



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:55 PM BST

PDB ID : 5EWL  
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE  
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX  
WITH MK-22  
Authors : Pandit, J.  
Deposited on : 2015-11-20  
Resolution : 2.98 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](mailto: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.

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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

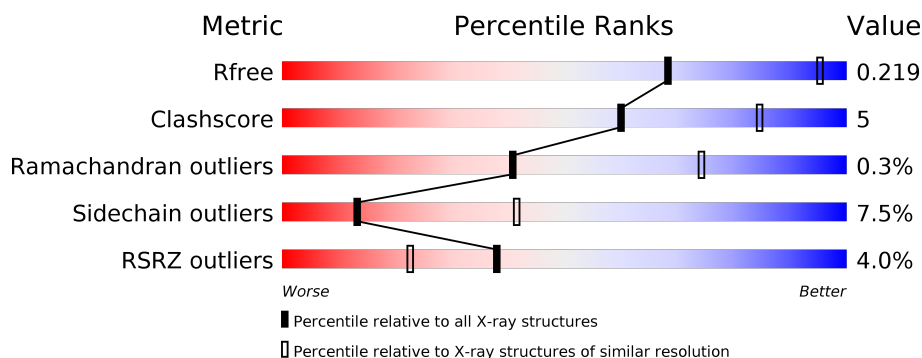
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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  $\geq 3$ , 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	390	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>• 8%</div> </div> </div>
1	C	390	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>• 9%</div> </div> </div>
2	B	364	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>
2	D	364	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
3	E	5	<div> <div></div> <div> <div></div> <div>60%</div> <div>40%</div> </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
5	NAG	B	501	-	-	-	X
5	NAG	B	502	-	-	-	X
5	NAG	D	501	-	-	-	X
5	NAG	D	502	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11493 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2752	1753	477	511	11			
1	C	356	Total	C	N	O	S	0	0	0
			2737	1741	479	507	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
A	409	LEU	-	expression tag	UNP Q91977
A	410	VAL	-	expression tag	UNP Q91977
A	411	PRO	-	expression tag	UNP Q91977
A	412	ARG	-	expression tag	UNP Q91977
C	61	GLN	ASN	engineered mutation	UNP Q91977
C	371	GLN	ASN	engineered mutation	UNP Q91977
C	409	LEU	-	expression tag	UNP Q91977
C	410	VAL	-	expression tag	UNP Q91977
C	411	PRO	-	expression tag	UNP Q91977
C	412	ARG	-	expression tag	UNP Q91977

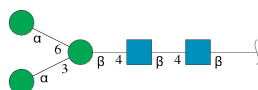
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2739	1766	432	526	15			
2	D	355	Total	C	N	O	S	0	0	0
			2789	1797	441	535	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q13224
D	348	ASP	ASN	engineered mutation	UNP Q13224

- 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.

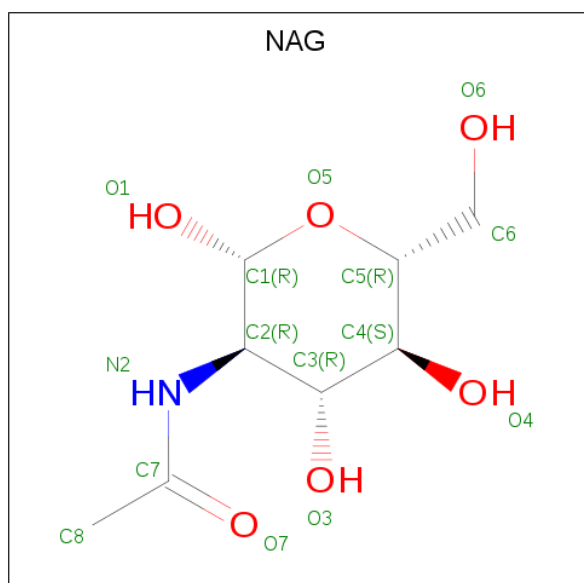


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

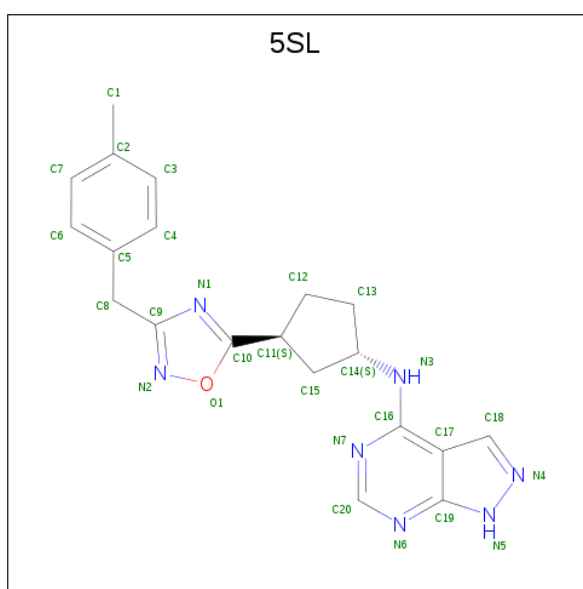
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	3	Total	Na	0	0
			3	3		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is {N}-(1 {S},3 {S})-3-[3-[(4-methylphenyl)methyl]-1,2,4-oxadiazol-5-yl]cyclopentyl]-1 {H}-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: 5SL) (formula: C<sub>20</sub>H<sub>21</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			28	20	7	1		
6	C	1	Total	C	N	O	0	0
			28	20	7	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	99	Total	O	0	0
			99	99		

