



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:04 AM EDT

PDB ID : 6E7U
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-31
Authors : Regan, M.C.; Furukawa, H.
Deposited on : 2018-07-27
Resolution : 2.27 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

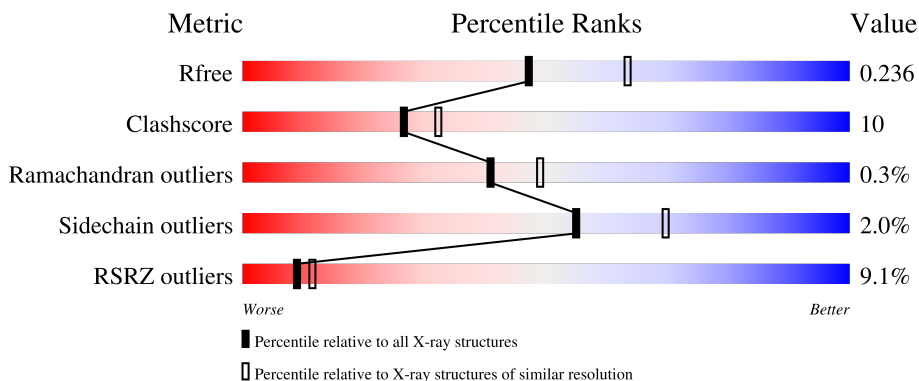
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 $\leq 5\%$. 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	385	 2% (poor fit), 78% (0-1 outliers), 15% (2 outliers), 7% (3+ outliers), 0% (not modelled)
1	C	385	 9% (poor fit), 73% (0-1 outliers), 18% (2 outliers), 7% (3+ outliers), 0% (not modelled)
2	B	363	 11% (poor fit), 84% (0-1 outliers), 14% (2 outliers), 0% (3+ outliers), 0% (not modelled)
2	D	363	 13% (poor fit), 82% (0-1 outliers), 16% (2 outliers), 0% (3+ outliers), 0% (not modelled)
3	E	5	 100% (0-1 outliers)

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
3	MAN	E	4	-	-	-	X
4	NAG	B	501	-	-	-	X
4	NAG	B	502	-	-	-	X
4	NAG	C	501	-	-	-	X
4	NAG	D	401	-	-	-	X
6	CL	A	509	-	-	X	-
6	CL	D	406	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 11538 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2765	1763	482	509	11	0	0	0
1	C	357	2728	1738	473	506	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
A	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	359	2771	1785	443	527	16	0	1	0
2	D	360	2720	1751	436	517	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

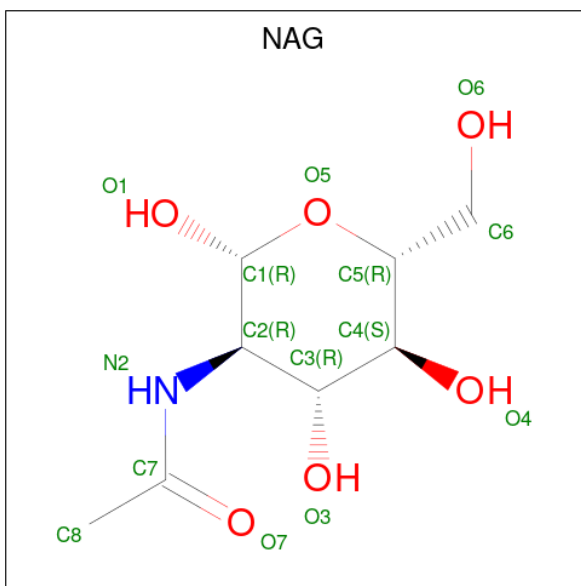
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- Molecule 3 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
			Total	C	N	O			
3	E	5	61	34	2	25	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

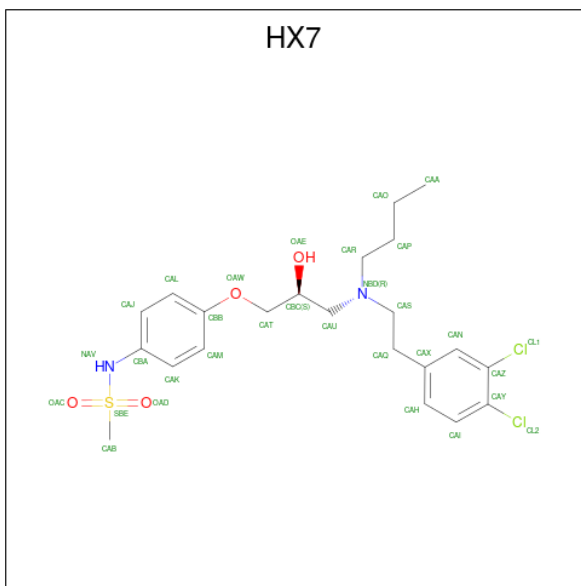
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	B	4	Total Cl 4 4	0	0
6	C	2	Total Cl 2 2	0	0
6	D	4	Total Cl 4 4	0	0

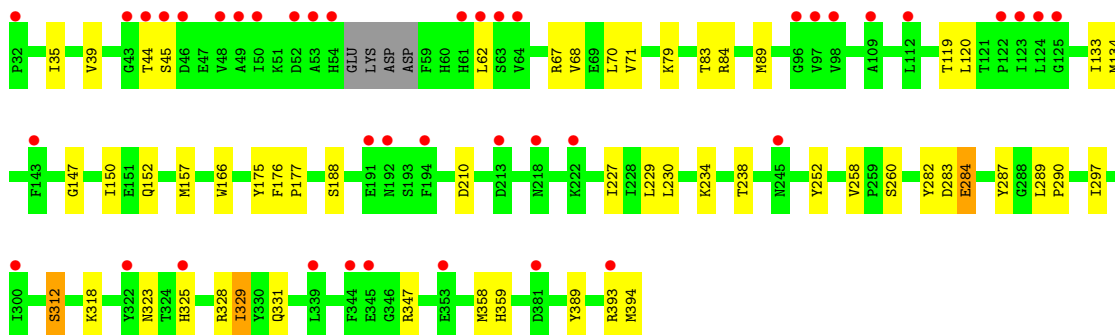
- Molecule 7 is N-{4-[(2S)-3-{butyl[2-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: HX7) (formula: C₂₂H₃₀Cl₂N₂O₄S) (labeled as "Ligand of Interest" by depositor).



