



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:09 AM BST

PDB ID : 6E7R
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-4
Authors : Regan, M.C.; Furukawa, H.
Deposited on : 2018-07-27
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

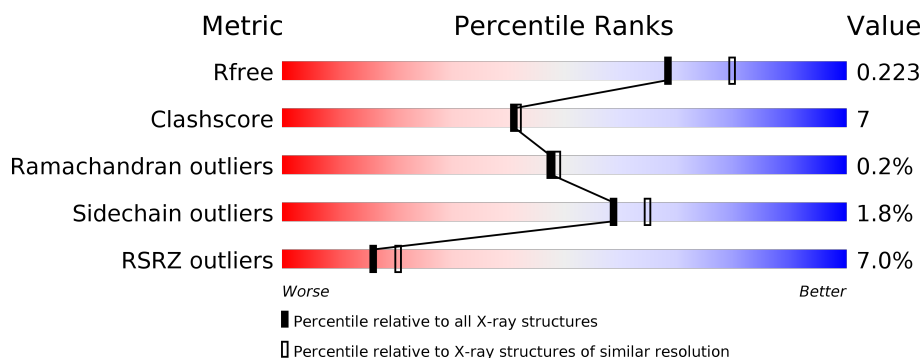
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
1	C	385	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
2	B	363	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	D	363	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
3	E	5	<div> <div></div> <div>100%</div> </div>
4	F	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	1	-	-	-	X
4	NAG	F	2	-	-	-	X
5	NAG	A	507	-	-	-	X
5	NAG	B	502	-	-	-	X
5	NAG	D	401	-	-	-	X
7	CL	A	510	-	-	X	-
7	CL	B	504	-	-	X	-
7	CL	B	507	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11522 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
1	A	358	Total	C	N	O	S	0	0	0
			2756	1759	479	508	10			
1	C	357	Total	C	N	O	S	0	0	0
			2714	1731	467	505	11			

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

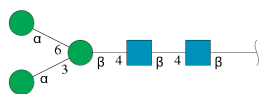
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2775	1787	439	534	15			
2	D	358	Total	C	N	O	S	0	0	0
			2698	1737	428	517	16			

There are 2 discrepancies between the modelled and reference sequences:

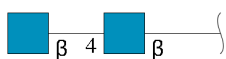
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- 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.



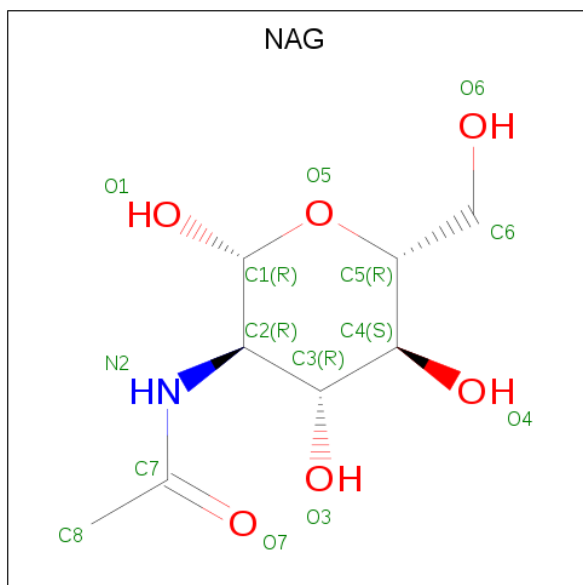
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			13	7	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

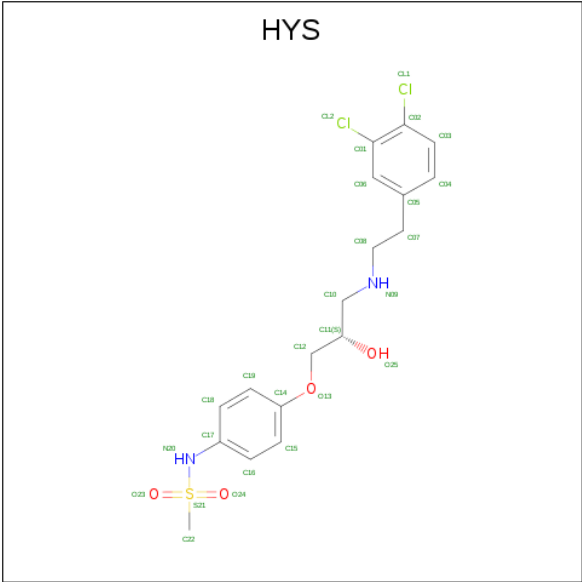
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is N-{4-[(2S)-3-{[2-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: HYS) (formula: C₁₈H₂₂Cl₂N₂O₄S) (labeled as "Ligand of Interest" by author).

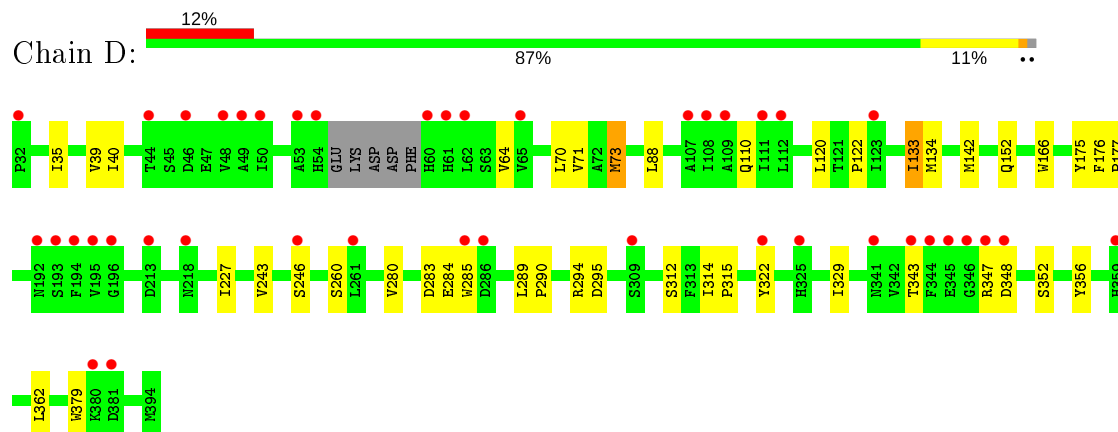


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	Cl	N	O	S	0	0
			27	18	2	2	4	1		
8	D	1	Total	C	Cl	N	O	S	0	0
			27	18	2	2	4	1		

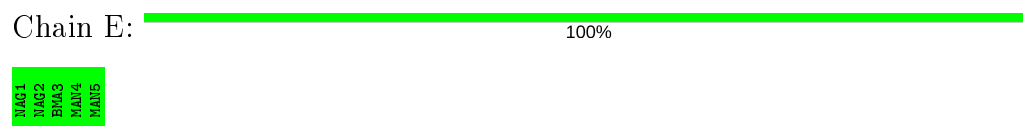
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	136	Total	O	0	0
			136	136		
9	B	80	Total	O	0	0
			80	80		
9	C	75	Total	O	0	0
			75	75		
9	D	48	Total	O	0	0
			48	48		