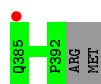
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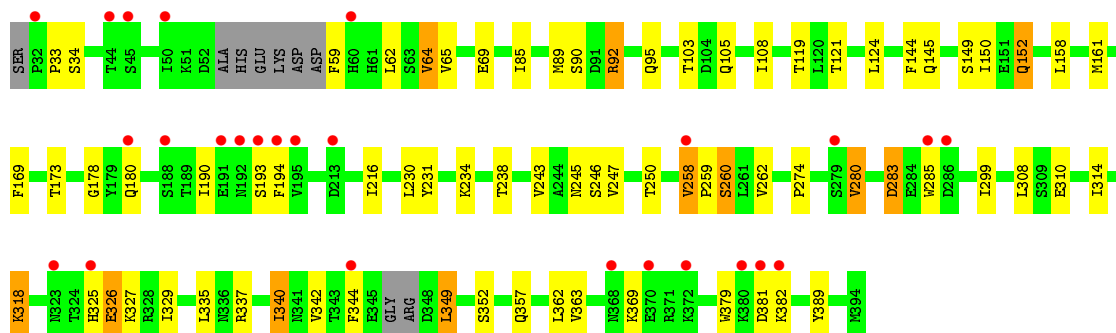
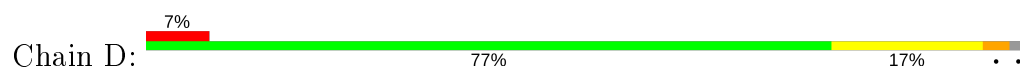
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	83	Total 83	O 83	0	0
7	C	39	Total 39	O 39	0	0
7	D	48	Total 48	O 48	0	0



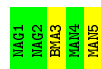




- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- 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, $\alpha$ , $\beta$ , $\gamma$	268.88Å 59.94Å 144.45Å 90.00° 116.51° 90.00°	Depositor
Resolution (Å)	30.04 – 2.98 29.97 – 2.98	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.04-2.98) 95.8 (29.97-2.98)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.162 , 0.217 0.166 , 0.219	Depositor DCC
$R_{free}$ test set	2068 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 80.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, BMA, NAG, 5SL, 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	0.57	0/2809	0.72	0/3819
1	C	0.49	0/2792	0.69	0/3794
2	B	0.53	0/2801	0.73	0/3814
2	D	0.50	0/2853	0.72	0/3879
All	All	0.52	0/11255	0.72	0/15306