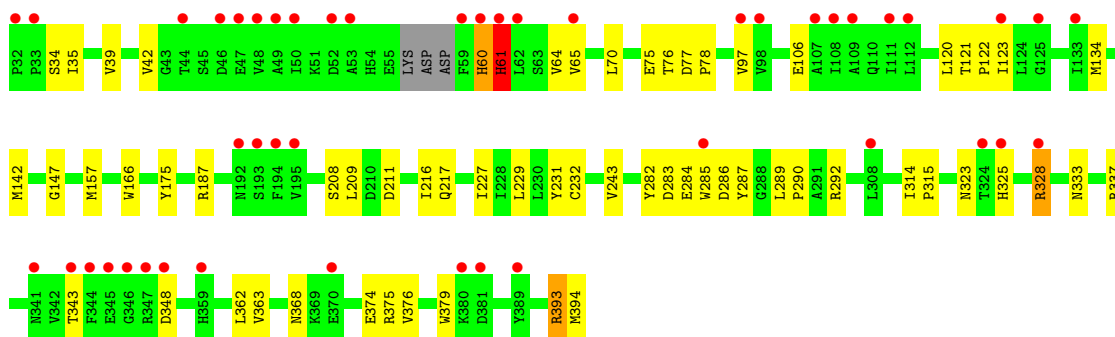
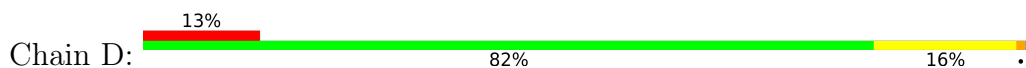
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	1	Total	C	Cl	N	O	S	0	0
			31	22	2	2	4	1		
7	D	1	Total	C	Cl	N	O	S	0	0
			31	22	2	2	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	135	Total 135	O 135	0	0
8	B	76	Total 76	O 76	0	0
8	C	75	Total 75	O 75	0	0
8	D	47	Total 47	O 47	0	0



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 3: 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.62Å 59.59Å 145.91Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	25.00 – 2.27 34.26 – 2.27	Depositor EDS
% Data completeness (in resolution range)	82.0 (25.00-2.27) 82.1 (34.26-2.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.27Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.237 0.207 , 0.236	Depositor DCC
R_{free} test set	3929 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: HX7, NAG, BMA, NA, MAN, 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	0.32	0/2822	0.36	0/3834
1	C	0.30	0/2783	0.35	0/3783
2	B	0.31	0/2838	0.36	0/3871
2	D	0.30	0/2781	0.36	0/3797
All	All	0.31	0/11224	0.36	0/15285

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	2
2	D	0	4
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	TYR	Sidechain
1	A	124	ARG	Sidechain
2	B	347	ARG	Sidechain
2	B	45	SER	Peptide
1	C	124	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	273	ARG	Sidechain
1	C	43	ARG	Sidechain
2	D	187	ARG	Sidechain
2	D	333	ASN	Peptide
2	D	393	ARG	Sidechain
2	D	61	HIS	Peptide

5.2 Too-close contacts [i](#)

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	2765	0	2731	47	0
1	C	2728	0	2694	63	2
2	B	2771	0	2637	50	2
2	D	2720	0	2563	60	0
3	E	61	0	52	0	0
4	A	14	0	13	0	0
4	B	28	0	26	3	0
4	C	28	0	26	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	3	0
6	B	4	0	0	2	0
6	C	2	0	0	0	0
6	D	4	0	0	3	0
7	B	31	0	0	4	0
7	D	31	0	0	5	0
8	A	135	0	0	5	0
8	B	76	0	0	8	0
8	C	75	0	0	4	0
8	D	47	0	0	3	0
All	All	11538	0	10755	225	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 10.

