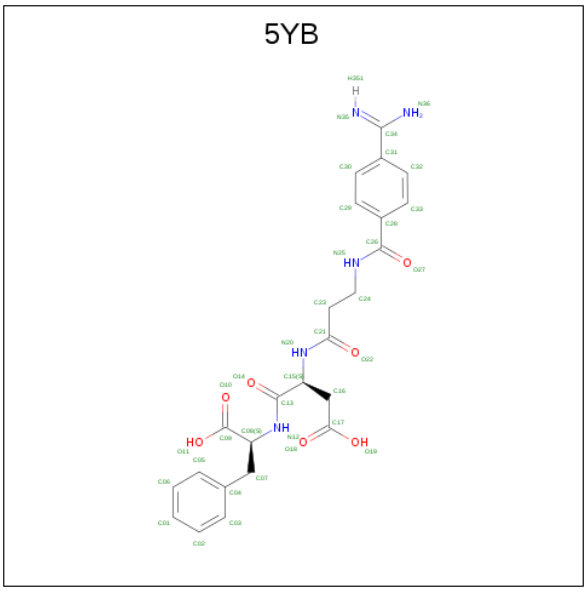
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Mg 1 1	0	0
11	D	1	Total Mg 1 1	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
12	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 13 is N-(4-carbamimidoylbenzoyl)-beta-alanyl-L-alpha-aspartyl-L-phenylalanine (three-letter code: 5YB) (formula: $C_{24}H_{27}N_5O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	0	0
			61	24	25	5	7		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total	C	H	N	O	0	0
			61	24	25	5	7		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	2	Total	Cl	0	0
			2	2		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	303	Total	O	0	0
			303	303		
15	B	175	Total	O	0	0
			175	175		
15	C	80	Total	O	0	0
			80	80		
15	D	96	Total	O	0	0
			96	96		
15	E	10	Total	O	0	0
			10	10		
15	F	13	Total	O	0	0
			13	13		
15	H	24	Total	O	0	0
			24	24		
15	L	41	Total	O	0	0
			41	41		

3 Residue-property plots (i)

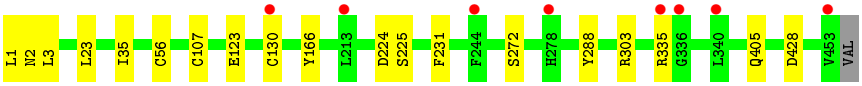
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

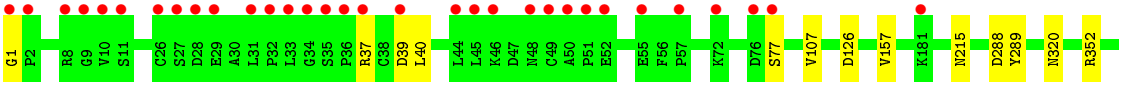
- Molecule 1: Integrin alpha-IIb

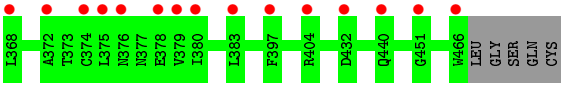
Chain C:



- Molecule 2: Integrin beta-3

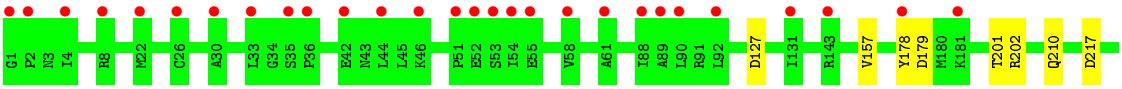
Chain B:

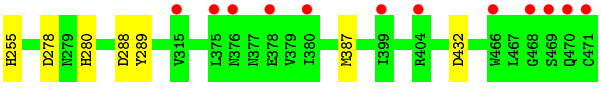




- Molecule 2: Integrin beta-3

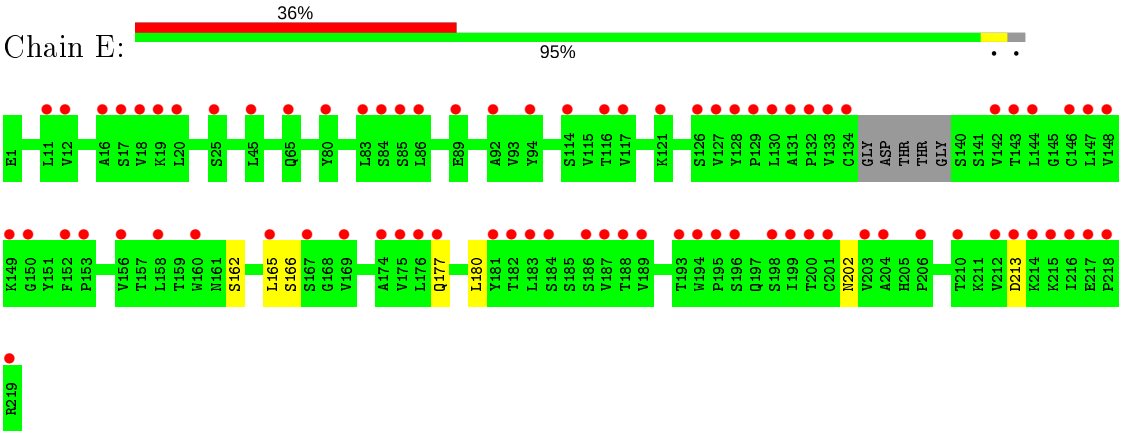
Chain D:





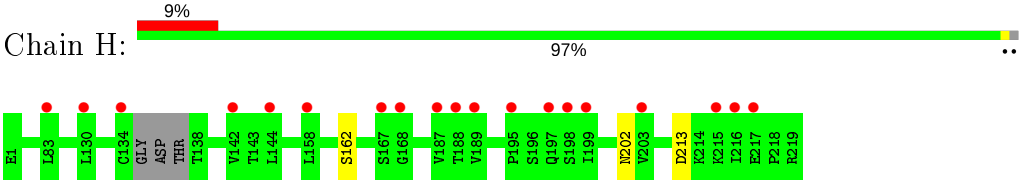
- Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain E:



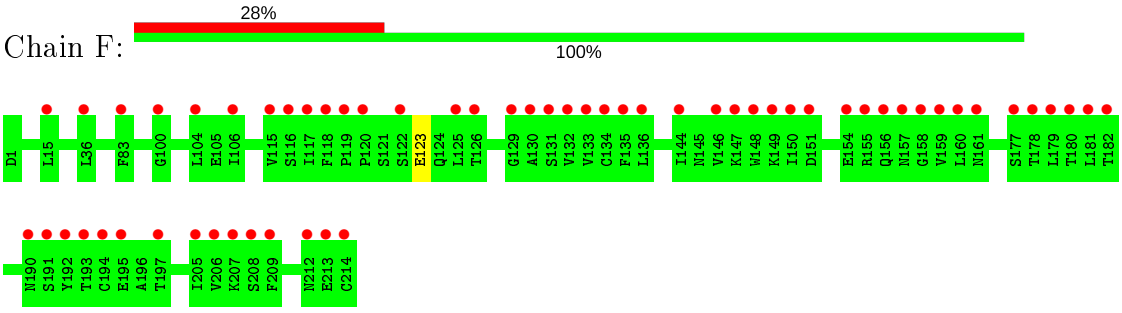
• Molecule 3: Monoclonal antibody 10E5 heavy chain

Chain H:



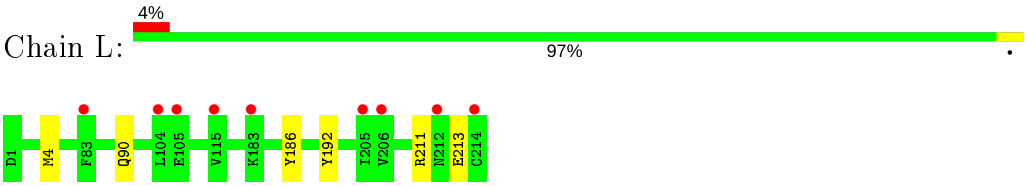
• Molecule 4: Monoclonal antibody 10E5 light chain

Chain F:



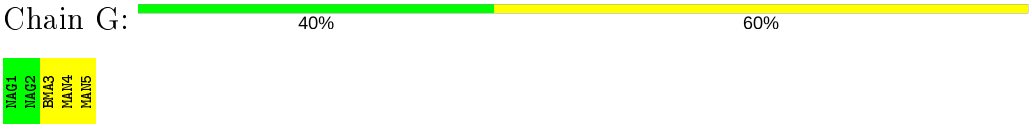
• Molecule 4: Monoclonal antibody 10E5 light chain

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:

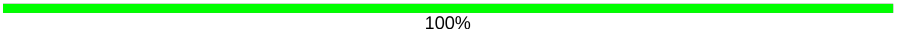


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	259.35Å 144.44Å 104.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.70 49.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.01-2.70) 85.7 (49.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.212 , 0.237 0.214 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	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	0.93	EDS
Total number of atoms	42246	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: GOL, MG, BMA, NAG, CL, CA, 5YB, SO4, MAN

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	0.27	0/3651	0.44	0/4975
1	C	0.25	0/3618	0.43	0/4930
2	B	0.24	0/3726	0.42	0/5051
2	D	0.24	0/3710	0.41	0/5029
3	E	0.24	0/1673	0.43	0/2290
3	H	0.24	0/1684	0.43	0/2305
4	F	0.24	0/1673	0.41	0/2269
4	L	0.24	0/1673	0.43	0/2269
All	All	0.25	0/21408	0.43	0/29118

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	3527	3381	3365	5	0
1	C	3502	3338	3320	8	0
2	B	3628	3556	3525	6	0
2	D	3631	3551	3539	8	0
3	E	1631	1590	1590	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1600	1600	2	0
4	F	1637	1553	1553	1	0
4	L	1637	1553	1553	3	0
5	G	61	52	52	0	0
6	I	28	25	25	1	0
6	K	28	25	25	0	0
7	J	50	43	43	0	0
8	A	15	0	0	0	0
8	C	10	0	0	0	0
8	L	5	0	0	0	0
9	A	6	8	8	0	0
10	A	4	0	0	0	0
10	B	1	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	14	13	13	0	0
12	D	14	13	13	0	0
13	B	36	25	24	1	0
13	D	36	25	24	1	0
14	C	2	0	0	0	0
15	A	303	0	0	1	1
15	B	175	0	0	3	0
15	C	80	0	0	1	1
15	D	96	0	0	4	0
15	E	10	0	0	0	0
15	F	13	0	0	0	0
15	H	24	0	0	0	0
15	L	41	0	0	0	0
All	All	21895	20351	20272	38	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 38 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:MET:O	15:D:2101:HOH:O	2.01	0.79
2:B:126[B]:ASP:OD1	15:B:2101:HOH:O	2.07	0.70
2:D:280:HIS:O	15:D:2102:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ASP:OD2	15:C:601:HOH:O	2.16	0.61
1:A:301:ASP:OD2	15:A:601:HOH:O	2.17	0.60

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:882:HOH:O	15:C:678:HOH:O[1_554]	1.96	0.24

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	461/454 (102%)	441 (96%)	19 (4%)	1 (0%)	47 73
1	C	457/454 (101%)	433 (95%)	23 (5%)	1 (0%)	47 73
2	B	472/471 (100%)	451 (96%)	20 (4%)	1 (0%)	47 73
2	D	471/471 (100%)	453 (96%)	17 (4%)	1 (0%)	47 73
3	E	210/219 (96%)	199 (95%)	11 (5%)	0	100 100
3	H	212/219 (97%)	200 (94%)	12 (6%)	0	100 100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100 100
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
All	All	2707/2716 (100%)	2580 (95%)	123 (4%)	4 (0%)	51 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	C	123	GLU
2	D	157	VAL

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Mol	Chain	Res	Type
2	B	157	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/362 (102%)	365 (99%)	5 (1%)	67 86
1	C	366/362 (101%)	362 (99%)	4 (1%)	73 90
2	B	420/416 (101%)	417 (99%)	3 (1%)	84 94
2	D	418/416 (100%)	415 (99%)	3 (1%)	84 94
3	E	186/189 (98%)	186 (100%)	0	100 100
3	H	187/189 (99%)	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	2323/2310 (101%)	2308 (99%)	15 (1%)	84 95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	77	SER
2	B	215	ASN
2	D	127	ASP
2	B	37	ARG
1	C	288	TYR