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 [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	2752	0	2717	24	0
1	C	2737	0	2705	17	0
2	B	2739	0	2649	27	0
2	D	2789	0	2707	34	0
3	E	61	0	52	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	26	0	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
6	A	28	0	0	1	0
6	C	28	0	0	0	0
7	A	99	0	0	1	0
7	B	83	0	0	0	0
7	C	39	0	0	0	0
7	D	48	0	0	0	0
All	All	11493	0	10908	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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:173:THR:HG22	2:D:231:TYR:HB3	1.59	0.84
2:D:344:PHE:HB2	2:D:349:LEU:HD11	1.60	0.82
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.61	0.80
2:D:85:ILE:HG22	2:D:89:MET:HE2	1.64	0.78
2:B:33:PRO:HG2	2:B:64:VAL:HG23	1.70	0.72
2:B:109:ALA:HB1	2:B:134:MET:HG3	1.76	0.67
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.76	0.67
1:A:376:ASN:HD22	1:A:378:GLN:HE21	1.43	0.66
2:D:33:PRO:HG2	2:D:64:VAL:HG23	1.77	0.66
1:A:57:LYS:HB2	7:A:670:HOH:O	1.95	0.66
1:C:167:VAL:HG12	1:C:243:SER:HB3	1.78	0.65
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.78	0.64
2:B:158:LEU:HA	2:B:161:MET:HE3	1.83	0.61
2:D:149:SER:H	2:D:152:GLN:HE21	1.47	0.60
2:D:158:LEU:HA	2:D:161:MET:HE3	1.83	0.60
1:A:376:ASN:HD21	1:A:401:ILE:H	1.50	0.60
2:B:327:LYS:O	2:B:331:GLN:HG3	2.02	0.60
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.37	0.60
2:B:149:SER:H	2:B:152:GLN:HE21	1.49	0.59
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.65	0.59
1:C:287:ILE:HG22	1:C:377:LEU:HB2	1.84	0.58
2:D:234:LYS:O	2:D:238:THR:HG23	2.04	0.57
1:C:262:THR:HB	1:C:284:PRO:HB3	1.86	0.56
2:B:258:VAL:HG13	2:B:262:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:O	2:B:238:THR:HG23	2.05	0.56
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.89	0.54
1:C:40:GLN:HG3	1:C:43:ARG:HH22	1.73	0.54
2:D:230:LEU:O	2:D:259:PRO:HD3	2.08	0.54
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.90	0.54
2:B:230:LEU:O	2:B:259:PRO:HD3	2.08	0.53
2:D:85:ILE:HG22	2:D:89:MET:CE	2.37	0.53
2:D:283:ASP:HA	2:D:285:TRP:HE3	1.73	0.53
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.73	0.53
2:B:250:THR:HB	2:B:274:PRO:HB3	1.92	0.52
1:A:322:ILE:HG23	1:A:338:THR:HG21	1.92	0.51
2:B:283:ASP:OD1	2:B:285:TRP:HB2	2.10	0.51
1:C:309:VAL:O	1:C:313:ILE:HG12	2.11	0.51
2:D:250:THR:HB	2:D:274:PRO:HB3	1.91	0.51
1:A:262:THR:HB	1:A:284:PRO:HB3	1.92	0.50
2:D:149:SER:H	2:D:152:GLN:NE2	2.08	0.50
2:B:193:SER:C	2:B:195:VAL:H	2.13	0.50
1:A:135:LEU:HD22	6:A:508:5SL:C15	2.42	0.50
2:D:318:LYS:H	2:D:318:LYS:CD	2.25	0.50
2:D:169:PHE:CZ	2:D:190:ILE:HD11	2.45	0.50
2:B:129:GLY:HA2	2:B:132:MET:SD	2.51	0.49
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.94	0.49
1:A:229:LEU:HD12	1:A:255:SER:HB2	1.93	0.49
1:C:144:TYR:CZ	1:C:273:ARG:HD2	2.48	0.48
2:B:149:SER:H	2:B:152:GLN:NE2	2.10	0.48
2:B:329:ILE:HG22	2:D:308:LEU:HD11	1.96	0.48
2:D:325:HIS:CD2	2:D:326:GLU:HG3	2.48	0.48
1:C:157:LEU:HD23	1:C:158:PHE:CE1	2.49	0.47
2:D:283:ASP:HA	2:D:285:TRP:CE3	2.49	0.47
1:A:226:THR:HG22	1:A:255:SER:HB3	1.96	0.47
1:A:33:LEU:O	1:A:66:THR:HA	2.15	0.47
2:B:318:LYS:H	2:B:318:LYS:CD	2.27	0.47
2:D:150:ILE:HD13	2:D:178:GLY:HA3	1.96	0.47
1:C:147:GLN:HE22	1:C:272:GLU:H	1.63	0.47
2:D:89:MET:HE3	2:D:119:THR:HG21	1.97	0.46
1:C:33:LEU:O	1:C:66:THR:HA	2.16	0.46
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.51	0.46
1:A:157:LEU:HD23	1:A:158:PHE:CE1	2.50	0.46
2:D:283:ASP:HB3	2:D:363:VAL:HG23	1.97	0.46
2:D:105:GLN:HB3	2:D:108:ILE:HD12	1.98	0.46
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HB3	1:A:270:VAL:HG23	1.98	0.45
1:C:242:LEU:HB3	1:C:270:VAL:HG23	1.99	0.45
1:A:135:LEU:H	1:A:135:LEU:HD23	1.81	0.45
2:B:216:ILE:HG22	2:B:243:VAL:HG11	1.99	0.45
2:D:92:ARG:O	2:D:92:ARG:HD3	2.16	0.45
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.98	0.45
2:D:144:PHE:HE1	2:D:340:ILE:HD12	1.81	0.45
1:A:133:ILE:HG22	1:A:134:HIS:CD2	2.52	0.44
2:B:344:PHE:HB3	2:B:349:LEU:HD11	1.99	0.44
2:B:220:LEU:HD12	2:B:243:VAL:HG12	2.00	0.44
2:B:109:ALA:CB	2:B:134:MET:HG3	2.45	0.43
1:A:41:ILE:HG22	1:A:302:ILE:HG21	2.01	0.43
2:B:50:ILE:HD11	2:B:289:LEU:HD23	2.00	0.43
2:D:247:VAL:O	2:D:247:VAL:HG12	2.18	0.42
2:D:318:LYS:H	2:D:318:LYS:HD3	1.83	0.42
2:B:161:MET:HE2	2:B:229:LEU:HD21	2.01	0.42
1:A:309:VAL:O	1:A:313:ILE:HG12	2.20	0.42
1:C:167:VAL:O	1:C:217:GLN:HA	2.20	0.42
2:D:124:LEU:HD23	2:D:144:PHE:HB2	2.01	0.42
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.95	0.42
1:C:47:ASN:HA	1:C:50:ASN:HD22	1.85	0.42
1:C:147:GLN:HE22	1:C:272:GLU:N	2.18	0.41
1:A:167:VAL:O	1:A:217:GLN:HA	2.21	0.41
2:B:299:ILE:HA	2:B:342:VAL:HG11	2.03	0.41
2:D:216:ILE:HG22	2:D:243:VAL:HG11	2.02	0.41
2:D:95:GLN:NE2	2:D:314:ILE:HD12	2.35	0.41
2:B:269:VAL:HG11	2:B:367:LEU:HD11	2.03	0.41
1:A:229:LEU:CD1	1:A:255:SER:HB2	2.51	0.40
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.56	0.40
2:B:121:THR:OG1	2:B:318:LYS:HE3	2.21	0.40
2:D:121:THR:OG1	2:D:318:LYS:HE3	2.20	0.40
1:A:350:LYS:HG2	1:A:360:GLU:HG2	2.03	0.40
1:C:30:GLY:HA2	1:C:63:THR:O	2.21	0.40
2:B:318:LYS:H	2:B:318:LYS:HD3	1.86	0.40
2:B:92:ARG:O	2:B:92:ARG:HD3	2.22	0.40
2:D:260:SER:HA	2:D:280:VAL:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	351/390 (90%)	339 (97%)	12 (3%)	0	100	100
1	C	350/390 (90%)	338 (97%)	12 (3%)	0	100	100
2	B	348/364 (96%)	320 (92%)	27 (8%)	1 (0%)	41	74
2	D	349/364 (96%)	316 (90%)	30 (9%)	3 (1%)	17	53
All	All	1398/1508 (93%)	1313 (94%)	81 (6%)	4 (0%)	41	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ASP
2	D	283	ASP
2	D	62	LEU
2	D	327	LYS