All (225) 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:283:ASP:O	2:D:285:TRP:HD1	1.12	1.30
2:D:283:ASP:O	2:D:285:TRP:CD1	1.93	1.21
1:C:237:ALA:O	8:C:601:HOH:O	1.70	1.07
1:A:270:VAL:CG1	1:A:274:GLU:HB2	1.89	1.02
1:C:41:ILE:HD13	1:C:299:SER:OG	1.73	0.88
1:C:229:LEU:HB3	1:C:261:MET:HE1	1.55	0.87
6:D:406:CL:CL	8:D:513:HOH:O	2.32	0.84
2:B:157:MET:HE3	2:B:229:LEU:HD22	1.62	0.81
1:A:270:VAL:CG1	1:A:274:GLU:CB	2.62	0.77
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.66	0.75
2:B:312:SER:O	8:B:601:HOH:O	2.03	0.75
2:D:314:ILE:HB	2:D:315:PRO:HD2	1.69	0.74
6:B:507:CL:CL	8:B:669:HOH:O	2.42	0.74
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.23	0.74
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.69	0.73
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.71	0.72
1:C:23:ASP:N	1:C:24:PRO:CD	2.52	0.72
1:A:270:VAL:HG11	1:A:274:GLU:HB2	1.72	0.72
2:B:234:LYS:O	2:B:238:THR:HG23	1.90	0.71
6:D:406:CL:CL	8:D:533:HOH:O	2.45	0.71
1:C:262:THR:HB	1:C:284:PRO:HB3	1.72	0.71
1:A:44:GLU:O	1:A:48:GLN:HG3	1.90	0.71
2:D:60:HIS:O	2:D:61:HIS:CB	2.38	0.71
2:D:120:LEU:C	2:D:142:MET:CE	2.59	0.70
2:B:133:ILE:HD12	2:B:150:ILE:CG1	2.20	0.70
7:B:503:HX7:OAE	7:B:503:HX7:CAR	2.39	0.70
4:B:502:NAG:H2	4:B:502:NAG:H61	1.73	0.70
2:D:343:THR:HG22	2:D:348:ASP:HA	1.72	0.70
7:D:402:HX7:OAE	7:D:402:HX7:CAR	2.39	0.70
2:D:122:PRO:HD3	2:D:142:MET:HE1	1.73	0.70
2:B:157:MET:CE	2:B:229:LEU:HD22	2.22	0.69
1:A:136:SER:HB3	8:A:626:HOH:O	1.93	0.69
2:D:285:TRP:CZ3	2:D:286:ASP:HB2	2.27	0.69
1:A:57:LYS:HG2	1:A:58:ILE:HG23	1.73	0.69
2:B:318:LYS:HD2	2:B:331:GLN:OE1	1.93	0.69
1:A:270:VAL:HG12	1:A:274:GLU:HB2	1.74	0.68
2:B:331:GLN:O	8:B:602:HOH:O	2.13	0.67
1:C:229:LEU:HB3	1:C:261:MET:CE	2.26	0.65
7:D:402:HX7:CAQ	7:D:402:HX7:CBC	2.73	0.65
7:B:503:HX7:CAQ	7:B:503:HX7:CBC	2.72	0.65
1:A:135:LEU:C	1:A:135:LEU:HD12	2.16	0.65
1:A:398:ARG:O	6:A:509:CL:CL	2.52	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:PRO:O	1:C:97:ALA:HB2	1.96	0.65
1:A:80:GLU:HG3	2:B:79:LYS:HE2	1.79	0.64
2:D:285:TRP:CE3	2:D:286:ASP:HB2	2.33	0.64
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.79	0.63
1:A:218:PHE:HB3	1:A:228:LEU:CD1	2.28	0.63
2:D:75:GLU:OE2	2:D:75:GLU:HA	1.98	0.63
2:D:368:ASN:HA	2:D:394:MET:CE	2.30	0.62
2:D:35:ILE:HG13	2:D:35:ILE:O	1.99	0.61
1:A:270:VAL:HG11	1:A:274:GLU:CB	2.26	0.61
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.81	0.61
2:D:157:MET:HE2	2:D:229:LEU:HD13	1.83	0.60
1:A:270:VAL:HG21	1:A:287:ILE:HD11	1.84	0.60
1:A:270:VAL:HG12	1:A:271:GLY:N	2.15	0.60
1:A:157:LEU:O	8:A:601:HOH:O	2.17	0.60
1:A:396:ASN:O	6:A:509:CL:CL	2.57	0.60
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.83	0.60
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.33	0.60
2:B:79:LYS:O	2:B:83:THR:HG23	2.02	0.59
1:C:135:LEU:C	1:C:135:LEU:HD12	2.21	0.59
2:D:120:LEU:C	2:D:142:MET:HE2	2.23	0.59
2:B:39:VAL:HB	2:B:70:LEU:HD23	1.83	0.59
2:D:286:ASP:OD1	2:D:375:ARG:NH2	2.36	0.59
1:C:136:SER:HB3	8:C:650:HOH:O	2.02	0.59
2:D:328:ARG:CZ	2:D:328:ARG:HB3	2.32	0.59
1:C:23:ASP:N	1:C:24:PRO:HD2	2.18	0.58
1:A:103:THR:HB	1:A:104:PRO:HD2	1.84	0.58
2:D:216:ILE:HD11	2:D:243:VAL:HG21	1.86	0.57
2:B:133:ILE:HD12	2:B:150:ILE:HG12	1.85	0.57
1:C:259:LEU:HD12	1:C:261:MET:CE	2.35	0.57
2:D:39:VAL:HB	2:D:70:LEU:HD23	1.85	0.57
2:B:283:ASP:O	2:B:284:GLU:C	2.42	0.57
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.86	0.56
1:C:68:ARG:HB3	1:C:69:PRO:HD2	1.87	0.56
1:C:135:LEU:HD23	7:D:402:HX7:CAM	2.35	0.56
2:D:157:MET:CE	2:D:229:LEU:HD22	2.33	0.56
2:D:285:TRP:CD1	2:D:285:TRP:N	2.72	0.56
2:D:157:MET:HE1	2:D:229:LEU:HB3	1.86	0.56
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.40	0.56
1:C:41:ILE:CD1	1:C:299:SER:OG	2.52	0.56
2:D:376:VAL:HG12	2:D:376:VAL:O	2.06	0.55
2:B:133:ILE:HG23	6:B:504:CL:CL	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ARG:HG3	1:C:344:ARG:HH11	1.70	0.55
2:B:133:ILE:CD1	2:B:150:ILE:HG12	2.37	0.54
1:C:344:ARG:HG3	1:C:344:ARG:NH1	2.21	0.54
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.23	0.54
2:B:120:LEU:O	2:B:318:LYS:HE3	2.08	0.54
1:A:103:THR:HB	1:A:104:PRO:CD	2.38	0.53
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.73	0.53
1:C:135:LEU:HD23	7:D:402:HX7:CBB	2.39	0.53
1:C:58:ILE:HD11	1:C:314:HIS:CD2	2.44	0.53
1:C:254:LYS:HE2	1:C:282:TYR:CE2	2.44	0.53
2:D:289:LEU:N	2:D:290:PRO:CD	2.72	0.53
2:D:157:MET:CE	2:D:229:LEU:HD13	2.39	0.52
1:C:30:GLY:N	1:C:87:VAL:CG2	2.72	0.52
1:A:105:THR:N	1:A:106:PRO:CD	2.72	0.52
1:A:149:LEU:HD23	1:A:183:LEU:HD11	1.90	0.52
2:B:67:ARG:O	2:B:67:ARG:HG2	2.09	0.52
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.91	0.52
2:B:323:ASN:HA	2:B:325:HIS:CE1	2.44	0.52
1:C:95:PRO:HG2	1:C:102:LEU:HD12	1.91	0.51
1:C:105:THR:N	1:C:106:PRO:CD	2.72	0.51
1:C:293:ILE:O	1:C:294:ASN:HB2	2.10	0.51
1:C:373:SER:HB3	1:C:375:MET:SD	2.50	0.51
1:A:150:VAL:O	1:A:154:MET:HG3	2.09	0.51
1:C:138:LEU:HD12	1:C:138:LEU:N	2.24	0.51
2:D:368:ASN:HA	2:D:394:MET:HE1	1.93	0.51
1:C:96:PRO:O	1:C:97:ALA:CB	2.59	0.51
1:C:153:GLU:OE2	1:C:156:ARG:NH1	2.44	0.51
2:B:238:THR:HG21	8:B:674:HOH:O	2.11	0.50
1:C:177:GLN:O	1:C:181:GLU:HG3	2.10	0.50