Some 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 (i)

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

5.5 Carbohydrates (i)

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	2,5	14,14,15	0.38	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.47	0
5	BMA	G	3	5	11,11,12	0.80	0	15,15,17	0.96	1 (6%)
5	MAN	G	4	5	11,11,12	0.63	0	15,15,17	0.94	1 (6%)
5	MAN	G	5	5	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.32	0	17,19,21	0.42	0
6	NAG	I	2	6	14,14,15	0.26	0	17,19,21	0.56	0
7	NAG	J	1	2,7	14,14,15	0.39	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.33	0	17,19,21	0.39	0
7	BMA	J	3	7	11,11,12	0.64	0	15,15,17	0.79	0
7	MAN	J	4	7	11,11,12	0.72	0	15,15,17	1.08	2 (13%)
6	NAG	K	1	2,6	14,14,15	0.36	0	17,19,21	0.39	0
6	NAG	K	2	6	14,14,15	0.12	0	17,19,21	0.47	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	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	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

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	5	MAN	C1-O5-C5	3.19	116.51	112.19
7	J	4	MAN	C1-O5-C5	3.03	116.29	112.19
7	J	4	MAN	O2-C2-C3	-2.24	105.64	110.14
5	G	4	MAN	O2-C2-C3	-2.20	105.74	110.14
5	G	5	MAN	O2-C2-C3	-2.18	105.77	110.14

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	1	NAG	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

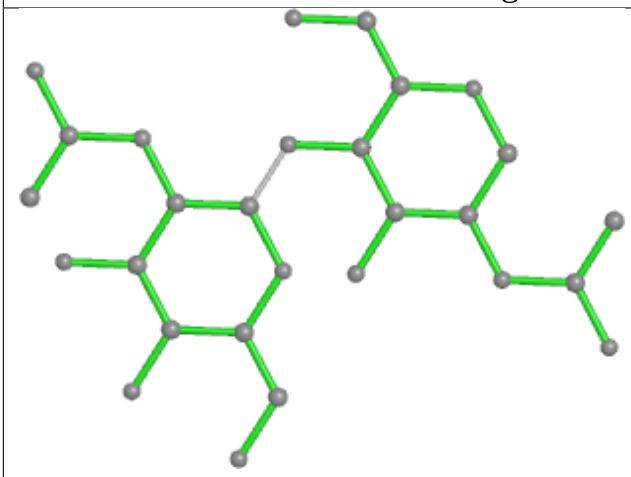
There are no ring outliers.

2 monomers are involved in 1 short contact:

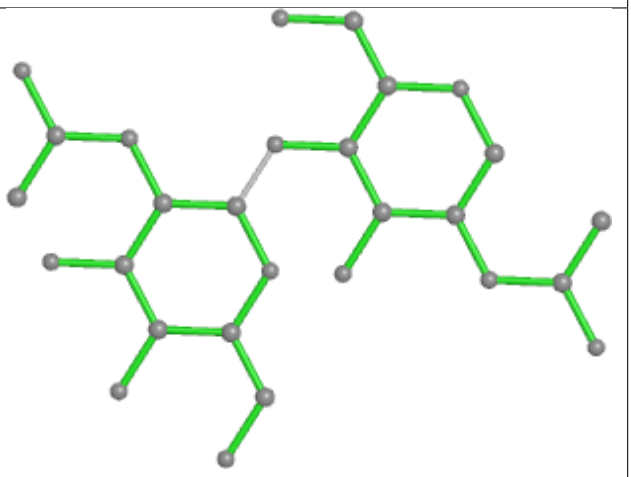
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0
6	I	2	NAG	1	0