- 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



- Molecule 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	267.95Å 59.90Å 145.29Å 90.00° 116.69° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 35.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.2 (25.00-2.10) 83.3 (35.02-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.218 0.197 , 0.223	Depositor DCC
R_{free} test set	5146 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11522	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, NA, HYS, 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	0.37	0/2814	0.36	0/3826
1	C	0.32	0/2770	0.35	0/3772
2	B	0.35	0/2837	0.36	0/3873
2	D	0.31	0/2760	0.35	0/3773
All	All	0.34	0/11181	0.35	0/15244

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	GLY	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	2756	0	2715	36	0
1	C	2714	0	2655	42	0
2	B	2775	0	2608	35	0
2	D	2698	0	2526	36	0
3	E	61	0	52	0	0
4	F	28	0	25	1	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
5	C	13	0	9	4	0
5	D	14	0	13	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	2	0
7	B	4	0	0	5	0
7	C	2	0	0	0	0
7	D	4	0	0	2	0
8	B	27	0	0	3	0
8	D	27	0	0	2	0
9	A	136	0	0	4	0
9	B	80	0	0	5	0
9	C	75	0	0	3	0
9	D	48	0	0	2	0
All	All	11522	0	10655	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (156) 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)
5:C:501:NAG:C8	5:C:501:NAG:O7	1.87	1.21
5:C:501:NAG:N2	5:C:501:NAG:O7	1.76	1.19
7:A:510:CL:CL	9:A:601:HOH:O	2.04	1.10
2:B:235:GLU:OE1	2:B:235:GLU:OE2	1.70	1.07
1:C:157:LEU:HD23	1:C:158:PHE:CE2	2.03	0.93
7:B:504:CL:CL	9:B:641:HOH:O	2.23	0.92
2:D:133:ILE:HG23	7:D:403:CL:CL	2.14	0.85
5:C:501:NAG:N2	5:C:501:NAG:C8	2.40	0.84
1:A:29:ILE:HD11	1:A:313:ILE:CD1	2.09	0.81
2:B:235:GLU:CG	2:B:235:GLU:OE2	2.32	0.78
2:B:318:LYS:HD2	2:B:331:GLN:OE1	1.84	0.78
2:B:235:GLU:OE1	2:B:235:GLU:CG	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:SER:O	9:B:601:HOH:O	2.02	0.76
1:C:157:LEU:HD23	1:C:158:PHE:CD2	2.20	0.76
2:B:375:ARG:NH1	9:B:603:HOH:O	2.17	0.76
2:D:120:LEU:C	2:D:142:MET:CE	2.56	0.74
1:C:222:THR:HB	1:C:225:LEU:HD21	1.72	0.71
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.71	0.71
2:B:193:SER:O	9:B:602:HOH:O	2.09	0.71
1:A:218:PHE:HB3	1:A:228:LEU:CD1	2.22	0.69
2:D:343:THR:HG22	2:D:348:ASP:HA	1.75	0.69
1:A:153:GLU:OE2	1:A:156:ARG:NH1	2.26	0.69
2:B:343:THR:HG22	2:B:348:ASP:HA	1.74	0.69
1:C:135:LEU:C	1:C:135:LEU:HD23	2.13	0.68
7:B:507:CL:CL	9:B:633:HOH:O	2.48	0.68
1:A:233:LYS:HE3	1:A:259:LEU:O	1.95	0.67
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.08	0.67
1:C:232:ALA:O	9:C:601:HOH:O	2.14	0.66
2:D:312:SER:O	9:D:501:HOH:O	2.12	0.66
1:A:68:ARG:HD2	9:A:712:HOH:O	1.95	0.65
1:A:29:ILE:HD11	1:A:313:ILE:HD11	1.79	0.65
2:B:328:ARG:O	9:D:501:HOH:O	2.15	0.64
1:C:41:ILE:HD13	1:C:299:SER:OG	1.98	0.64
2:D:283:ASP:O	2:D:285:TRP:CD1	2.51	0.64
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.80	0.64
1:C:229:LEU:HD12	1:C:255:SER:HB2	1.80	0.62
2:D:120:LEU:C	2:D:142:MET:HE2	2.19	0.62
1:C:69:PRO:HD2	1:C:73:GLN:OE1	1.99	0.62
1:C:262:THR:HB	1:C:284:PRO:HB3	1.81	0.62
1:A:150:VAL:O	1:A:154:MET:HG3	2.00	0.61
1:C:157:LEU:CD2	1:C:158:PHE:CE2	2.82	0.60
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.84	0.60
1:C:135:LEU:HD23	1:C:136:SER:N	2.17	0.60
2:B:133:ILE:HG23	7:B:504:CL:CL	2.39	0.60
2:B:55:GLU:C	2:B:57:ASP:H	2.05	0.60
1:C:218:PHE:HB3	1:C:228:LEU:CD1	2.33	0.59
2:D:40:ILE:HG12	2:D:71:VAL:CG2	2.34	0.57
2:D:176:PHE:CD1	2:D:177:PRO:HD2	2.39	0.57
1:A:395:GLN:NE2	7:A:510:CL:CL	2.74	0.57
1:C:273:ARG:HD3	9:C:640:HOH:O	2.04	0.57
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.88	0.56
1:C:229:LEU:CD1	1:C:255:SER:HB2	2.36	0.55
1:C:228:LEU:HD23	1:C:228:LEU:C	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:O	9:C:602:HOH:O	2.18	0.55
2:D:314:ILE:HB	2:D:315:PRO:HD2	1.88	0.55
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.88	0.55
1:A:68:ARG:CD	9:A:712:HOH:O	2.54	0.55
1:A:136:SER:HB3	9:A:665:HOH:O	2.06	0.55
2:D:39:VAL:HB	2:D:70:LEU:HD23	1.88	0.55
8:B:503:HYS:O25	8:B:503:HYS:C08	2.55	0.54
1:A:105:THR:N	1:A:106:PRO:CD	2.71	0.54
2:D:40:ILE:HG21	2:D:73:MET:HE2	1.90	0.54
1:C:396:ASN:C	1:C:396:ASN:OD1	2.46	0.53
2:B:35:ILE:HG23	2:B:64:VAL:HG21	1.91	0.53
1:C:261:MET:HA	1:C:266:TYR:CE2	2.44	0.52
1:A:135:LEU:HD12	1:A:135:LEU:C	2.30	0.52