### 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	292/336 (87%)	274 (94%)	18 (6%)	18	50
1	C	289/336 (86%)	271 (94%)	18 (6%)	18	50
2	B	297/326 (91%)	276 (93%)	21 (7%)	14	44
2	D	307/326 (94%)	275 (90%)	32 (10%)	7	26
All	All	1185/1324 (90%)	1096 (92%)	89 (8%)	13	41

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ILE
1	A	136	SER
1	A	182	THR
1	A	223	LYS
1	A	226	THR
1	A	230	LEU
1	A	255	SER
1	A	270	VAL
1	A	285	ASP
1	A	320	GLU
1	A	335	ILE
1	A	353	ASP
1	A	367	ARG
1	A	380	ARG
1	A	382	LEU
1	A	387	ILE
1	A	392	TYR
1	A	399	LYS
2	B	64	VAL
2	B	65	VAL
2	B	69	GLU
2	B	90	SER
2	B	91	ASP
2	B	92	ARG
2	B	152	GLN
2	B	190	ILE
2	B	246	SER
2	B	258	VAL
2	B	260	SER
2	B	308	LEU
2	B	310	GLU
2	B	318	LYS
2	B	329	ILE
2	B	335	LEU
2	B	349	LEU
2	B	357	GLN
2	B	378	LYS
2	B	380	LYS
2	B	381	ASP
1	C	27	VAL
1	C	54	PHE
1	C	55	THR

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Mol	Chain	Res	Type
1	C	58	ILE
1	C	127	ILE
1	C	135	LEU
1	C	136	SER
1	C	229	LEU
1	C	270	VAL
1	C	273	ARG
1	C	285	ASP
1	C	335	ILE
1	C	353	ASP
1	C	364	ASP
1	C	367	ARG
1	C	377	LEU
1	C	378	GLN
1	C	387	ILE
2	D	34	SER
2	D	59	PHE
2	D	64	VAL
2	D	65	VAL
2	D	69	GLU
2	D	90	SER
2	D	92	ARG
2	D	103	THR
2	D	145	GLN
2	D	152	GLN
2	D	180	GLN
2	D	193	SER
2	D	194	PHE
2	D	245	ASN
2	D	246	SER
2	D	258	VAL
2	D	260	SER
2	D	280	VAL
2	D	310	GLU
2	D	318	LYS
2	D	326	GLU
2	D	329	ILE
2	D	335	LEU
2	D	337	ARG
2	D	340	ILE
2	D	349	LEU
2	D	352	SER

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Mol	Chain	Res	Type
2	D	357	GLN
2	D	369	LYS
2	D	381	ASP
2	D	382	LYS
2	D	389	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	384	GLN
2	B	110	GLN
2	B	118	GLN
2	B	152	GLN
2	B	311	HIS
1	C	28	ASN
1	C	147	GLN
1	C	376	ASN
1	C	384	GLN
2	D	95	GLN
2	D	118	GLN
2	D	152	GLN
2	D	311	HIS

### 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	0.27	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.78	0
3	BMA	E	3	3	11,11,12	0.31	0	15,15,17	0.82	1 (6%)
3	MAN	E	4	3	11,11,12	0.42	0	15,15,17	1.09	0
3	MAN	E	5	3	11,11,12	0.43	0	15,15,17	0.91	1 (6%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MAN	C1-O5-C5	2.61	115.72	112.19
3	E	3	BMA	C1-O5-C5	2.03	114.95	112.19