1:A:385:VAL:O	6:A:509:CL:CL	2.66	0.50
1:C:30:GLY:N	1:C:87:VAL:HG21	2.26	0.50
1:A:293:ILE:O	1:A:294:ASN:HB2	2.12	0.50
1:C:396:ASN:C	1:C:396:ASN:OD1	2.50	0.49
1:A:53:HIS:O	8:A:603:HOH:O	2.20	0.49
2:B:35:ILE:HG13	2:B:35:ILE:O	2.12	0.49
1:A:64:SER:O	8:A:602:HOH:O	2.19	0.49
1:C:124:ARG:O	1:C:143:PRO:HA	2.13	0.49
1:C:354:GLY:HA3	1:C:359:ILE:HD11	1.93	0.49
2:D:285:TRP:CE3	2:D:286:ASP:CB	2.95	0.48
2:D:323:ASN:HA	2:D:325:HIS:CE1	2.47	0.48
1:A:270:VAL:CG1	1:A:271:GLY:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ILE:HG12	2:B:329:ILE:O	2.13	0.48
2:D:120:LEU:O	2:D:142:MET:CE	2.61	0.48
1:C:402:TRP:HB2	1:C:406:GLU:CB	2.44	0.47
2:D:175:TYR:HB2	7:D:402:HX7:CAB	2.44	0.47
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.95	0.47
2:D:120:LEU:C	2:D:142:MET:HE3	2.35	0.47
2:B:252:TYR:OH	2:B:393:ARG:HG2	2.15	0.47
1:C:273:ARG:HD3	8:C:629:HOH:O	2.15	0.47
1:C:354:GLY:HA3	1:C:359:ILE:CD1	2.45	0.47
1:C:402:TRP:HB3	1:C:403:PRO:HD2	1.97	0.47
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.95	0.47
2:B:289:LEU:N	2:B:290:PRO:CD	2.78	0.47
2:B:175:TYR:HB2	7:B:503:HX7:CAB	2.44	0.47
2:B:84:ARG:HB2	8:B:657:HOH:O	2.15	0.46
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.45	0.46
2:D:97:VAL:HB	2:D:123:ILE:HG12	1.97	0.46
2:D:282:TYR:CE1	2:D:285:TRP:HZ2	2.33	0.46
2:B:393:ARG:HG2	2:B:394:MET:N	2.31	0.46
2:D:147:GLY:HA3	8:D:504:HOH:O	2.15	0.46
2:B:119:THR:O	2:B:318:LYS:HE3	2.16	0.46
1:A:30:GLY:HA2	1:A:63:THR:O	2.16	0.46
1:C:39:GLU:OE1	1:C:64:SER:OG	2.25	0.46
2:B:328:ARG:O	8:B:602:HOH:O	2.20	0.46
1:A:330:VAL:HG23	2:B:79:LYS:HD3	1.98	0.45
1:C:231:GLU:O	1:C:235:LEU:HG	2.16	0.45
4:B:502:NAG:H61	4:B:502:NAG:C2	2.42	0.45
1:C:105:THR:HB	1:C:106:PRO:HD3	1.98	0.45
1:C:23:ASP:N	1:C:23:ASP:OD1	2.49	0.45
2:D:231:TYR:O	2:D:232:CYS:HB3	2.16	0.45
2:B:44:THR:HG21	2:B:289:LEU:CD2	2.46	0.45
1:A:281:ARG:NH1	1:A:281:ARG:HB2	2.32	0.45
2:D:216:ILE:HG13	2:D:217:GLN:N	2.30	0.45
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.51	0.45
1:C:275:ILE:HD13	1:C:289:GLY:HA3	1.99	0.45
2:D:75:GLU:OE2	2:D:75:GLU:CA	2.65	0.44
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.99	0.44
1:A:344:ARG:HG3	1:A:344:ARG:NH1	2.33	0.44
2:D:285:TRP:CE3	2:D:363:VAL:HG21	2.52	0.44
1:A:128:TYR:HA	1:A:134:HIS:CD2	2.53	0.44
2:B:157:MET:HE1	2:B:229:LEU:HB3	1.98	0.44
2:B:147:GLY:HA3	8:B:660:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ARG:HH11	1:C:344:ARG:CG	2.31	0.44
2:B:133:ILE:O	2:B:133:ILE:HG13	2.17	0.44
1:C:70:ASN:C	1:C:70:ASN:OD1	2.56	0.44
2:D:121:THR:N	2:D:142:MET:HE3	2.32	0.44
2:D:374:GLU:O	2:D:376:VAL:HG23	2.18	0.44
2:D:285:TRP:CE3	2:D:363:VAL:CG2	3.00	0.44
2:B:133:ILE:CD1	2:B:150:ILE:CG1	2.92	0.43
1:C:87:VAL:CG2	1:C:89:ALA:O	2.65	0.43
1:C:233:LYS:O	8:C:602:HOH:O	2.21	0.43
2:D:285:TRP:CG	2:D:286:ASP:N	2.86	0.43
1:A:57:LYS:HB3	8:A:667:HOH:O	2.18	0.43
1:C:37:LYS:HA	1:C:37:LYS:HD2	1.89	0.43
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.00	0.43
1:A:270:VAL:HG11	1:A:274:GLU:HB3	2.01	0.43
1:C:30:GLY:HA3	1:C:87:VAL:HG21	2.00	0.43
1:C:347:MET:HE3	1:C:347:MET:HB3	1.87	0.43
2:D:77:ASP:HB2	2:D:78:PRO:HD2	2.01	0.43
2:D:120:LEU:O	2:D:142:MET:HE2	2.17	0.43
2:B:71:VAL:HG13	2:B:84:ARG:HH21	1.82	0.42
2:D:35:ILE:HG23	2:D:64:VAL:CG1	2.49	0.42
1:A:23:ASP:N	1:A:24:PRO:CD	2.82	0.42
1:C:103:THR:HB	1:C:104:PRO:HD2	2.01	0.42
2:D:285:TRP:CD2	2:D:286:ASP:N	2.81	0.42
1:C:87:VAL:HG22	1:C:89:ALA:O	2.20	0.42
2:D:362:LEU:HB2	2:D:379:TRP:HB3	2.01	0.42
1:A:359:ILE:HD13	1:A:367:ARG:CZ	2.49	0.42
2:B:282:TYR:HH	2:B:287:TYR:HD2	1.64	0.42
2:D:106:GLU:OE2	6:D:406:CL:CL	2.75	0.42
2:D:283:ASP:CG	2:D:284:GLU:H	2.23	0.41
2:D:289:LEU:N	2:D:290:PRO:HD2	2.36	0.41
1:C:241:ILE:HA	1:C:269:LEU:O	2.20	0.41
2:B:44:THR:HG21	2:B:289:LEU:HD21	2.01	0.41
1:C:343:LYS:NZ	2:D:208:SER:OG	2.48	0.41
1:A:241:ILE:HA	1:A:269:LEU:O	2.21	0.41
1:A:250:THR:HG22	1:A:254:LYS:HE3	2.01	0.41
2:B:89:MET:HE3	2:B:318:LYS:HB2	2.02	0.41
1:A:339:GLY:N	1:A:340:PRO:CD	2.83	0.41
4:B:502:NAG:C2	4:B:502:NAG:C6	2.99	0.41
1:A:138:LEU:HD12	1:A:138:LEU:N	2.36	0.41
1:C:259:LEU:CD1	1:C:261:MET:CE	2.99	0.41
2:B:67:ARG:O	2:B:67:ARG:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LEU:N	2:B:290:PRO:HD2	2.36	0.41
1:C:233:LYS:HG3	1:C:266:TYR:OH	2.21	0.41
1:C:242:LEU:HB3	1:C:270:VAL:HG12	2.03	0.41
2:D:34:SER:HA	2:D:65:VAL:O	2.21	0.41
2:D:211:ASP:OD2	2:D:216:ILE:HG12	2.21	0.41
1:C:135:LEU:C	1:C:135:LEU:CD1	2.89	0.41
1:C:214:LYS:NZ	1:C:231:GLU:OE2	2.54	0.41
1:A:135:LEU:HD23	7:B:503:HX7:CBB	2.51	0.40
1:A:154:MET:HG2	1:A:393:ILE:HD11	2.03	0.40
2:B:120:LEU:HD13	2:B:331:GLN:HB3	2.04	0.40
2:B:318:LYS:HE2	8:B:658:HOH:O	2.20	0.40
2:D:368:ASN:OD1	2:D:368:ASN:C	2.60	0.40
1:A:344:ARG:NE	2:B:210:ASP:OD1	2.50	0.40
2:B:68:VAL:HG11	2:B:297:ILE:HD13	2.04	0.40
1:C:343:LYS:HD3	2:D:209:LEU:HD23	2.02	0.40
2:B:318:LYS:N	2:B:318:LYS:HD3	2.35	0.40
1:C:95:PRO:HA	1:C:96:PRO:HD3	1.88	0.40
1:A:33:LEU:O	1:A:66:THR:HA	2.21	0.40
2:D:376:VAL:O	2:D:376:VAL:CG1	2.69	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)
2:B:393:ARG:NH2	1:C:384:GLN:OE1[4_7510]	1.92	0.28
2:B:389:TYR:O	1:C:380:ARG:NH1[4_7510]	2.18	0.02