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

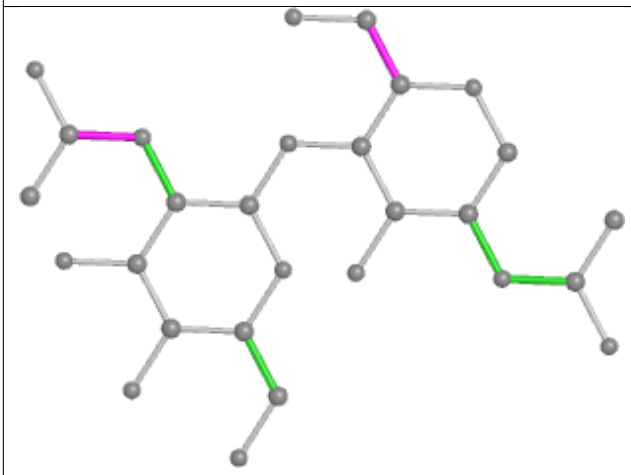
Oligosaccharide Chain I



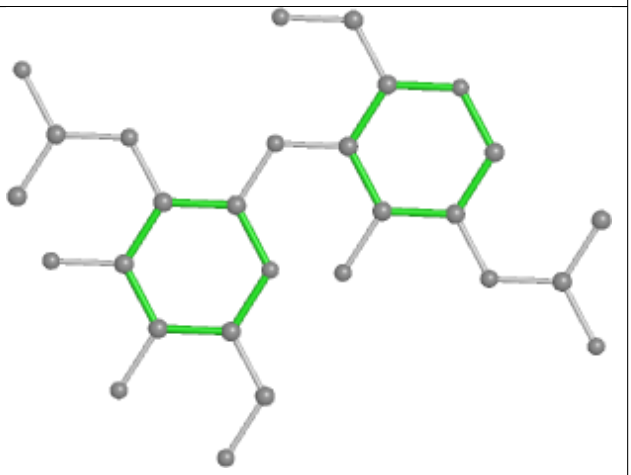
Bond lengths



Bond angles

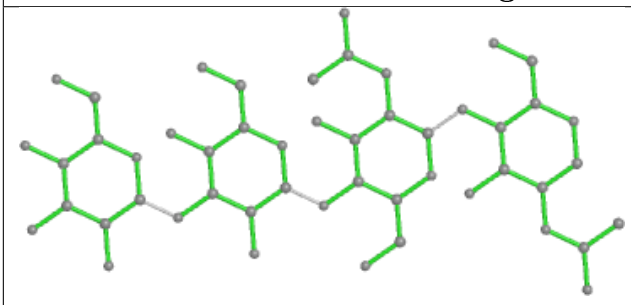


Torsions

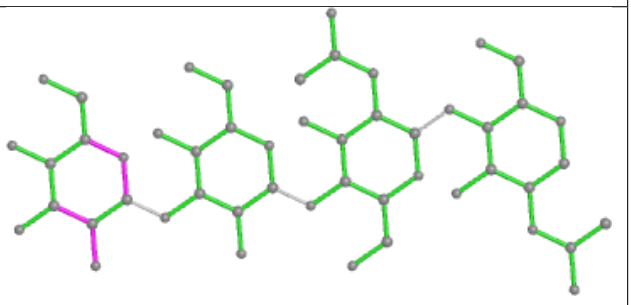


Rings

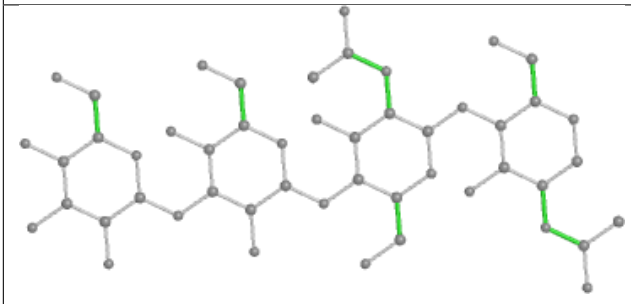
Oligosaccharide Chain J



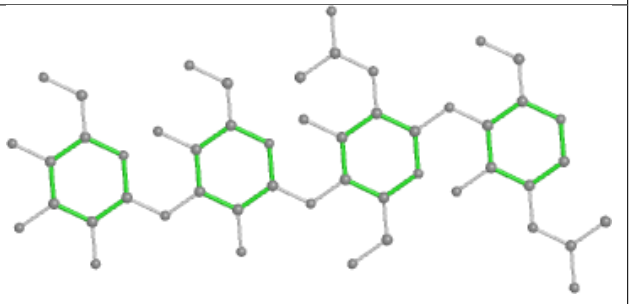
Bond lengths



Bond angles

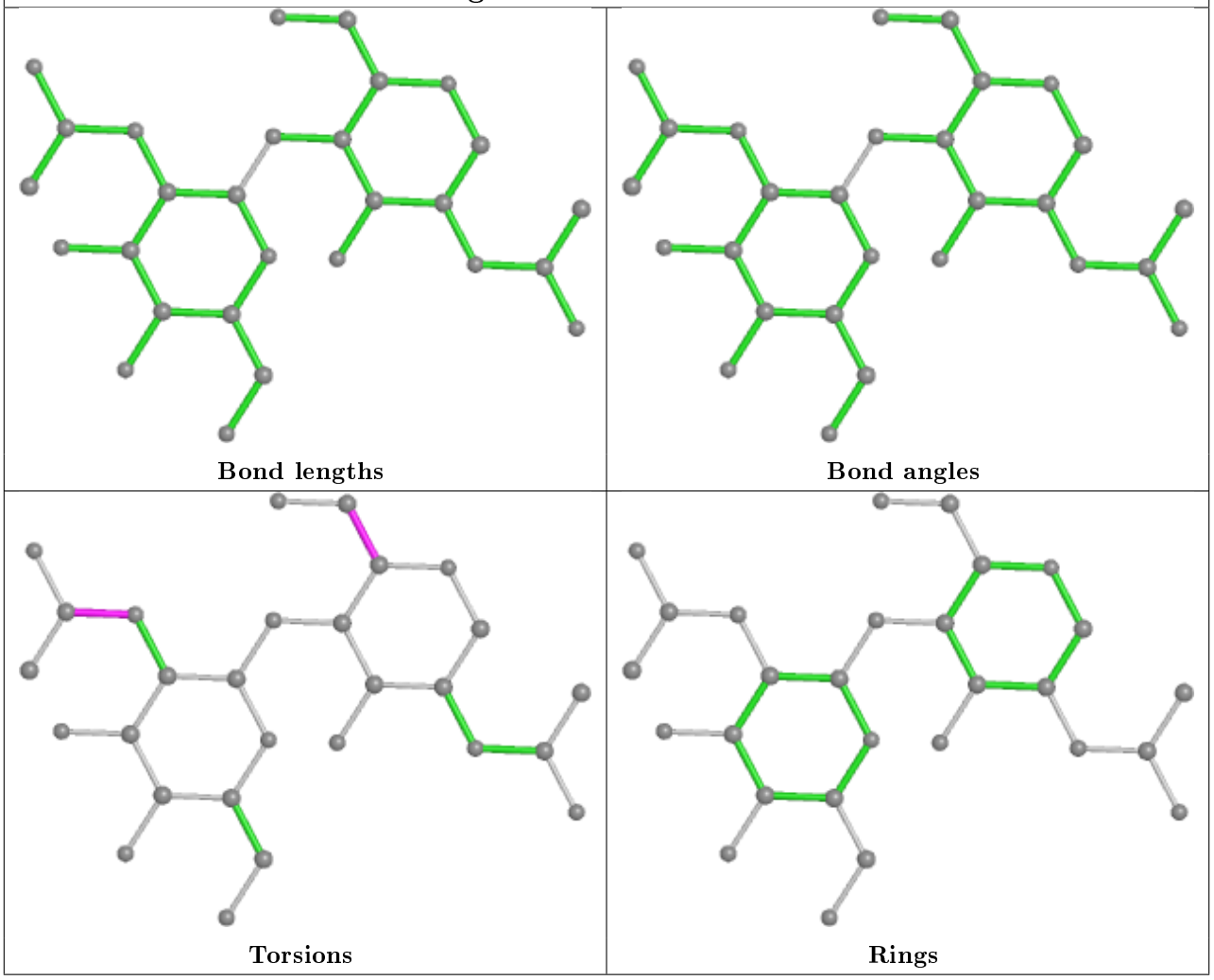


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
9	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.24	0
8	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.07	0
8	SO4	A	501	-	4,4,4	0.17	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	5YB	D	501	11	31,37,37	2.51	8 (25%)	36,49,49	1.14	3 (8%)
12	NAG	D	505	2	14,14,15	0.41	0	17,19,21	0.53	0
8	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.18	0
8	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.07	0
12	NAG	B	2003	2	14,14,15	0.28	0	17,19,21	0.42	0
13	5YB	B	2011	11	31,37,37	2.48	8 (25%)	36,49,49	1.16	3 (8%)
8	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.12	0
8	SO4	A	502	-	4,4,4	0.15	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