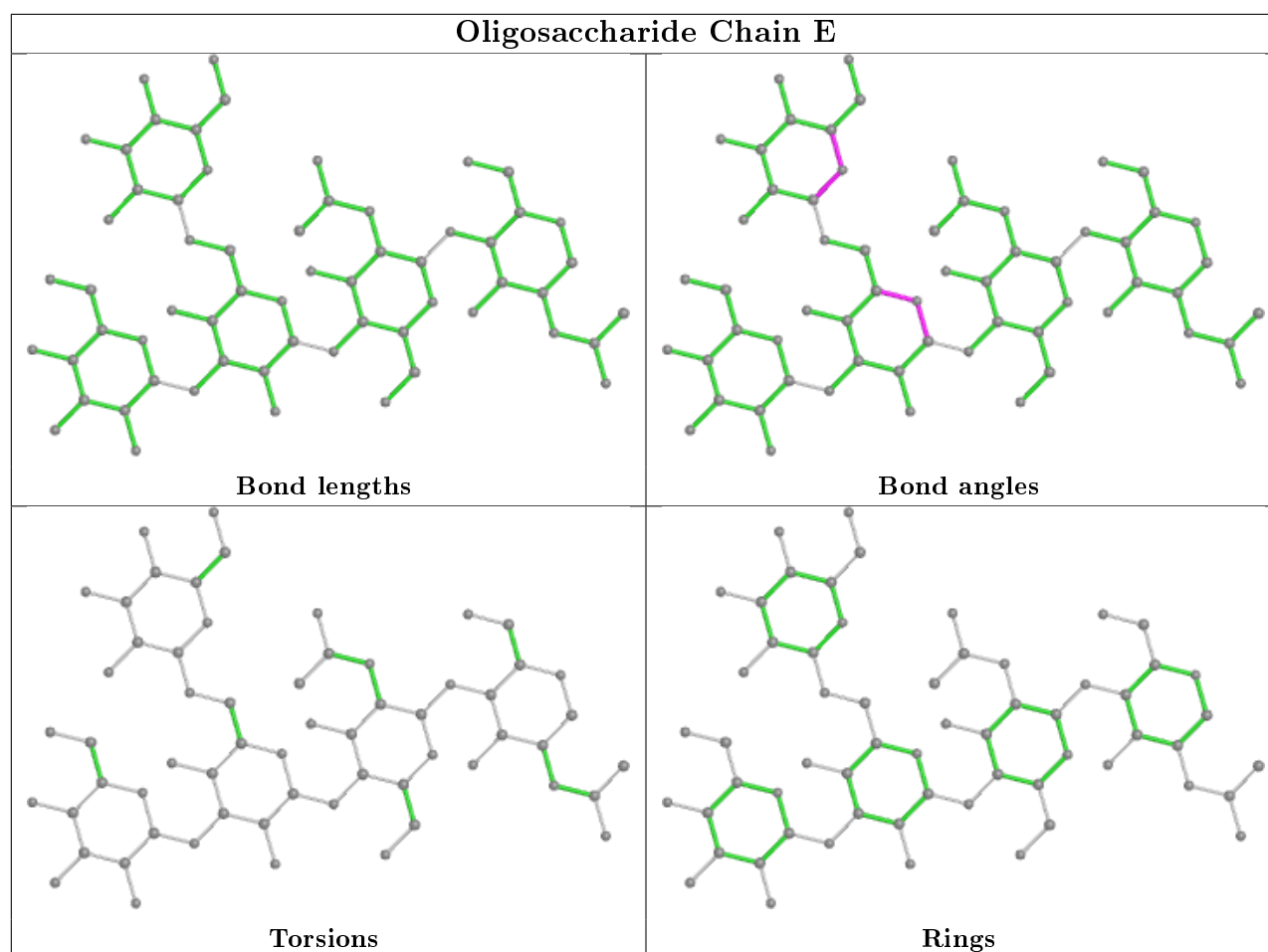
There are no chirality outliers.

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 14 ligands modelled in this entry, 6 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$
6	5SL	A	508	-	27,32,32	0.71	0	31,45,45	0.91	2 (6%)
5	NAG	C	502	1	14,14,15	0.40	0	17,19,21	1.05	1 (5%)
5	NAG	A	502	1	14,14,15	0.23	0	17,19,21	1.73	4 (23%)
5	NAG	B	502	2	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
5	NAG	D	501	2	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	D	502	2	14,14,15	0.33	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	501	2	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
6	5SL	C	503	-	27,32,32	0.75	0	31,45,45	0.99	2 (6%)

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
6	5SL	A	508	-	-	0/8/21/21	0/5/5/5
5	NAG	C	502	1	-	1/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	B	502	2	-	2/6/23/26	0/1/1/1
5	NAG	D	501	2	-	1/6/23/26	0/1/1/1
5	NAG	D	502	2	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	1/6/23/26	0/1/1/1
6	5SL	C	503	-	-	1/8/21/21	0/5/5/5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	NAG	O5-C1-C2	-4.49	104.19	111.29
6	C	503	5SL	C15-C11-C10	-3.64	107.47	114.39
5	C	502	NAG	C1-C2-N2	3.54	116.53	110.49
5	A	502	NAG	C3-C4-C5	3.20	115.95	110.24
6	A	508	5SL	C15-C11-C10	-2.78	109.11	114.39
5	A	502	NAG	C1-O5-C5	2.66	115.80	112.19
5	B	502	NAG	C1-O5-C5	2.58	115.69	112.19
6	A	508	5SL	C11-C10-N1	2.55	129.94	125.08
6	C	503	5SL	C11-C10-N1	2.48	129.81	125.08
5	B	501	NAG	O5-C1-C2	2.18	114.73	111.29
5	A	502	NAG	C1-C2-N2	-2.06	106.96	110.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6