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	353/385 (92%)	338 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	351/385 (91%)	339 (97%)	11 (3%)	1 (0%)	41	49
2	B	356/363 (98%)	337 (95%)	18 (5%)	1 (0%)	41	49
2	D	356/363 (98%)	341 (96%)	13 (4%)	2 (1%)	25	29
All	All	1416/1496 (95%)	1355 (96%)	57 (4%)	4 (0%)	41	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	284	GLU
2	D	61	HIS
2	D	60	HIS
1	C	96	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/331 (87%)	285 (99%)	4 (1%)	67	79
1	C	287/331 (87%)	281 (98%)	6 (2%)	53	68
2	B	293/326 (90%)	283 (97%)	10 (3%)	37	49
2	D	281/326 (86%)	277 (99%)	4 (1%)	67	79
All	All	1150/1314 (88%)	1126 (98%)	24 (2%)	55	68

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	258	MET
1	A	281	ARG
1	A	380	ARG
2	B	62	LEU
2	B	134	MET
2	B	152	GLN

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Mol	Chain	Res	Type
2	B	188	SER
2	B	260	SER
2	B	312	SER
2	B	329	ILE
2	B	358	MET
2	B	359[A]	HIS
2	B	359[B]	HIS
1	C	23	ASP
1	C	258	MET
1	C	281	ARG
1	C	299	SER
1	C	347	MET
1	C	363	GLU
2	D	134	MET
2	D	328	ARG
2	D	337	ARG
2	D	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	61	GLN
1	A	321	ASN
1	C	73	GLN
2	D	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.37	0	17,19,21	0.62	0
3	NAG	E	2	3	14,14,15	0.38	0	17,19,21	0.75	0
3	BMA	E	3	3	11,11,12	0.39	0	15,15,17	0.61	0
3	MAN	E	4	3	11,11,12	0.39	0	15,15,17	0.82	0
3	MAN	E	5	3	11,11,12	0.29	0	15,15,17	0.62	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

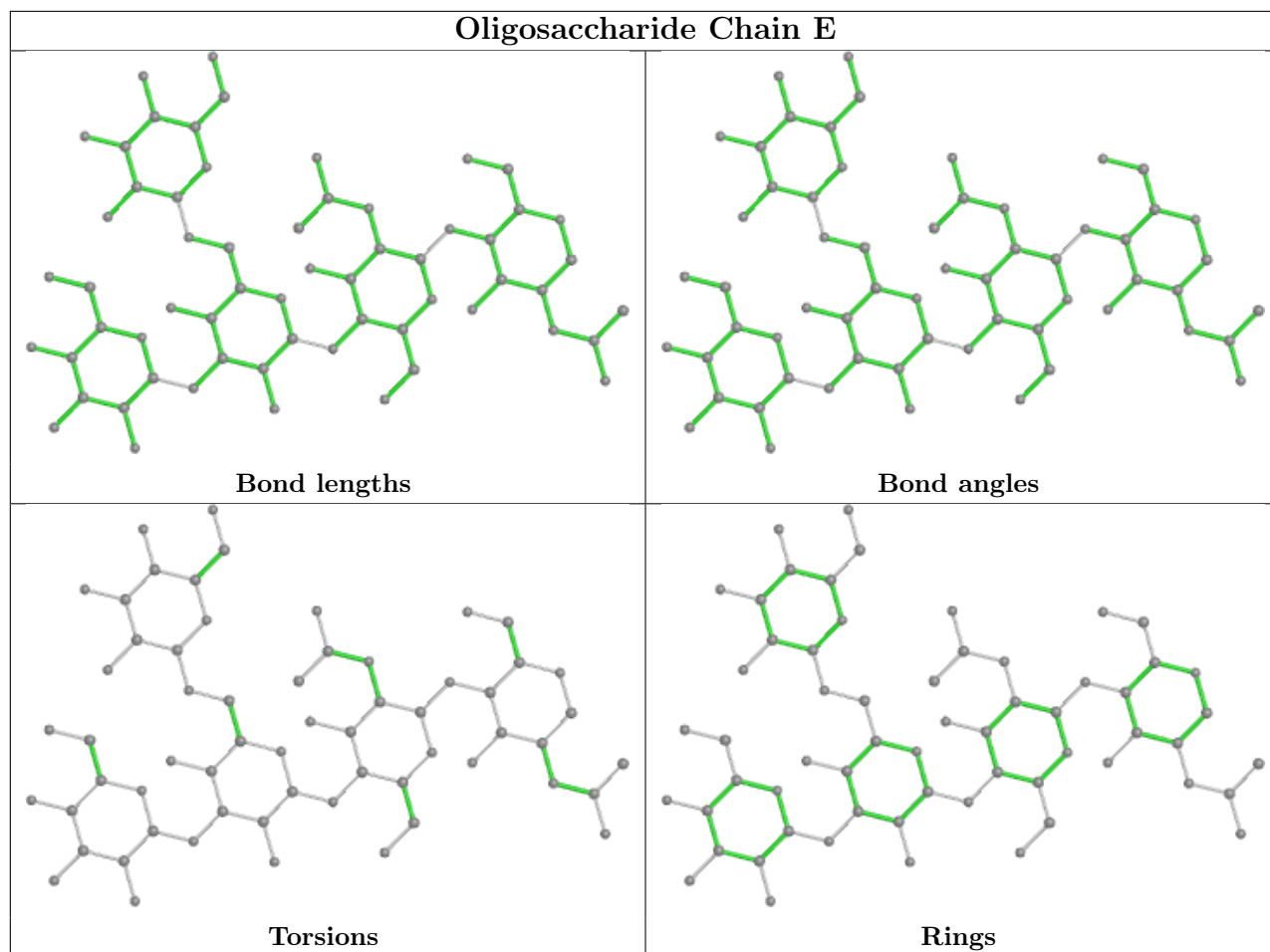
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.