2:D:283:ASP:O	2:D:285:TRP:HD1	1.93	0.52
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.90	0.52
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.45	0.52
2:D:243:VAL:O	2:D:246:SER:HB2	2.10	0.51
1:C:70:ASN:C	1:C:70:ASN:OD1	2.47	0.51
2:D:35:ILE:HG23	2:D:64:VAL:HG11	1.92	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.10	0.51
2:D:329:ILE:HG12	2:D:329:ILE:O	2.10	0.51
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.43	0.51
2:B:133:ILE:HD12	2:B:150:ILE:HG12	1.92	0.51
2:D:295:ASP:OD2	2:D:347:ARG:NH2	2.43	0.51
2:B:57:ASP:C	2:B:59:PHE:H	2.13	0.51
2:D:120:LEU:O	2:D:142:MET:CE	2.58	0.51
2:B:234:LYS:HG3	2:B:262:VAL:O	2.11	0.51
2:D:73:MET:HG2	7:D:404:CL:CL	2.47	0.51
2:D:71:VAL:HG11	2:D:88:LEU:HD21	1.93	0.50
2:D:40:ILE:HA	2:D:71:VAL:HG23	1.94	0.50
1:C:293:ILE:O	1:C:294:ASN:HB2	2.11	0.50
1:A:304:ASP:HB3	1:A:359:ILE:CD1	2.42	0.50
2:D:284:GLU:O	2:D:284:GLU:HG3	2.13	0.49
1:C:105:THR:N	1:C:106:PRO:CD	2.75	0.49
2:D:314:ILE:HB	2:D:315:PRO:CD	2.42	0.49
1:A:242:LEU:HB3	1:A:270:VAL:HG12	1.94	0.49
1:C:389:ASN:C	1:C:389:ASN:OD1	2.50	0.49
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.93	0.48
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.95	0.48
2:B:54:HIS:CG	2:B:54:HIS:O	2.66	0.48
1:C:138:LEU:N	1:C:138:LEU:HD12	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:CG1	2:B:84:ARG:NH2	2.76	0.48
1:C:154:MET:HG2	1:C:393:ILE:HD11	1.95	0.48
2:D:260:SER:HA	2:D:280:VAL:O	2.13	0.48
1:C:229:LEU:HD12	1:C:255:SER:CB	2.43	0.47
2:D:40:ILE:HG12	2:D:71:VAL:HG21	1.95	0.47
1:A:30:GLY:HA2	1:A:63:THR:O	2.14	0.47
1:C:241:ILE:HA	1:C:269:LEU:O	2.15	0.47
1:C:363:GLU:CD	1:C:363:GLU:H	2.17	0.47
1:A:135:LEU:HD23	8:B:503:HYS:C14	2.44	0.47
2:B:260:SER:HA	2:B:280:VAL:O	2.15	0.47
2:D:110:GLN:CD	8:D:402:HYS:O25	2.52	0.47
2:D:122:PRO:HD3	2:D:142:MET:HE1	1.96	0.46
1:A:363:GLU:H	1:A:363:GLU:CD	2.17	0.46
1:A:68:ARG:NH1	1:A:68:ARG:HG2	2.30	0.46
1:C:124:ARG:O	1:C:143:PRO:HA	2.15	0.46
2:D:133:ILE:HB	2:D:356:TYR:OH	2.16	0.45
1:C:155:MET:HE1	1:C:163:VAL:HG21	1.98	0.45
1:A:293:ILE:O	1:A:294:ASN:HB2	2.16	0.45
1:A:214:LYS:HG3	1:A:215:VAL:N	2.32	0.45
5:C:501:NAG:O7	5:C:501:NAG:C2	2.61	0.45
1:A:338:THR:O	1:A:338:THR:HG22	2.17	0.45
2:D:35:ILE:HG23	2:D:64:VAL:CG1	2.47	0.44
1:C:73:GLN:HE21	2:D:322:TYR:CB	2.31	0.44
2:D:175:TYR:HB2	8:D:402:HYS:C22	2.47	0.44
1:A:29:ILE:CD1	1:A:313:ILE:HD11	2.47	0.44
2:B:284:GLU:HG2	2:B:284:GLU:O	2.18	0.44
2:B:55:GLU:C	2:B:57:ASP:N	2.69	0.44
1:C:394:ILE:HD11	4:F:1:NAG:H61	2.00	0.44
2:B:295:ASP:OD2	2:B:347:ARG:NH2	2.43	0.44
2:D:289:LEU:N	2:D:290:PRO:CD	2.81	0.44
1:A:304:ASP:HB3	1:A:359:ILE:HD11	2.00	0.44
2:B:247:VAL:HG23	2:B:249:LEU:HG	2.00	0.44
2:B:289:LEU:N	2:B:290:PRO:CD	2.80	0.44
1:A:70:ASN:OD1	1:A:70:ASN:C	2.56	0.43
1:C:154:MET:HG2	1:C:393:ILE:CD1	2.48	0.43
1:A:343:LYS:O	1:A:347:MET:HG2	2.18	0.43
2:D:39:VAL:HB	2:D:70:LEU:CD2	2.48	0.43
2:B:235:GLU:HB2	7:B:507:CL:CL	2.56	0.43
1:C:344:ARG:NH1	1:C:344:ARG:HG3	2.34	0.42
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.84	0.42
2:B:35:ILE:HG23	2:B:64:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.55	0.42
2:B:56:LYS:O	2:B:59:PHE:CB	2.68	0.42
2:B:166:TRP:HB3	2:B:227:ILE:HG13	2.01	0.42
2:D:120:LEU:CA	2:D:142:MET:HE2	2.49	0.42
1:C:275:ILE:O	1:C:280:LEU:HG	2.20	0.42
1:C:338:THR:O	1:C:338:THR:HG22	2.20	0.41
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.56	0.41
2:B:314:ILE:HB	2:B:315:PRO:CD	2.50	0.41
2:B:106:GLU:OE1	7:B:507:CL:CL	2.75	0.41
1:A:135:LEU:HD23	8:B:503:HYS:C19	2.51	0.41
1:A:320:GLU:O	1:A:321:ASN:HB2	2.20	0.41
1:A:402:TRP:HB3	1:A:403:PRO:HD2	2.03	0.41
2:B:283:ASP:O	2:B:284:GLU:C	2.59	0.41
1:A:344:ARG:NH1	1:A:344:ARG:HG3	2.36	0.41
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.85	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.96	0.40
1:A:396:ASN:C	1:A:396:ASN:OD1	2.59	0.40
1:C:362:ASN:C	1:C:362:ASN:OD1	2.60	0.40
1:A:144:TYR:HB2	1:A:172:GLU:OE2	2.22	0.40
2:B:314:ILE:HB	2:B:315:PRO:HD2	2.04	0.40
1:C:154:MET:CE	1:C:158:PHE:HE2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/385 (91%)	342 (97%)	9 (3%)	1 (0%)	41	41
1	C	351/385 (91%)	340 (97%)	10 (3%)	1 (0%)	41	41
2	B	361/363 (99%)	348 (96%)	12 (3%)	1 (0%)	41	41
2	D	354/363 (98%)	342 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1418/1496 (95%)	1372 (97%)	43 (3%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	LYS
1	C	96	PRO
1	A	96	PRO