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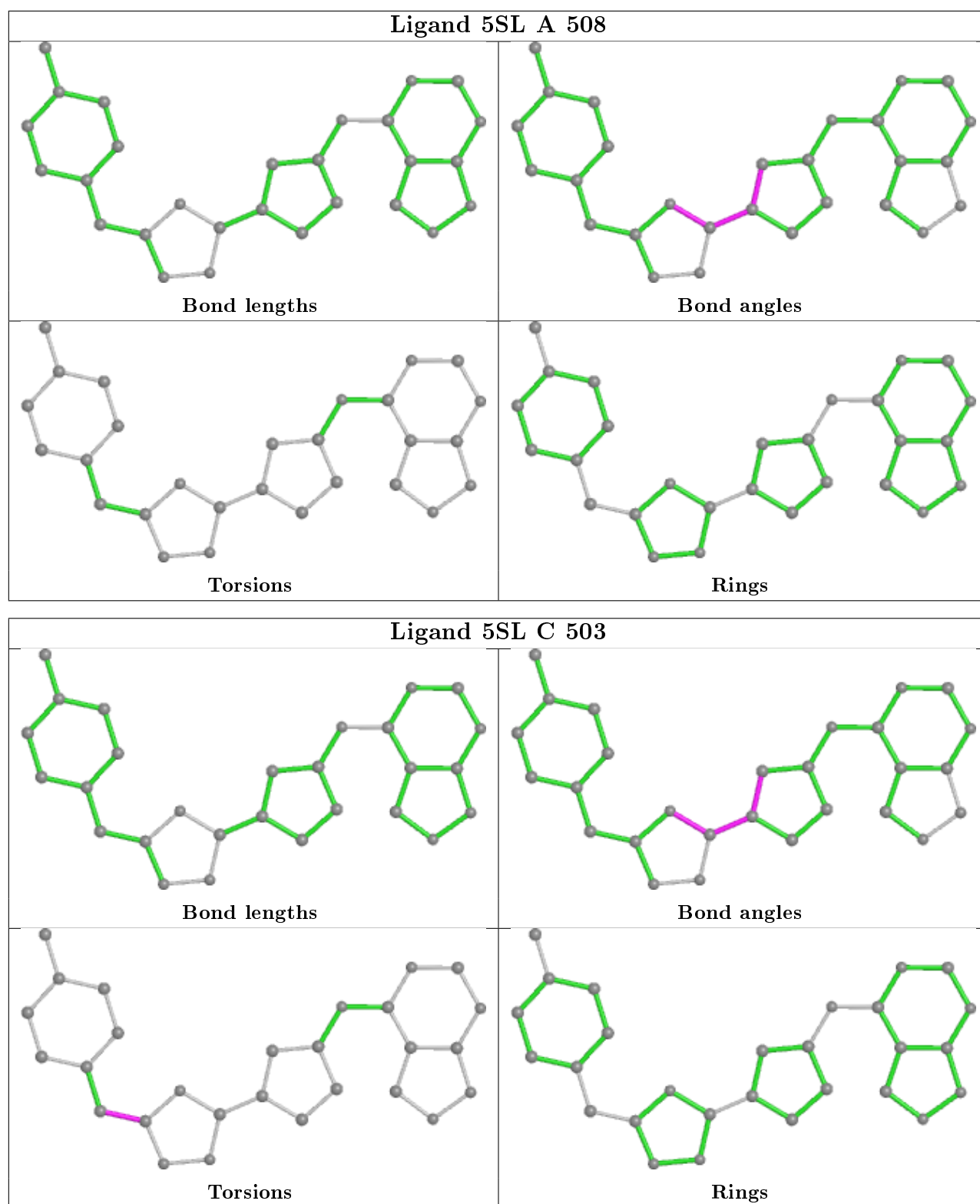
Mol	Chain	Res	Type	Atoms
5	D	502	NAG	C4-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
5	B	502	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
6	C	503	5SL	C5-C8-C9-N2
5	C	502	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	508	5SL	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	357/390 (91%)	-0.26	3 (0%) 86 71	35, 52, 84, 109	0
1	C	356/390 (91%)	0.11	20 (5%) 24 13	56, 78, 110, 137	0
2	B	352/364 (96%)	-0.02	8 (2%) 60 40	36, 66, 98, 119	0
2	D	355/364 (97%)	0.12	26 (7%) 15 7	53, 78, 119, 136	0
All	All	1420/1508 (94%)	-0.01	57 (4%) 38 23	35, 71, 108, 137	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	THR	5.5
2	D	193	SER	4.6
1	C	56	ARG	4.5
2	B	32	PRO	4.1
2	D	381	ASP	4.1
2	D	50	ILE	4.0
1	C	397	ASP	3.9
1	C	406	GLU	3.4
2	D	192	ASN	3.4
2	B	380	LYS	3.4
1	C	54	PHE	3.3
2	D	380	LYS	3.2
2	D	195	VAL	3.2
1	C	353	ASP	3.2
1	C	220	PRO	3.2
1	C	57	LYS	3.2
2	D	44	THR	3.1
1	C	394	ILE	2.9
2	D	344	PHE	2.9
1	C	405	GLY	2.9
2	B	382	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	264	ALA	2.8
1	C	321	ASN	2.7
2	D	325	HIS	2.7
1	A	405	GLY	2.7
2	B	49	ALA	2.7
2	D	213	ASP	2.7
1	C	210	PRO	2.6
1	C	209	GLY	2.6
1	A	320	GLU	2.6
1	C	404	GLY	2.6
2	D	194	PHE	2.5
2	D	382	LYS	2.5
1	C	259	LEU	2.4
2	D	286	ASP	2.3
2	D	372	LYS	2.3
1	C	169	ASP	2.3
1	A	407	THR	2.3
2	B	285	TRP	2.3
1	C	23	ASP	2.2
2	D	323	ASN	2.2
2	B	283	ASP	2.2
2	D	258	VAL	2.2
2	D	279	SER	2.2
1	C	69	PRO	2.2
2	D	180	GLN	2.2
2	D	285	TRP	2.2
2	D	45	SER	2.1
2	D	60	HIS	2.1
2	D	191	GLU	2.1
1	C	327	ARG	2.1
2	D	32	PRO	2.1
2	D	370	GLU	2.1
2	D	368	ASN	2.1
2	D	188	SER	2.0
2	B	64	VAL	2.0
2	B	385	GLN	2.0