5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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$
4	NAG	B	502	2	14,14,15	0.45	0	17,19,21	0.77	1 (5%)
7	HX7	B	503	-	32,32,32	1.74	7 (21%)	43,43,43	2.13	4 (9%)
4	NAG	A	501	1	14,14,15	0.27	0	17,19,21	0.73	0
4	NAG	D	401	2	14,14,15	0.86	1 (7%)	17,19,21	1.52	3 (17%)
7	HX7	D	402	-	32,32,32	1.67	8 (25%)	43,43,43	2.10	3 (6%)
4	NAG	C	502	1	14,14,15	0.34	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	501	2	14,14,15	0.41	0	17,19,21	0.61	0
4	NAG	C	501	1	14,14,15	0.64	1 (7%)	17,19,21	0.63	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
4	NAG	B	502	2	-	2/6/23/26	0/1/1/1
7	HX7	B	503	-	-	9/23/23/23	0/2/2/2
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	2	-	4/6/23/26	0/1/1/1
7	HX7	D	402	-	-	12/23/23/23	0/2/2/2
4	NAG	C	502	1	-	3/6/23/26	0/1/1/1
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
4	NAG	C	501	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503	HX7	SBE-NAV	6.71	1.72	1.63
7	D	402	HX7	SBE-NAV	6.22	1.71	1.63
7	B	503	HX7	OAW-CBB	3.01	1.44	1.37
7	B	503	HX7	CAB-SBE	2.94	1.82	1.75
7	D	402	HX7	CAB-SBE	2.90	1.82	1.75
7	D	402	HX7	OAW-CBB	2.88	1.44	1.37
7	B	503	HX7	CBA-NAV	2.56	1.47	1.43
7	B	503	HX7	CAY-CL2	2.45	1.79	1.73
7	D	402	HX7	CAY-CL2	2.30	1.79	1.73
7	D	402	HX7	OAC-SBE	2.27	1.47	1.43
7	D	402	HX7	CBA-NAV	2.24	1.46	1.43
4	D	401	NAG	O5-C1	2.16	1.47	1.43
7	D	402	HX7	CAZ-CL1	2.15	1.78	1.73
7	D	402	HX7	OAD-SBE	2.13	1.47	1.43
7	B	503	HX7	OAC-SBE	2.05	1.47	1.43
4	C	501	NAG	C1-C2	2.01	1.55	1.52
7	B	503	HX7	OAD-SBE	2.01	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503	HX7	OAD-SBE-OAC	-12.21	101.29	118.85
7	D	402	HX7	OAD-SBE-OAC	-11.96	101.66	118.85
4	D	401	NAG	C1-O5-C5	4.79	118.68	112.19
7	D	402	HX7	CAB-SBE-NAV	3.49	110.61	106.63
7	B	503	HX7	CAB-SBE-NAV	3.38	110.49	106.63
4	D	401	NAG	O5-C1-C2	2.36	115.02	111.29
7	D	402	HX7	OAC-SBE-NAV	2.10	111.39	107.10
4	D	401	NAG	O5-C5-C6	2.10	110.49	107.20
4	B	502	NAG	O5-C5-C6	2.06	110.43	107.20
7	B	503	HX7	OAD-SBE-NAV	2.03	111.24	107.10
7	B	503	HX7	OAC-SBE-NAV	2.03	111.24	107.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	402	HX7	NBD-CAU-CBC-CAT
7	B	503	HX7	CAQ-CAS-NBD-CAU
7	D	402	HX7	CAQ-CAS-NBD-CAU
4	D	401	NAG	O5-C5-C6-O6
4	D	401	NAG	C4-C5-C6-O6
4	B	502	NAG	C8-C7-N2-C2
4	B	502	NAG	O7-C7-N2-C2
4	C	502	NAG	C8-C7-N2-C2
4	C	502	NAG	O7-C7-N2-C2
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
7	D	402	HX7	NBD-CAU-CBC-OAE
7	D	402	HX7	CAX-CAQ-CAS-NBD
7	B	503	HX7	CAS-CAQ-CAX-CAN
7	B	503	HX7	CAX-CAQ-CAS-NBD
7	B	503	HX7	CAS-CAQ-CAX-CAH
7	D	402	HX7	CAS-CAQ-CAX-CAH
7	D	402	HX7	CAS-CAQ-CAX-CAN
7	B	503	HX7	CAO-CAP-CAR-NBD
7	D	402	HX7	CAP-CAR-NBD-CAS
7	D	402	HX7	CBA-NAV-SBE-OAD
7	D	402	HX7	CAQ-CAS-NBD-CAR
7	B	503	HX7	NBD-CAU-CBC-OAE
7	B	503	HX7	CAQ-CAS-NBD-CAR
4	C	502	NAG	C4-C5-C6-O6
7	B	503	HX7	CAM-CBB-OAW-CAT
7	D	402	HX7	OAW-CAT-CBC-CAU

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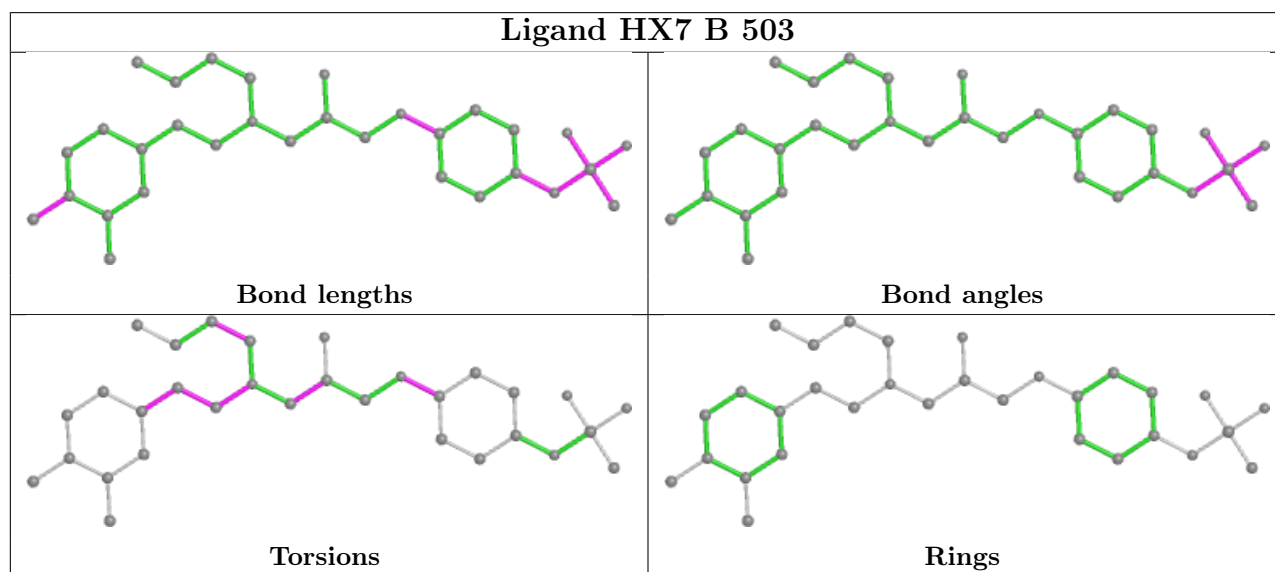
Mol	Chain	Res	Type	Atoms
7	D	402	HX7	OAW-CAT-CBC-OAE
7	D	402	HX7	CAP-CAR-NBD-CAU
7	B	503	HX7	NBD-CAU-CBC-CAT