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	288/331 (87%)	287 (100%)	1 (0%)	92	95
1	C	283/331 (86%)	276 (98%)	7 (2%)	47	52
2	B	288/326 (88%)	281 (98%)	7 (2%)	49	53
2	D	280/326 (86%)	274 (98%)	6 (2%)	53	59
All	All	1139/1314 (87%)	1118 (98%)	21 (2%)	59	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	SER
2	B	73	MET
2	B	92	ARG
2	B	134	MET
2	B	318	LYS
2	B	328	ARG
2	B	358	MET
2	B	371	ARG
1	C	135	LEU
1	C	146	HIS
1	C	226	THR
1	C	230	LEU

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Mol	Chain	Res	Type
1	C	280	LEU
1	C	291	GLN
1	C	377	LEU
2	D	73	MET
2	D	133	ILE
2	D	134	MET
2	D	152	GLN
2	D	294	ARG
2	D	352	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	152	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](#)

7 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	0.23	0	17,19,21	0.65	0
3	NAG	E	2	3	14,14,15	0.40	0	17,19,21	0.79	0
3	BMA	E	3	3	11,11,12	0.26	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	4	3	11,11,12	0.21	0	15,15,17	0.66	0
3	MAN	E	5	3	11,11,12	0.29	0	15,15,17	0.60	0
4	NAG	F	1	1,4	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.66	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	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.90	116.13	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

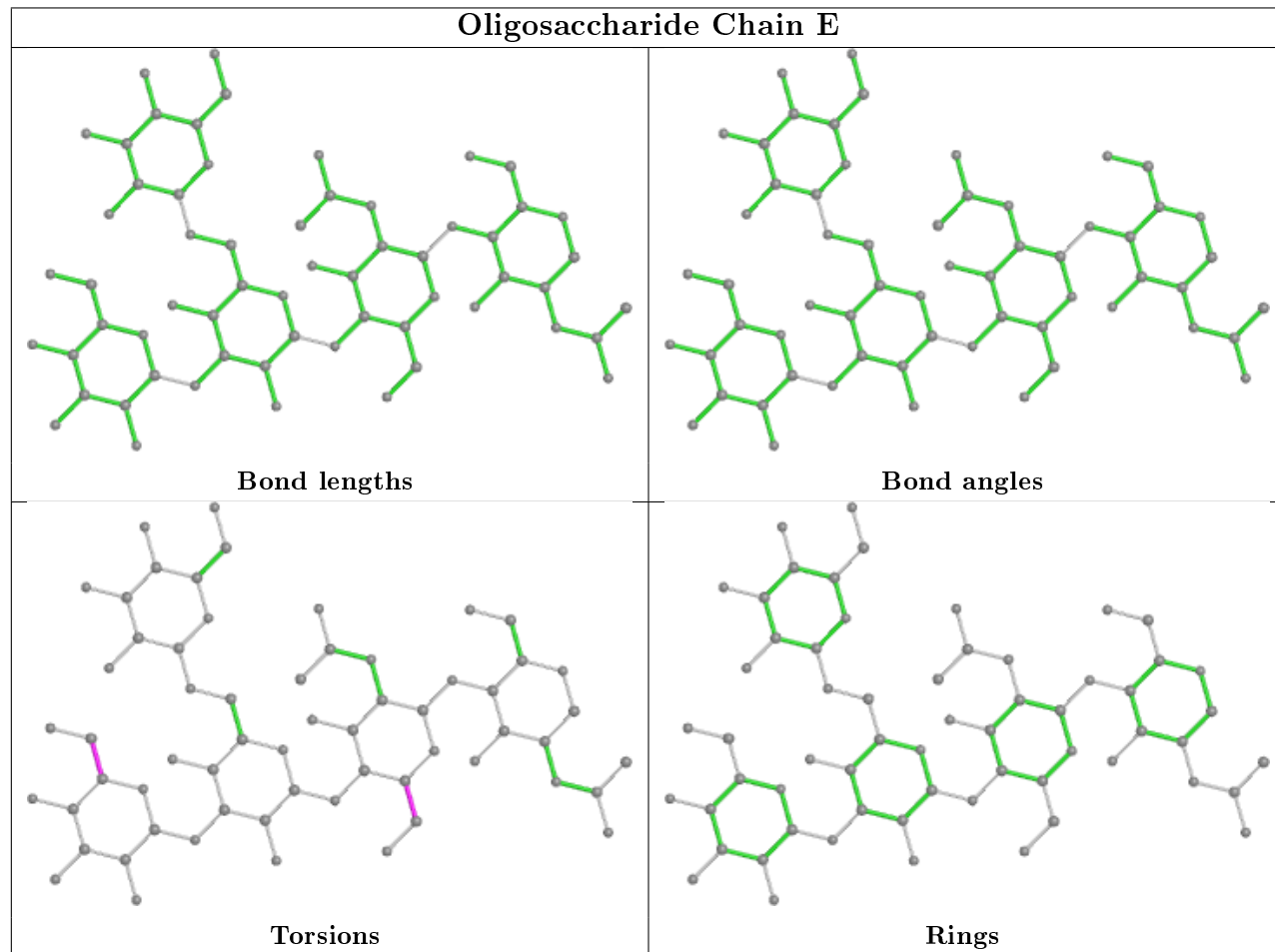
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7