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

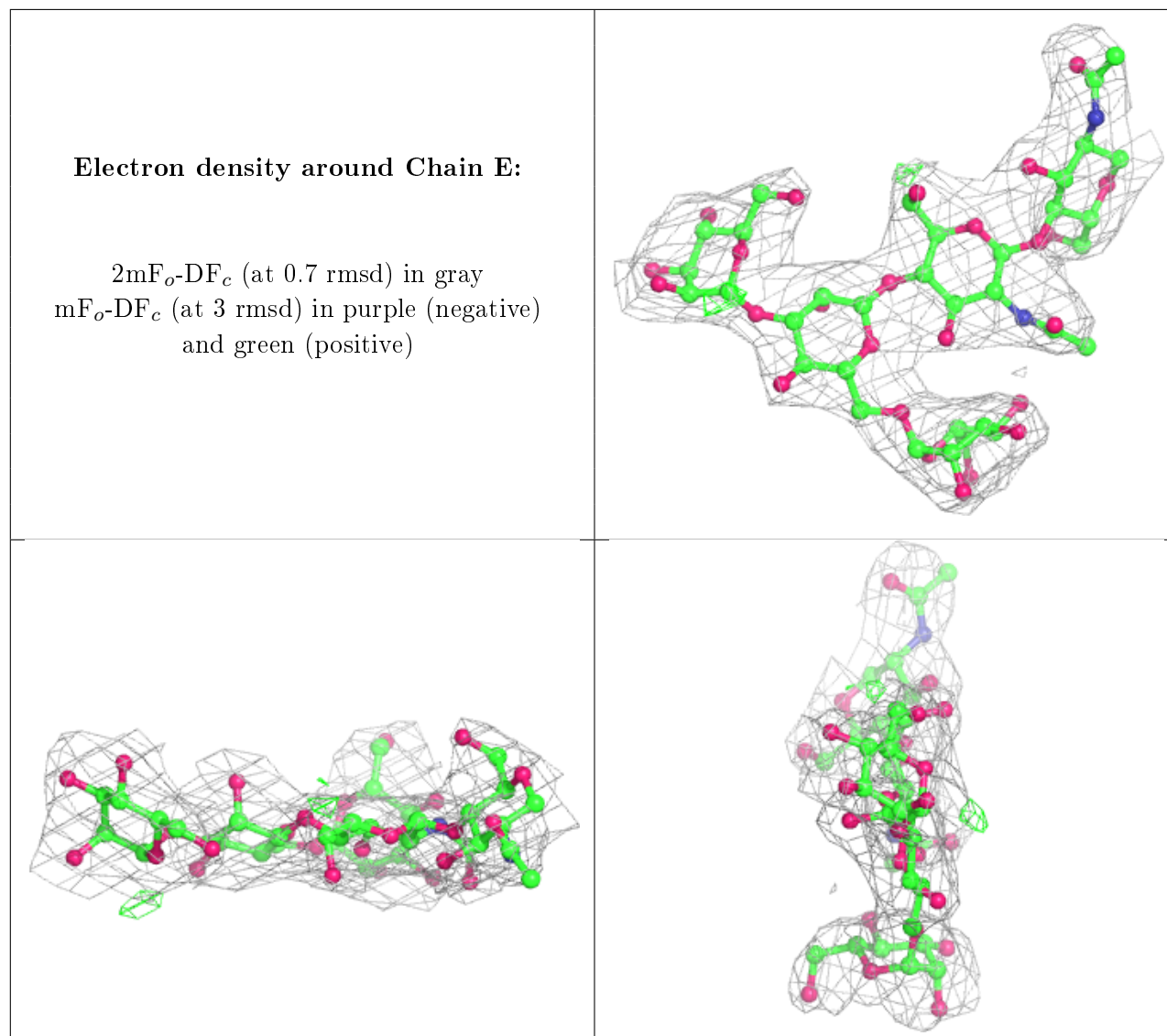
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MAN	E	4	11/12	0.89	0.20	76,80,86,88	0
3	MAN	E	5	11/12	0.96	0.21	59,62,68,69	0
3	BMA	E	3	11/12	0.96	0.20	68,73,82,85	0
3	NAG	E	1	14/15	0.97	0.23	60,70,78,80	0
3	NAG	E	2	14/15	0.97	0.29	64,68,75,75	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