9	GOL	A	504	-	-	2/4/4/4	-
12	NAG	D	505	2	-	0/6/23/26	0/1/1/1
12	NAG	B	2003	2	-	0/6/23/26	0/1/1/1
13	5YB	D	501	11	-	7/32/38/38	0/2/2/2
13	5YB	B	2011	11	-	5/32/38/38	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	2011	5YB	C13-N12	7.45	1.50	1.34
13	D	501	5YB	C13-N12	7.44	1.50	1.34
13	D	501	5YB	C21-N20	6.13	1.47	1.34
13	B	2011	5YB	C21-N20	5.97	1.46	1.34
13	D	501	5YB	C26-N25	5.19	1.45	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	2011	5YB	C23-C21-N20	2.95	120.95	115.83
13	D	501	5YB	C23-C21-N20	2.79	120.66	115.83
13	D	501	5YB	C28-C26-N25	2.34	122.12	117.09
13	B	2011	5YB	C08-N12-C13	-2.34	119.69	123.19
13	D	501	5YB	C08-N12-C13	-2.26	119.80	123.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

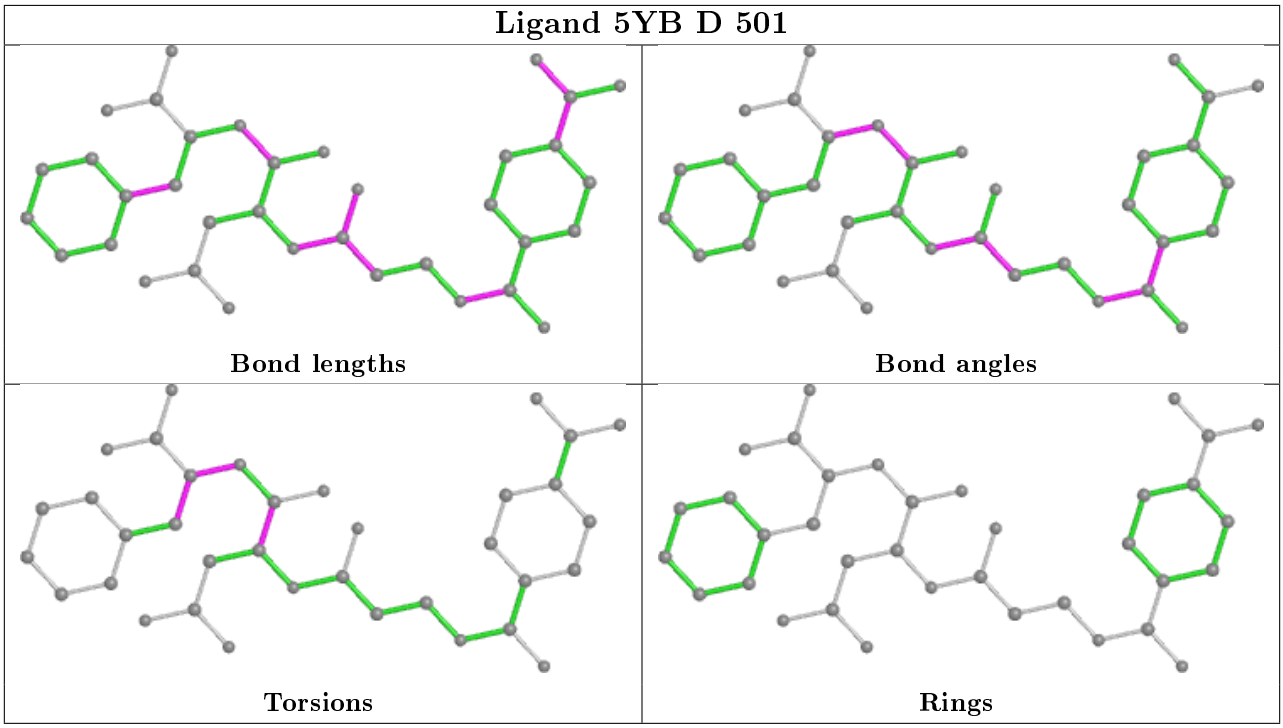
Mol	Chain	Res	Type	Atoms
13	D	501	5YB	C09-C08-N12-C13
13	B	2011	5YB	C09-C08-N12-C13
13	B	2011	5YB	C07-C08-N12-C13
9	A	504	GOL	O1-C1-C2-C3
9	A	504	GOL	O1-C1-C2-O2

There are no ring outliers.

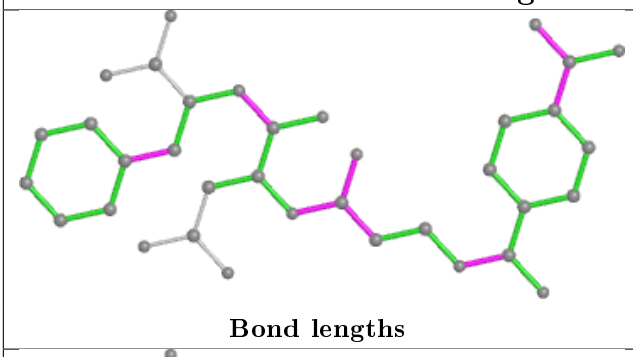
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	501	5YB	1	0
13	B	2011	5YB	1	0

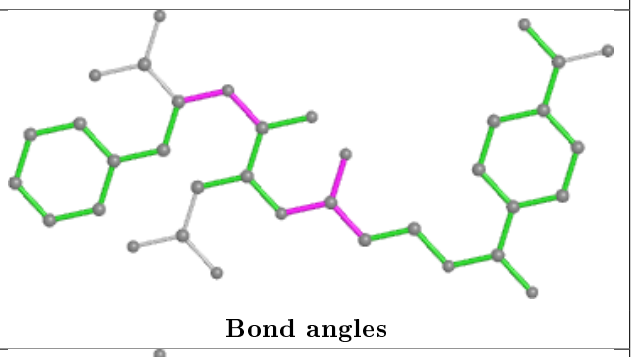
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