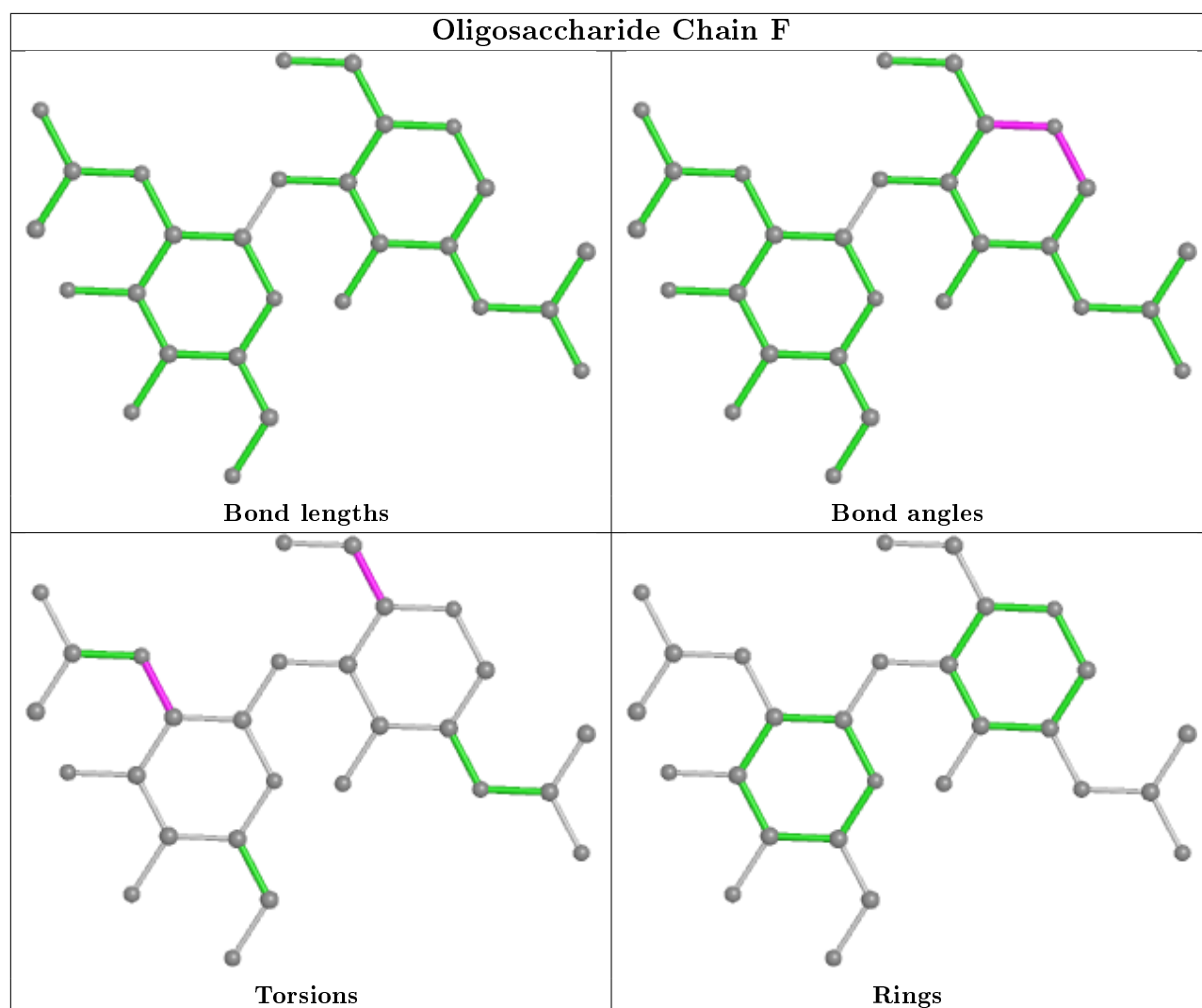
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0

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





5.6 Ligand geometry [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	$\# Z > 2$
5	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.60	0
5	NAG	B	501	2	14,14,15	0.40	0	17,19,21	0.74	0
8	HYS	D	402	-	28,28,28	1.59	2 (7%)	36,38,38	2.23	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	502	2	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
5	NAG	A	507	1	14,14,15	0.36	0	17,19,21	0.70	0
5	NAG	D	401	2	14,14,15	0.31	0	17,19,21	0.63	0
8	HYS	B	503	-	28,28,28	1.59	2 (7%)	36,38,38	2.25	2 (5%)
5	NAG	C	501	1	11,11,15	0.40	0	12,15,21	0.69	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	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
8	HYS	D	402	-	-	7/17/17/17	0/2/2/2
5	NAG	B	502	2	-	4/6/23/26	0/1/1/1
5	NAG	A	507	1	-	2/6/23/26	0/1/1/1
5	NAG	D	401	2	-	3/6/23/26	0/1/1/1
8	HYS	B	503	-	-	4/17/17/17	0/2/2/2
5	NAG	C	501	1	-	0/2/19/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	402	HYS	S21-N20	6.17	1.71	1.63
8	B	503	HYS	S21-N20	6.04	1.71	1.63
8	B	503	HYS	C17-N20	2.53	1.47	1.43
8	D	402	HYS	C17-N20	2.20	1.46	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	HYS	O24-S21-O23	-11.95	101.67	118.85
8	D	402	HYS	O24-S21-O23	-11.88	101.77	118.85
8	B	503	HYS	C22-S21-N20	3.16	110.23	106.63
8	D	402	HYS	C22-S21-N20	3.02	110.08	106.63
8	D	402	HYS	O23-S21-N20	2.13	111.45	107.10
5	B	502	NAG	C4-C3-C2	2.07	114.05	111.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	402	HYS	C05-C07-C08-N09
8	D	402	HYS	N09-C10-C11-C12
8	B	503	HYS	C05-C07-C08-N09
8	B	503	HYS	C10-C11-C12-O13
8	B	503	HYS	O25-C11-C12-O13
5	B	501	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	A	507	NAG	C4-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	A	507	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	B	502	NAG	C8-C7-N2-C2
5	B	502	NAG	O7-C7-N2-C2
5	D	401	NAG	C8-C7-N2-C2
5	D	401	NAG	O7-C7-N2-C2
5	B	502	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
8	D	402	HYS	C06-C05-C07-C08
8	D	402	HYS	C04-C05-C07-C08
8	B	503	HYS	C11-C10-N09-C08
8	D	402	HYS	N09-C10-C11-O25
8	D	402	HYS	C17-N20-S21-O24
8	D	402	HYS	C07-C08-N09-C10
5	D	401	NAG	O5-C5-C6-O6