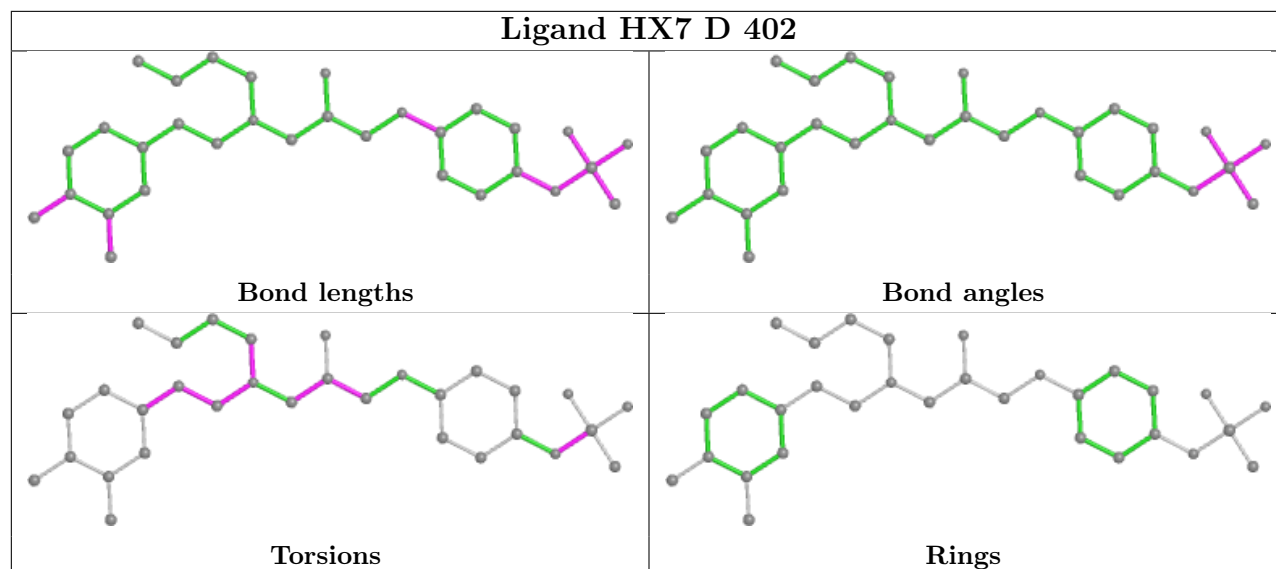
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	NAG	3	0
7	B	503	HX7	4	0
7	D	402	HX7	5	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	359/385 (93%)	0.11	9 (2%) 57 63	17, 30, 60, 74	0
1	C	357/385 (92%)	0.44	35 (9%) 7 9	22, 42, 69, 83	0
2	B	359/363 (98%)	0.59	41 (11%) 5 6	17, 43, 70, 83	0
2	D	360/363 (99%)	0.62	46 (12%) 3 4	22, 43, 77, 93	0
All	All	1435/1496 (95%)	0.44	131 (9%) 9 11	17, 39, 69, 93	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	VAL	9.2
2	D	194	PHE	7.7
2	D	48	VAL	6.1
2	D	344	PHE	5.8
1	C	97	ALA	5.3
1	C	266	TYR	5.1
1	C	321	ASN	4.9
2	D	49	ALA	4.8
2	B	381	ASP	4.7
2	D	381	ASP	4.4
1	C	259	LEU	4.4
1	C	157	LEU	4.3
2	D	359	HIS	4.3
2	B	49	ALA	4.2
2	B	52	ASP	4.1
1	A	23	ASP	4.0
2	D	345	GLU	4.0
2	D	60	HIS	4.0
2	D	195	VAL	4.0
2	B	46	ASP	3.9
2	D	380	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	325	HIS	3.9
2	D	192	ASN	3.8
1	C	264	ALA	3.8
2	B	44	THR	3.8
1	C	406	GLU	3.8
2	B	32	PRO	3.6
2	D	347	ARG	3.6
2	D	50	ILE	3.6
2	D	44	THR	3.5
2	B	61	HIS	3.5
2	D	32	PRO	3.5
2	D	346	GLY	3.5
1	C	258	MET	3.5
2	D	97	VAL	3.5
2	D	53	ALA	3.5
1	C	158	PHE	3.4
1	C	405	GLY	3.4
2	D	52	ASP	3.3
2	D	193	SER	3.3
2	D	46	ASP	3.3
2	B	123	ILE	3.3
2	D	343	THR	3.3
1	C	257	ALA	3.3
2	B	213	ASP	3.3
1	C	397	ASP	3.2
2	B	344	PHE	3.2
2	D	348	ASP	3.2
2	D	59	PHE	3.2
2	B	393	ARG	3.2
2	B	62	LEU	3.2
2	B	191	GLU	3.1
1	C	394	ILE	3.1
2	D	123	ILE	3.1
2	B	218	ASN	3.0
1	C	102	LEU	3.0
1	A	209	GLY	3.0
2	D	125	GLY	3.0
2	D	61	HIS	3.0
1	A	221	GLY	3.0
1	A	234	GLU	3.0
1	C	96	PRO	2.9
2	D	285	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	194	PHE	2.9
1	A	236	GLU	2.8
2	B	124	LEU	2.8
1	A	96	PRO	2.8
1	C	58	ILE	2.8
2	B	97	VAL	2.8
2	D	341	ASN	2.8
1	C	223	LYS	2.8
2	B	345	GLU	2.8
2	B	50	ILE	2.8
1	C	265	GLY	2.8
1	C	353	ASP	2.8
2	D	47	GLU	2.8
1	C	209	GLY	2.7
2	B	43	GLY	2.7
1	C	159	ASN	2.7
2	D	108	ILE	2.7
2	D	62	LEU	2.6
2	B	98	VAL	2.6
2	B	109	ALA	2.5
2	B	45	SER	2.5
2	B	122	PRO	2.5
1	C	23	ASP	2.5
2	B	53	ALA	2.5
2	D	107	ALA	2.5
2	B	245	ASN	2.5
1	C	382	LEU	2.5
1	C	224	ASN	2.5
1	C	260	ASP	2.4
2	D	112	LEU	2.4
2	B	325	HIS	2.4
2	D	324	THR	2.4
2	B	112	LEU	2.4
2	D	370	GLU	2.4
1	A	185	GLU	2.4
2	B	54	HIS	2.3
2	B	353	GLU	2.3
2	B	192	ASN	2.3
1	A	186	GLY	2.3
2	D	328	ARG	2.3
2	B	63	SER	2.3
2	D	109	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	125	GLY	2.2
2	D	98	VAL	2.2
2	B	300	ILE	2.2
2	B	64	VAL	2.2
1	C	391	SER	2.2
1	C	56	ARG	2.2
1	C	358	ARG	2.2
1	C	282	TYR	2.2
2	B	322	TYR	2.2
1	C	290	LEU	2.1
1	C	352	PRO	2.1
1	C	404	GLY	2.1
2	D	389	TYR	2.1
2	D	33	PRO	2.1
1	C	227	ALA	2.1
2	B	222	LYS	2.1
2	B	143	PHE	2.1
2	B	339	LEU	2.0
2	D	111	ILE	2.0
2	D	133	ILE	2.0
1	C	263	GLY	2.0
2	B	96	GLY	2.0
1	C	222	THR	2.0
2	D	65	VAL	2.0
2	D	308	LEU	2.0
1	A	407	THR	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.