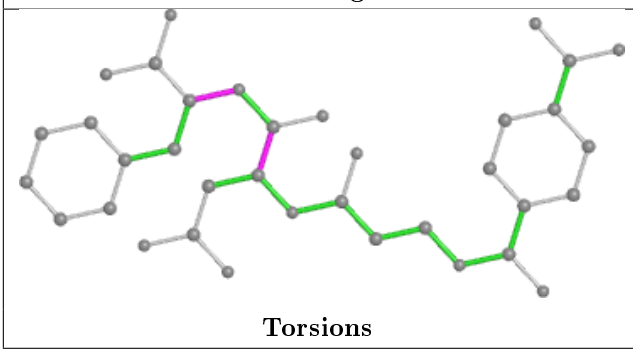
Ligand 5YB B 2011



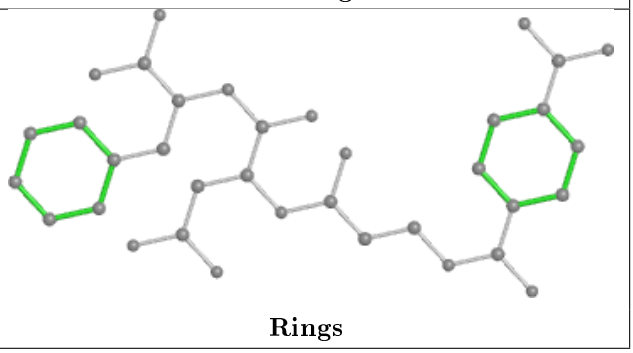
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.33	3 (0%) 87 89	35, 49, 78, 127	0
1	C	453/454 (99%)	0.40	8 (1%) 68 70	45, 71, 105, 148	0
2	B	466/471 (98%)	0.57	47 (10%) 7 5	39, 81, 171, 207	1 (0%)
2	D	471/471 (100%)	0.65	40 (8%) 10 9	54, 96, 146, 220	1 (0%)
3	E	214/219 (97%)	1.79	79 (36%) 0 0	82, 145, 210, 246	0
3	H	216/219 (98%)	0.49	19 (8%) 10 8	56, 108, 164, 212	0
4	F	214/214 (100%)	1.54	59 (27%) 0 0	88, 138, 210, 235	0
4	L	214/214 (100%)	0.43	9 (4%) 36 35	63, 96, 126, 196	0
All	All	2702/2716 (99%)	0.67	264 (9%) 7 5	35, 87, 174, 246	2 (0%)

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	12.8
4	F	130	ALA	9.0
3	E	147	LEU	8.9
2	D	469	SER	8.3
2	B	33	LEU	8.2

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

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

6.3 Carbohydrates

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,

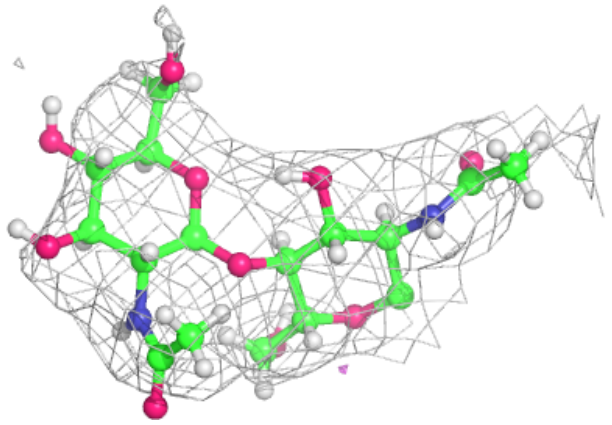
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

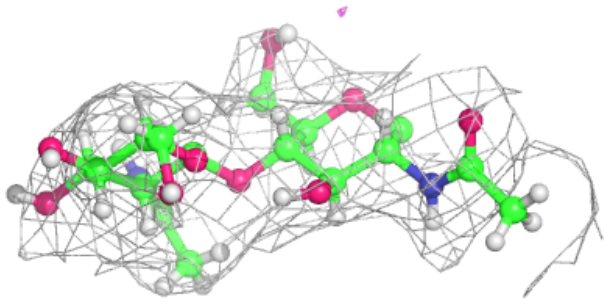
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	G	5	11/12	0.78	0.22	118,137,164,166	0
5	BMA	G	3	11/12	0.79	0.16	110,142,177,177	0
7	BMA	J	3	11/12	0.82	0.24	118,141,169,169	0
6	NAG	K	2	14/15	0.82	0.21	128,154,185,204	0
6	NAG	I	2	14/15	0.85	0.25	126,160,184,202	0
5	NAG	G	2	14/15	0.88	0.24	104,134,157,176	0
5	MAN	G	4	11/12	0.89	0.18	109,130,153,158	0
7	MAN	J	4	11/12	0.89	0.18	125,145,174,175	0
6	NAG	I	1	14/15	0.90	0.24	105,134,169,169	0
6	NAG	K	1	14/15	0.90	0.21	102,140,174,174	0
7	NAG	J	2	14/15	0.91	0.21	108,141,179,183	0
7	NAG	J	1	14/15	0.92	0.17	81,115,156,158	0
5	NAG	G	1	14/15	0.96	0.19	55,79,95,98	0

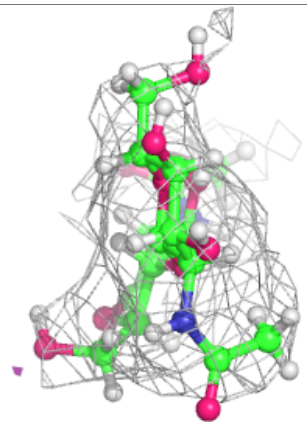
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