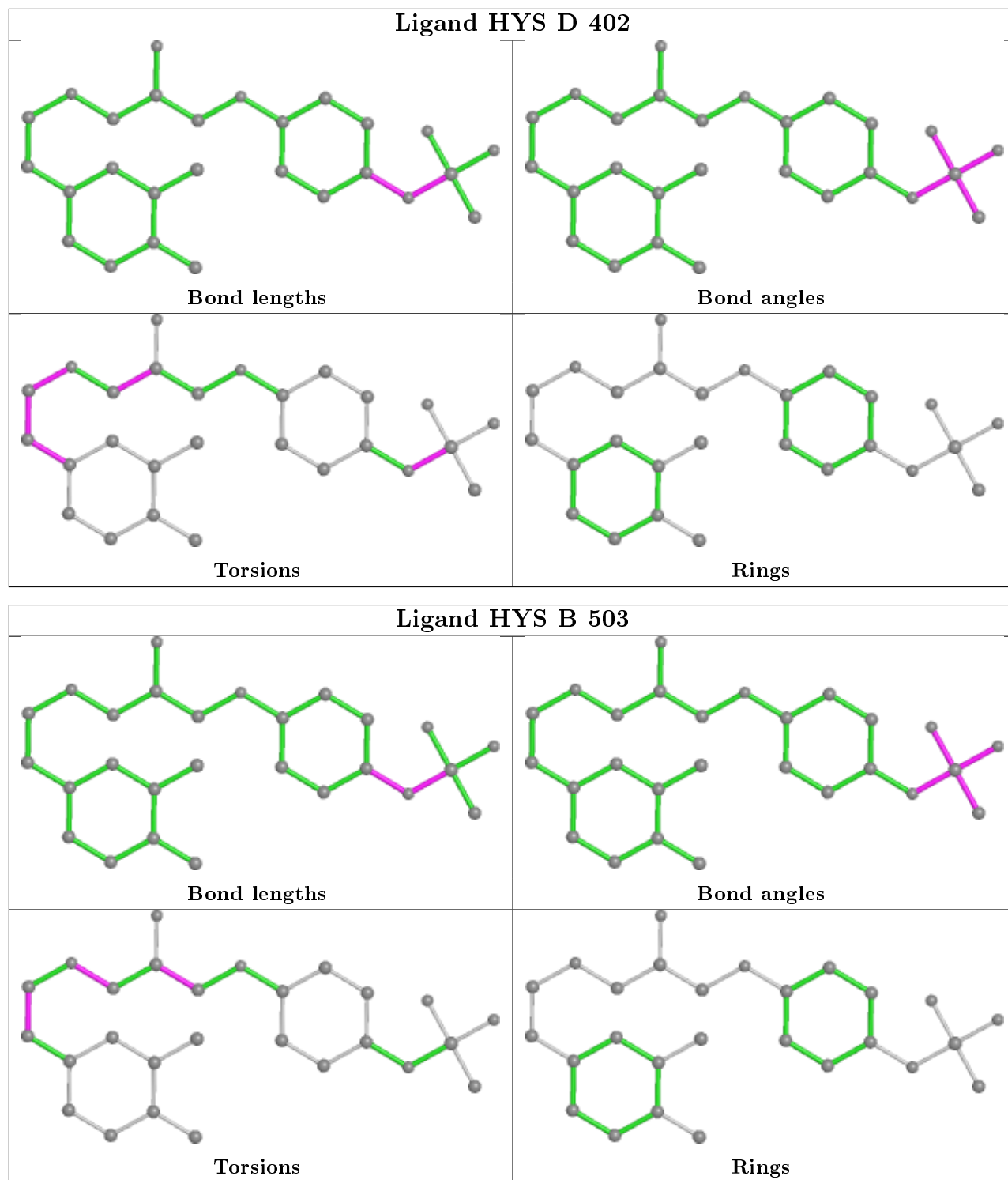
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	402	HYS	2	0
8	B	503	HYS	3	0
5	C	501	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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, 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	358/385 (92%)	-0.05	9 (2%) 57 62	11, 27, 60, 95	0
1	C	357/385 (92%)	0.22	21 (5%) 22 27	21, 40, 78, 102	0
2	B	363/363 (100%)	0.35	29 (7%) 12 16	11, 38, 78, 109	0
2	D	358/363 (98%)	0.52	42 (11%) 4 6	21, 42, 79, 125	0
All	All	1436/1496 (95%)	0.26	101 (7%) 16 20	11, 37, 75, 125	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	344	PHE	7.2
2	D	194	PHE	6.8
2	B	55	GLU	6.7
2	B	58	ASP	6.4
2	B	48	VAL	5.6
2	D	346	GLY	5.4
2	D	48	VAL	5.3
2	D	343	THR	4.9
2	D	53	ALA	4.9
2	D	195	VAL	4.8
2	B	44	THR	4.8
1	C	101	HIS	4.5
2	D	192	ASN	4.5
1	C	265	GLY	4.3
2	D	49	ALA	4.3
2	D	62	LEU	4.2
1	C	264	ALA	4.1
2	B	52	ASP	4.1
2	B	394	MET	4.0
2	D	347	ARG	4.0
1	A	102	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	44	THR	3.9
2	D	348	ASP	3.9
2	D	46	ASP	3.7
2	B	49	ALA	3.7
1	C	158	PHE	3.7
1	A	97	ALA	3.7
2	D	381	ASP	3.7
1	A	234	GLU	3.5
2	D	32	PRO	3.4
1	C	321	ASN	3.3
2	D	359	HIS	3.2
2	D	345	GLU	3.2
1	C	258	MET	3.2
2	B	54	HIS	3.2
2	D	61	HIS	3.2
2	D	325	HIS	3.2
1	C	397	ASP	3.1
1	A	186	GLY	3.1
2	B	346	GLY	3.1
2	B	61	HIS	3.1
2	D	380	LYS	3.1
1	C	102	LEU	3.0
2	D	193	SER	3.0
2	D	65	VAL	2.9
1	C	257	ALA	2.9
1	A	230	LEU	2.9
1	C	266	TYR	2.9
1	C	157	LEU	2.9
2	B	57	ASP	2.9
2	B	59	PHE	2.9
1	A	101	HIS	2.8
1	C	54	PHE	2.8
1	C	97	ALA	2.8
2	D	60	HIS	2.8
2	D	123	ILE	2.8
2	D	111	ILE	2.8
1	C	69	PRO	2.7
2	B	213	ASP	2.6
2	B	192	ASN	2.6
2	D	109	ALA	2.6
1	A	96	PRO	2.6
2	B	381	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	108	ILE	2.5
2	B	46	ASP	2.5
2	B	212	GLY	2.5
1	A	236	GLU	2.5
2	D	246	SER	2.4
2	B	56	LYS	2.4
2	D	50	ILE	2.4
1	C	259	LEU	2.4
2	D	112	LEU	2.4
2	B	325	HIS	2.4
1	C	159	ASN	2.3
1	C	226	THR	2.3
2	D	341	ASN	2.3
2	B	359	HIS	2.3
2	D	286	ASP	2.3
2	B	53	ALA	2.3
2	B	111	ILE	2.3
2	B	345	GLU	2.3
1	C	222	THR	2.2
2	D	218	ASN	2.2
2	D	309	SER	2.2
2	D	107	ALA	2.2
1	C	391	SER	2.2
2	D	322	TYR	2.2
2	B	328	ARG	2.2
2	B	112	LEU	2.2
2	B	191	GLU	2.2
2	D	196	GLY	2.2
1	A	265	GLY	2.1
2	D	285	TRP	2.1
1	C	389	ASN	2.1
2	B	123	ILE	2.1
2	D	213	ASP	2.1
2	B	309	SER	2.1
2	D	54	HIS	2.1
2	D	261	LEU	2.1
2	B	32	PRO	2.1
1	C	318	GLU	2.0