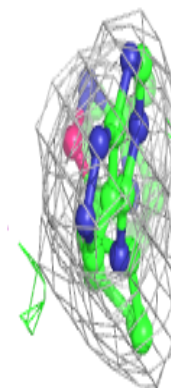
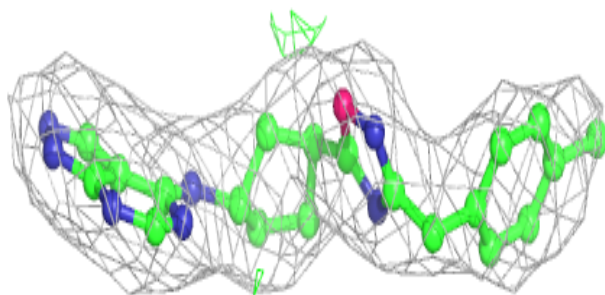
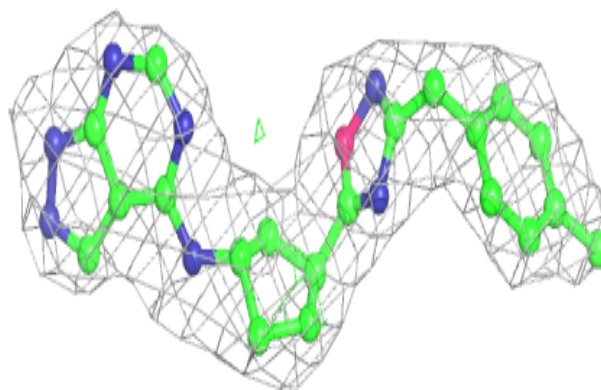
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	502	14/15	0.43	0.41	146,150,157,160	0
5	NAG	D	501	14/15	0.59	0.48	145,147,152,154	0
5	NAG	D	502	14/15	0.66	0.48	165,171,173,175	0
5	NAG	B	501	14/15	0.74	0.52	127,135,141,141	0
5	NAG	C	502	14/15	0.84	0.40	72,80,89,94	0
4	NA	A	509	1/1	0.87	0.19	49,49,49,49	0
4	NA	A	501	1/1	0.89	0.42	66,66,66,66	0
4	NA	B	504	1/1	0.94	0.10	60,60,60,60	0
5	NAG	A	502	14/15	0.95	0.28	60,68,75,79	0
4	NA	A	510	1/1	0.95	0.06	43,43,43,43	0
4	NA	C	501	1/1	0.96	0.30	70,70,70,70	0
6	5SL	A	508	28/28	0.98	0.14	33,42,55,58	0
4	NA	B	503	1/1	0.98	0.07	67,67,67,67	0
6	5SL	C	503	28/28	0.98	0.14	52,60,64,65	0

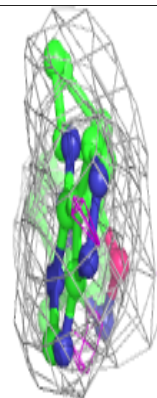
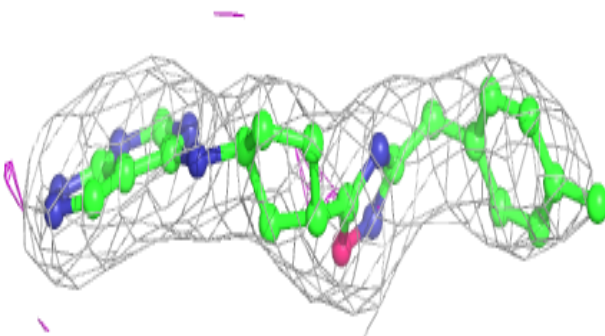
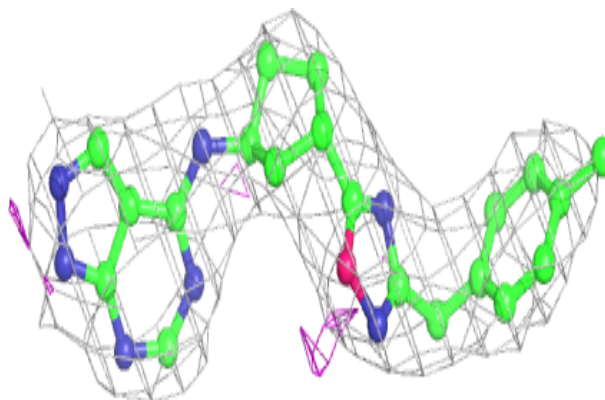
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5SL A 508:**

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

**Electron density around 5SL C 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.