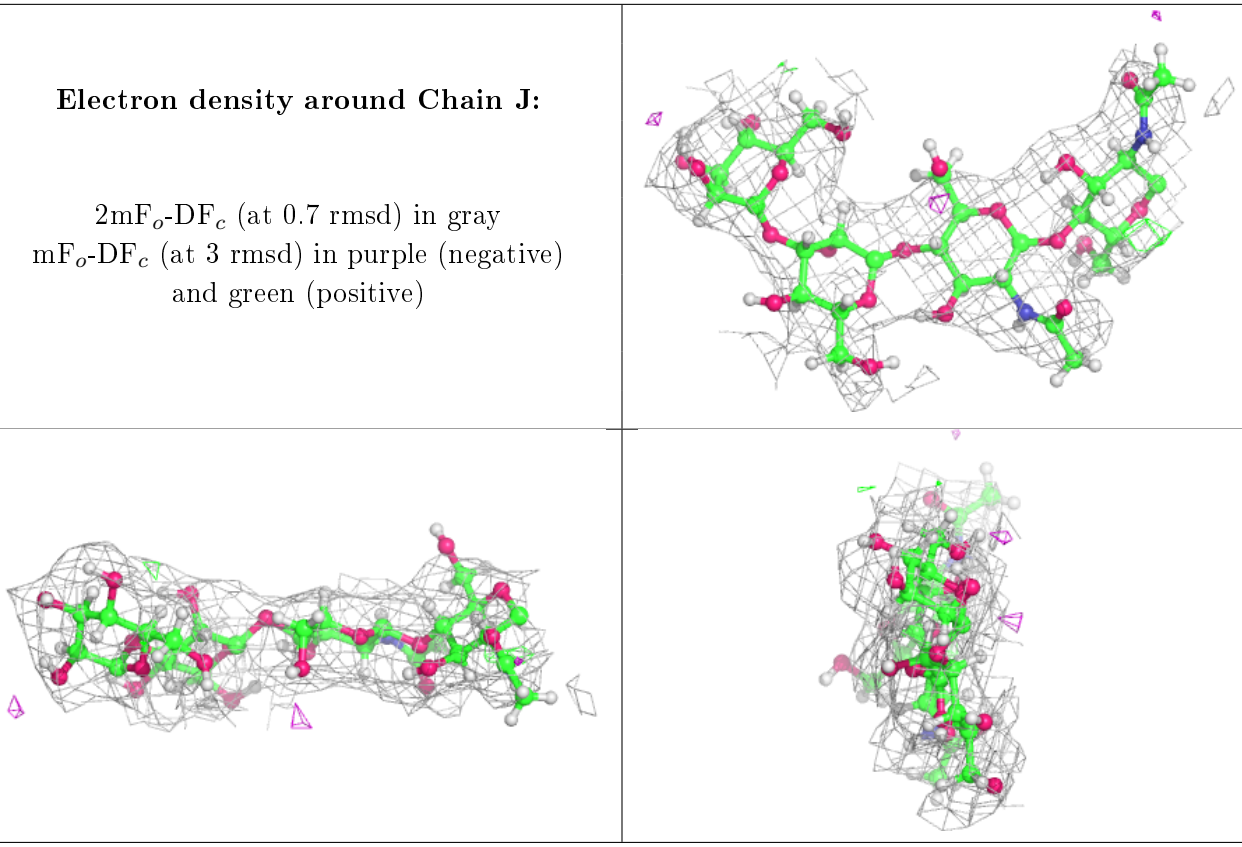






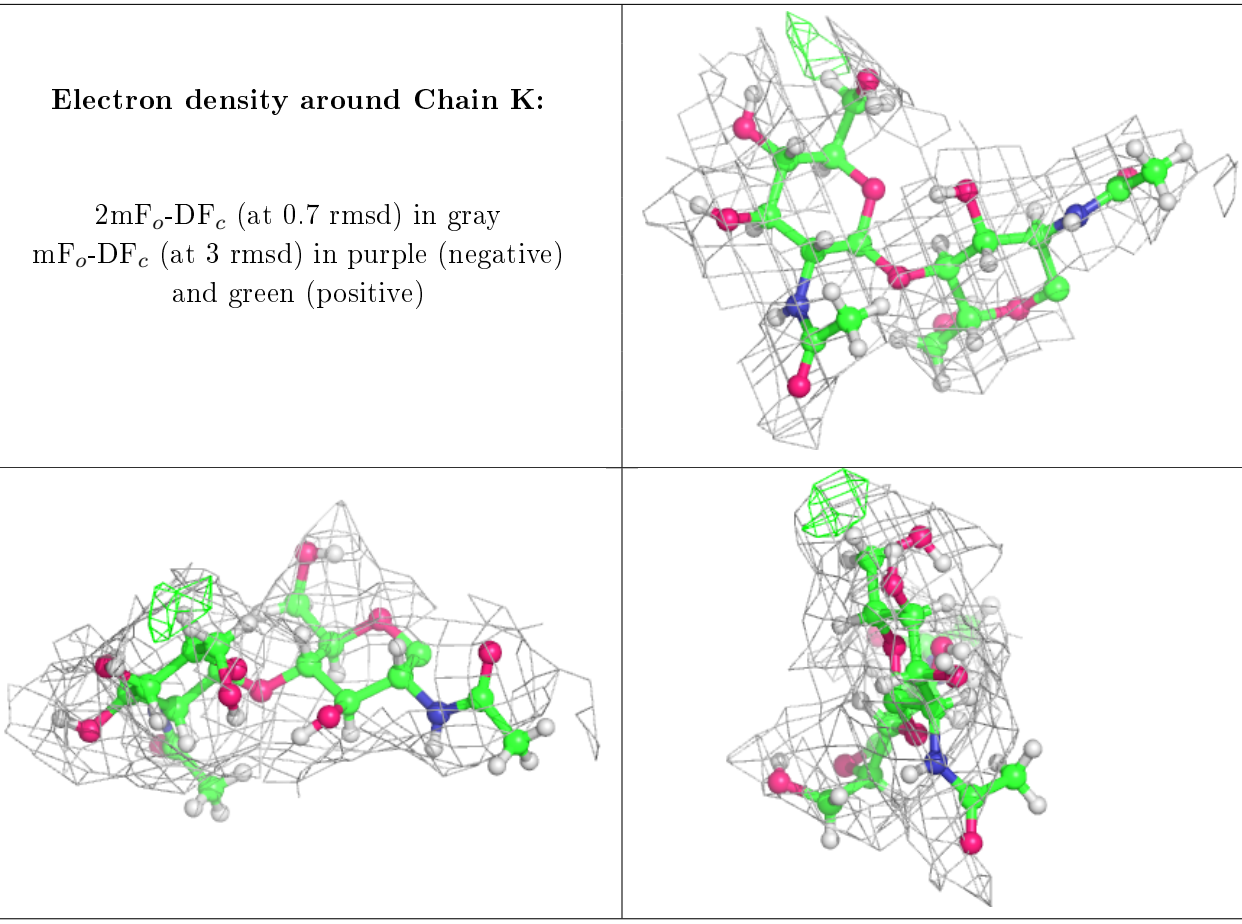
Electron density around Chain J:

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



Electron density around Chain K:

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



6.4 Ligands (i)

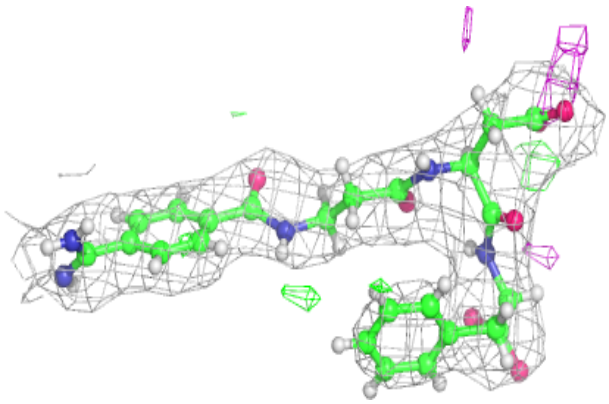
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

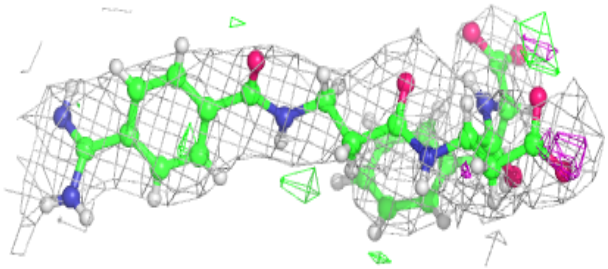
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CA	C	505	1/1	0.04	0.20	174,174,174,174	0
14	CL	C	504	1/1	0.65	0.17	100,100,100,100	0
10	CA	D	503	1/1	0.72	0.48	210,210,210,210	0
8	SO4	A	501	5/5	0.83	0.50	169,171,181,184	0
14	CL	C	503	1/1	0.84	0.20	81,81,81,81	0
12	NAG	D	505	14/15	0.85	0.25	104,142,170,170	0
10	CA	A	506	1/1	0.86	0.23	68,68,68,68	0
8	SO4	C	501	5/5	0.87	0.41	176,179,182,182	0
9	GOL	A	504	6/6	0.88	0.32	86,104,123,124	0
8	SO4	C	502	5/5	0.89	0.22	188,191,193,193	0
12	NAG	B	2003	14/15	0.89	0.29	111,144,173,174	0
10	CA	A	505	1/1	0.91	0.11	62,62,62,62	0
10	CA	A	507	1/1	0.92	0.38	79,79,79,79	0
13	5YB	B	2011	36/36	0.92	0.26	34,77,107,118	0
11	MG	B	2001	1/1	0.92	0.22	31,31,31,31	0
10	CA	C	506	1/1	0.93	0.04	67,67,67,67	0
10	CA	C	507	1/1	0.93	0.12	56,56,56,56	0
8	SO4	L	301	5/5	0.93	0.16	176,178,179,181	0
8	SO4	A	502	5/5	0.93	0.36	134,139,148,154	0
13	5YB	D	501	36/36	0.94	0.23	45,85,116,122	0
11	MG	D	502	1/1	0.95	0.15	47,47,47,47	0
8	SO4	A	503	5/5	0.95	0.22	97,111,113,122	0
10	CA	C	508	1/1	0.98	0.15	62,62,62,62	0
10	CA	D	504	1/1	0.98	0.17	50,50,50,50	0
10	CA	B	2002	1/1	0.99	0.15	31,31,31,31	0
10	CA	A	508	1/1	0.99	0.19	38,38,38,38	0

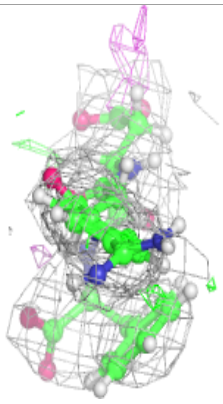
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5YB B 2011:

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

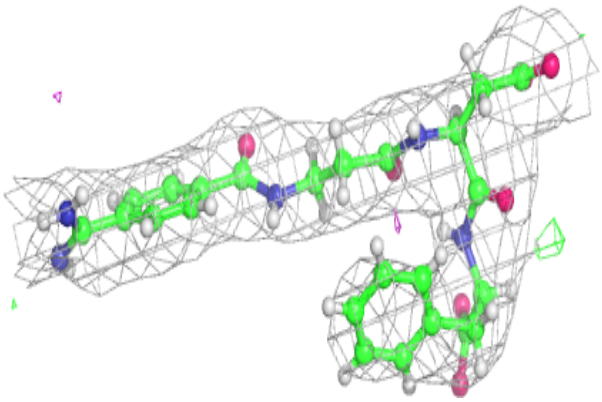


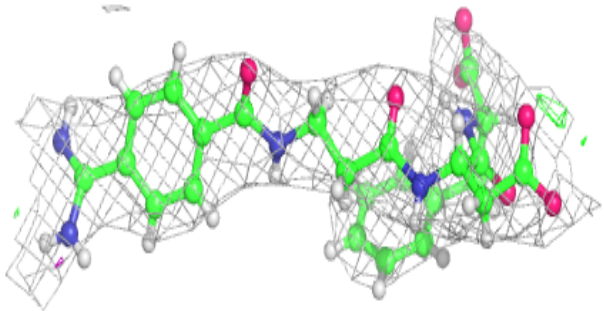


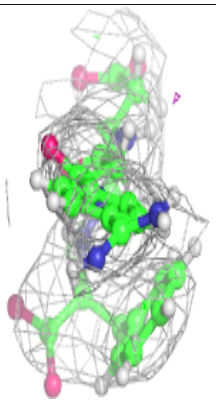


Electron density around 5YB D 501:

$2mF_o$-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.