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

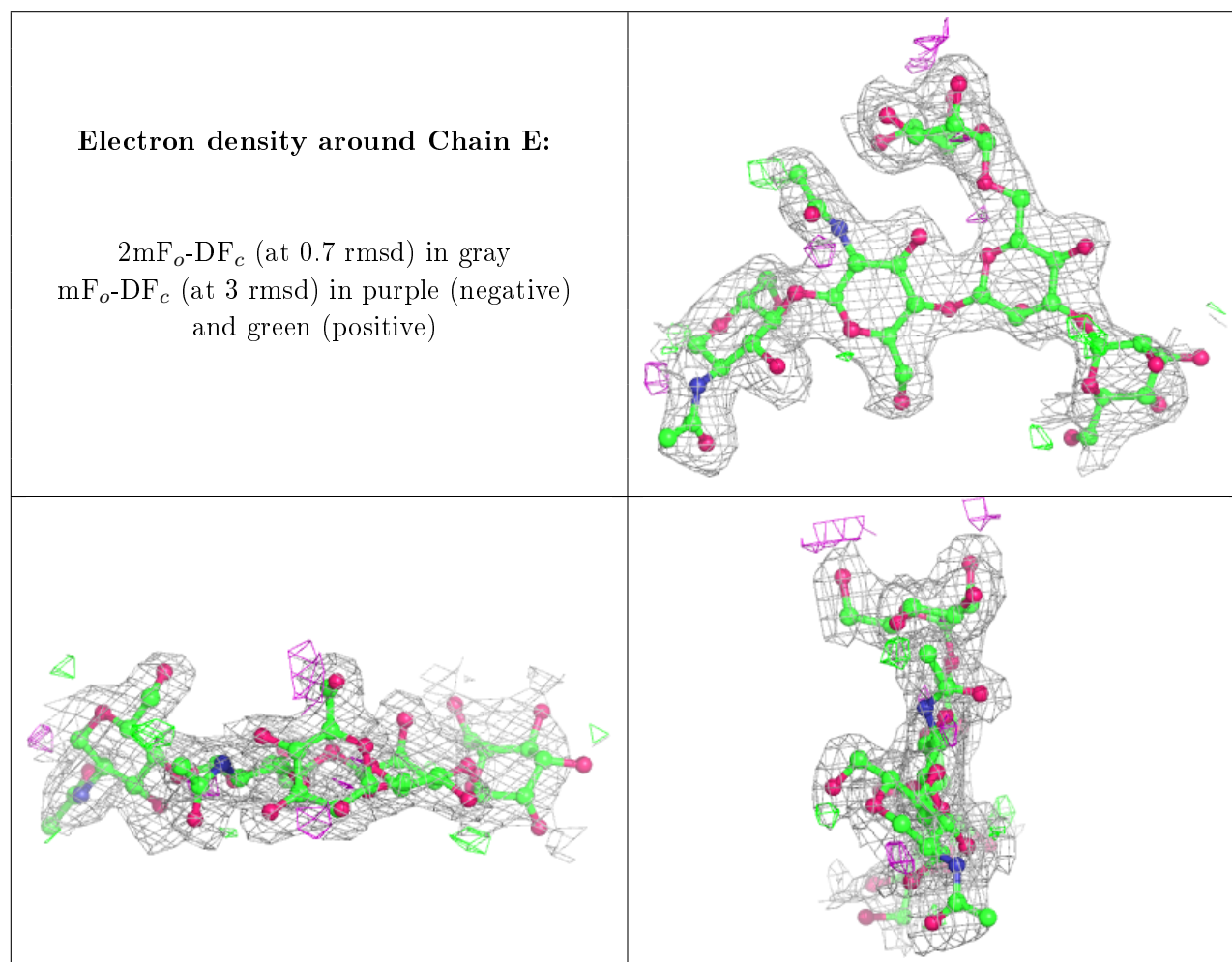
There are no non-standard protein/DNA/RNA residues in this entry.

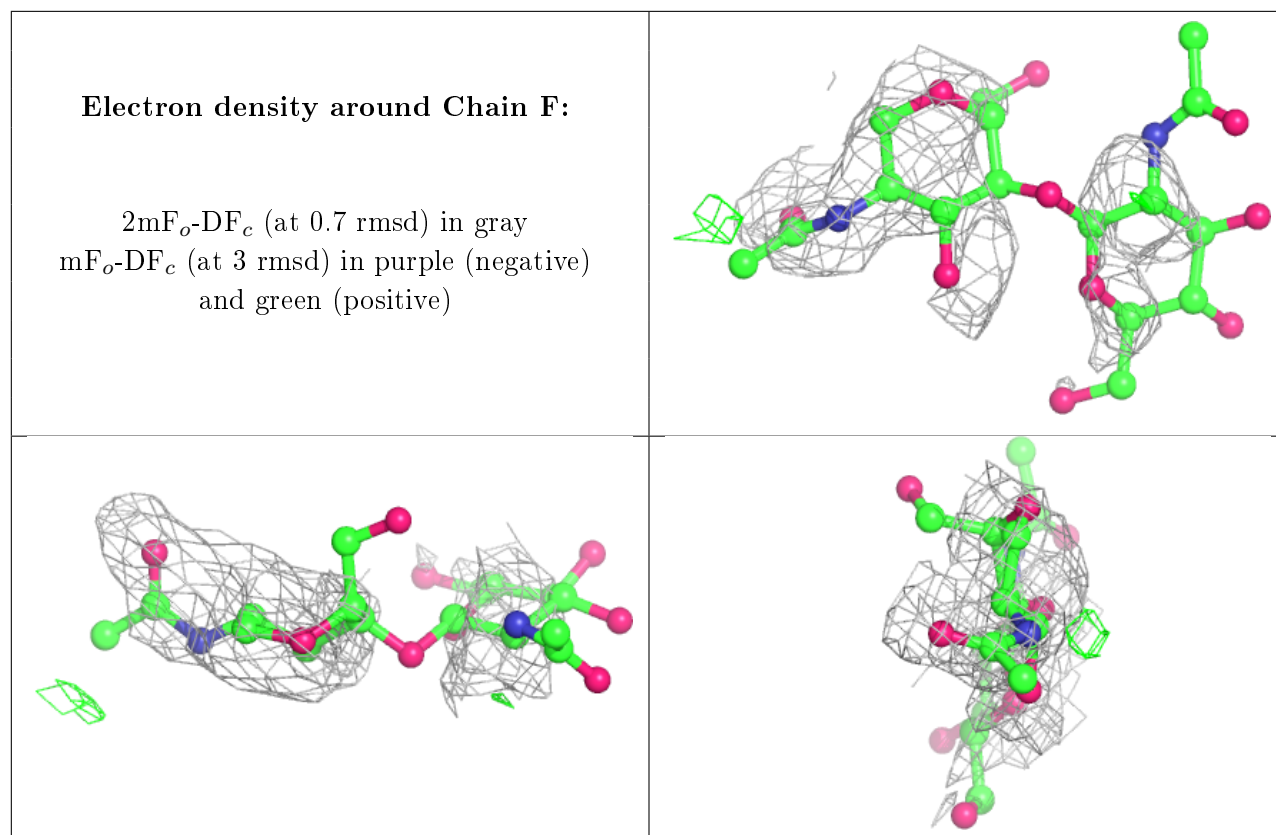
6.3 Carbohydrates ⓘ

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, 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
4	NAG	F	2	14/15	0.62	0.72	113,143,161,182	0
4	NAG	F	1	14/15	0.68	0.49	86,111,128,141	0
3	MAN	E	4	11/12	0.80	0.28	103,108,114,125	0
3	BMA	E	3	11/12	0.89	0.18	57,67,76,97	0
3	NAG	E	2	14/15	0.90	0.13	49,55,60,70	0
3	NAG	E	1	14/15	0.91	0.13	37,42,48,51	0
3	MAN	E	5	11/12	0.92	0.12	46,50,55,56	0