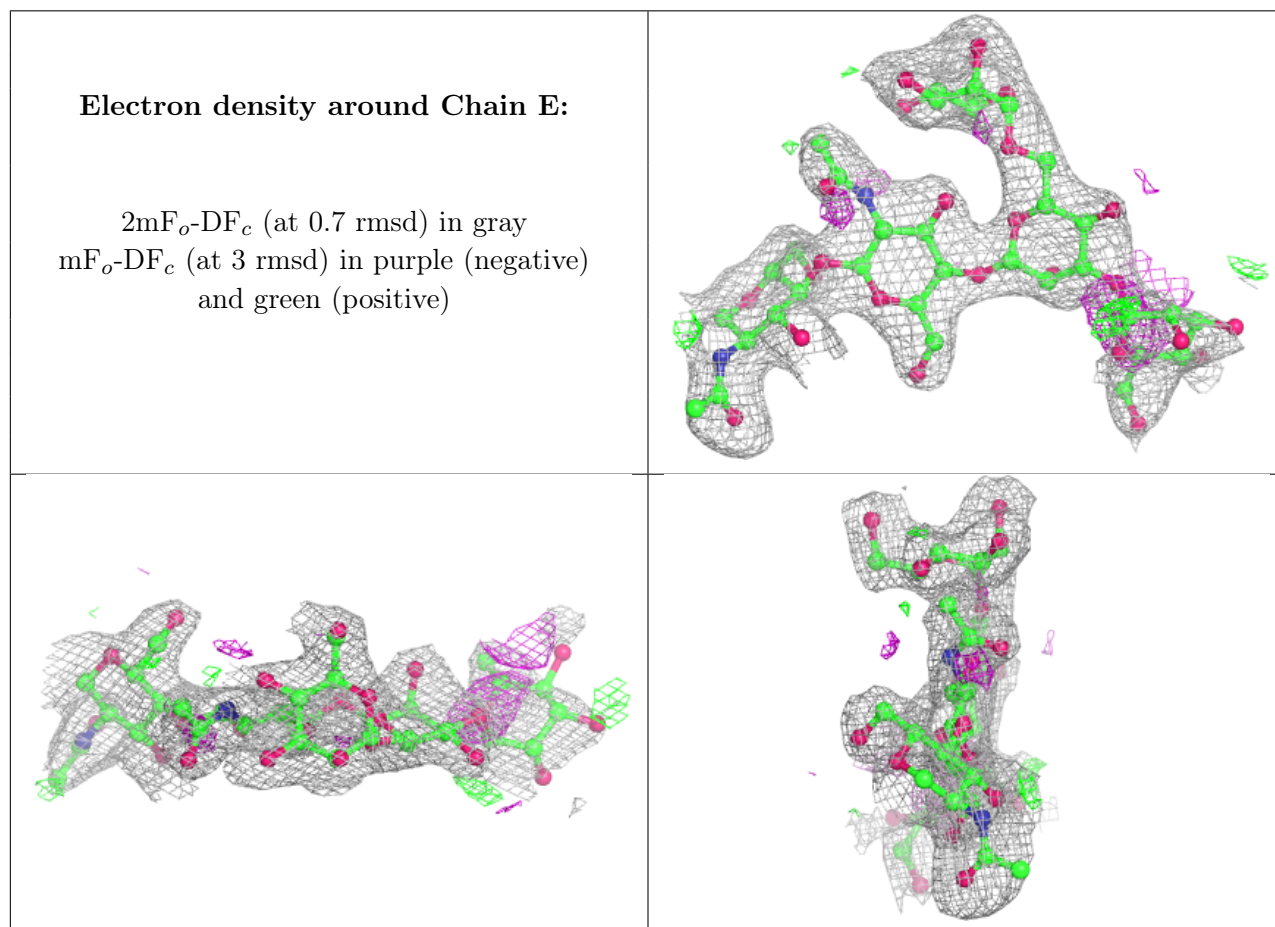
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	4	11/12	0.66	0.46	82,85,91,94	0
3	MAN	E	5	11/12	0.80	0.16	63,68,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	1	14/15	0.87	0.16	41,46,51,52	0
3	BMA	E	3	11/12	0.88	0.26	69,73,79,81	0
3	NAG	E	2	14/15	0.91	0.20	56,58,64,66	0

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



6.4 Ligands 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
4	NAG	B	502	14/15	0.58	0.59	72,76,81,84	0
4	NAG	D	401	14/15	0.69	0.51	74,77,82,84	0
4	NAG	B	501	14/15	0.72	0.41	61,66,70,71	0

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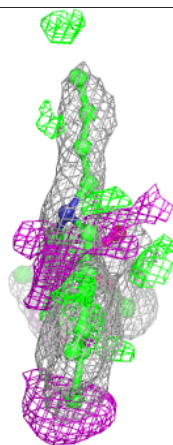
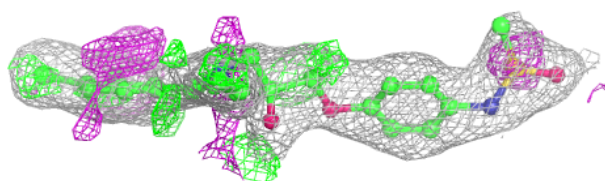
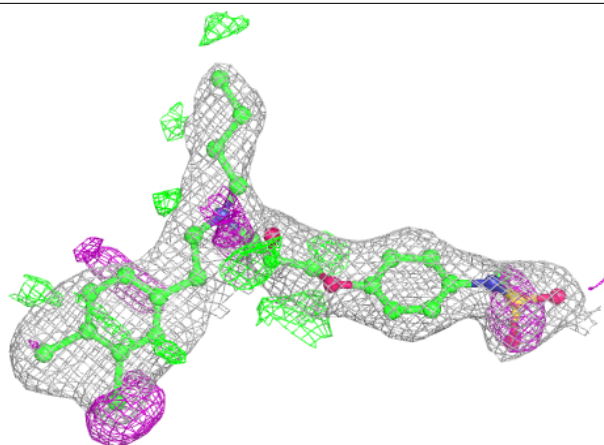
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	501	14/15	0.79	0.46	65,74,81,81	0
6	CL	B	506	1/1	0.86	0.12	53,53,53,53	0
6	CL	D	403	1/1	0.87	0.28	57,57,57,57	0
6	CL	B	504	1/1	0.88	0.21	53,53,53,53	0
6	CL	D	405	1/1	0.88	0.10	66,66,66,66	0
7	HX7	B	503	31/31	0.88	0.20	34,38,42,43	0
4	NAG	C	502	14/15	0.89	0.16	44,47,51,52	0
4	NAG	A	501	14/15	0.91	0.23	35,38,40,41	0
6	CL	A	509	1/1	0.91	0.07	48,48,48,48	0
6	CL	C	504	1/1	0.91	0.17	69,69,69,69	0
7	HX7	D	402	31/31	0.91	0.18	34,40,46,52	0
6	CL	A	508	1/1	0.92	0.06	57,57,57,57	0
6	CL	D	404	1/1	0.93	0.20	77,77,77,77	0
6	CL	D	406	1/1	0.94	0.08	70,70,70,70	0
6	CL	B	507	1/1	0.95	0.12	61,61,61,61	0
6	CL	B	505	1/1	0.95	0.17	72,72,72,72	0
6	CL	C	505	1/1	0.95	0.08	43,43,43,43	0
5	NA	C	503	1/1	0.98	0.05	28,28,28,28	0
5	NA	A	507	1/1	0.99	0.10	19,19,19,19	0

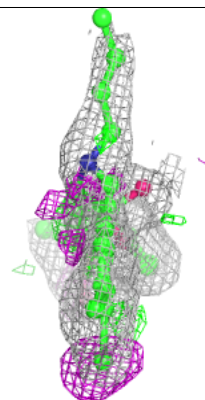
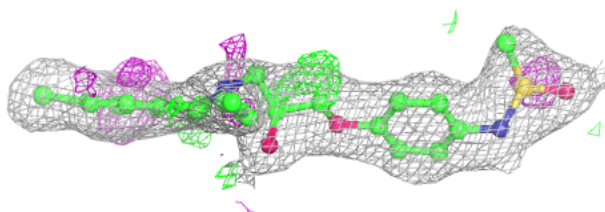
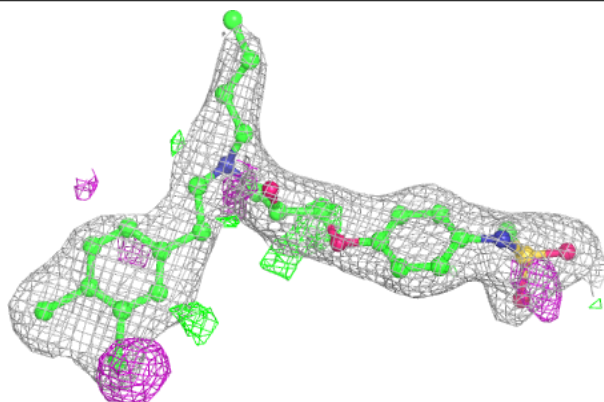
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HX7 B 503:

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

**Electron density around HX7 D 402:**

$2mF_o-DF_c$ (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.