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	507	14/15	0.46	0.59	86,104,127,140	0
5	NAG	B	502	14/15	0.50	0.55	95,113,118,123	0
5	NAG	B	501	14/15	0.63	0.35	69,86,92,95	0
5	NAG	D	401	14/15	0.70	0.48	95,102,112,115	0
7	CL	D	404	1/1	0.74	0.25	77,77,77,77	0
7	CL	D	406	1/1	0.75	0.12	75,75,75,75	0
7	CL	C	505	1/1	0.78	0.20	71,71,71,71	0
7	CL	B	506	1/1	0.81	0.14	53,53,53,53	0
7	CL	B	505	1/1	0.90	0.11	68,68,68,68	0
7	CL	D	405	1/1	0.90	0.13	71,71,71,71	0
5	NAG	C	501	13/15	0.91	0.17	43,52,59,64	0
5	NAG	A	501	14/15	0.91	0.17	31,40,45,54	0
7	CL	D	403	1/1	0.93	0.21	58,58,58,58	0
8	HYS	B	503	27/27	0.94	0.18	19,31,51,57	0

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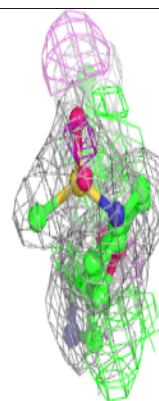
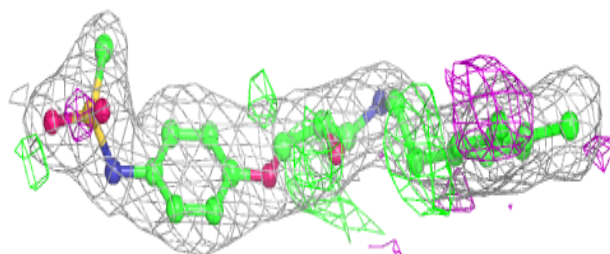
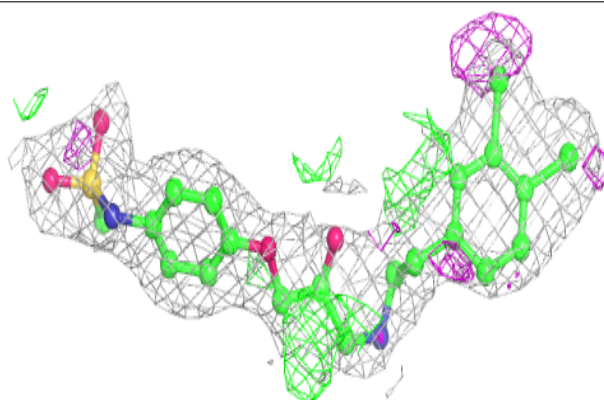
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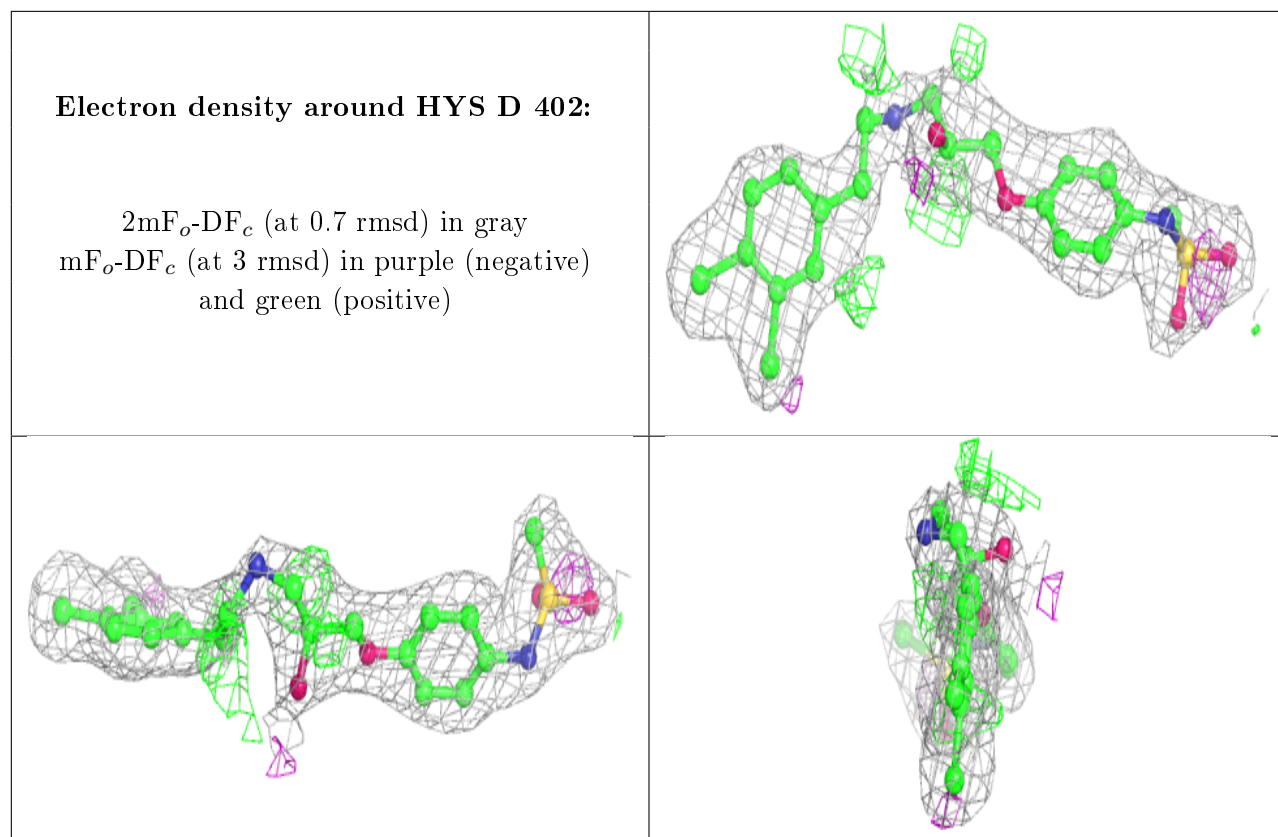
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CL	A	509	1/1	0.94	0.06	53,53,53,53	0
8	HYS	D	402	27/27	0.95	0.13	29,40,53,65	0
6	NA	A	508	1/1	0.97	0.11	18,18,18,18	0
7	CL	B	507	1/1	0.97	0.08	57,57,57,57	0
6	NA	C	504	1/1	0.97	0.09	25,25,25,25	0
7	CL	A	510	1/1	0.98	0.13	42,42,42,42	0
7	CL	B	504	1/1	0.98	0.05	46,46,46,46	0
7	CL	C	506	1/1	0.98	0.06	47,47,47,47	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 HYS 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.