



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:08 PM BST

PDB ID : 6E7W  
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-115  
Authors : Regan, M.C.; Furukawa, H.  
Deposited on : 2018-07-27  
Resolution : 2.67 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

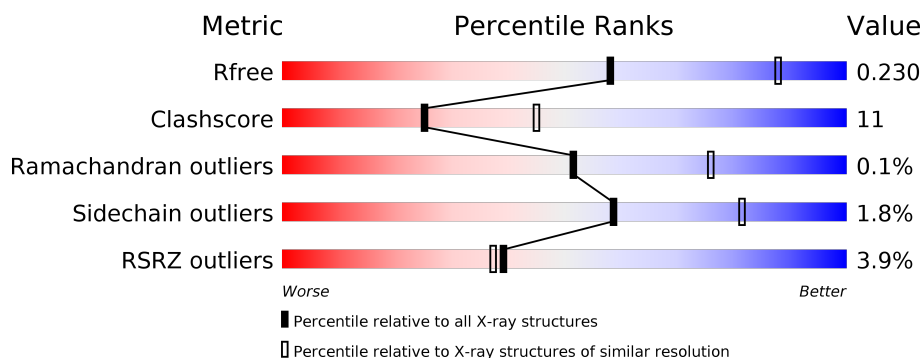
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	385	<div> <div>74%</div> <div>18%</div> <div>7%</div> </div>
1	C	385	<div> <div>4%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>
2	B	363	<div> <div>3%</div> <div>84%</div> <div>14%</div> </div>
2	D	363	<div> <div>7%</div> <div>77%</div> <div>22%</div> </div>
3	E	5	<div> <div>100%</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	A	507	-	-	-	X
4	NAG	B	502	-	-	-	X
4	NAG	C	502	-	-	-	X
4	NAG	C	503	-	-	-	X
6	CL	A	510	-	-	X	-
6	CL	D	504	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11315 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
			2753	1756	481	505	11			
1	C	357	Total	C	N	O	S	0	0	0
			2691	1716	464	500	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

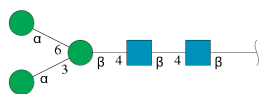
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2692	1736	429	512	15			
2	D	363	Total	C	N	O	S	0	0	0
			2702	1739	428	519	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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

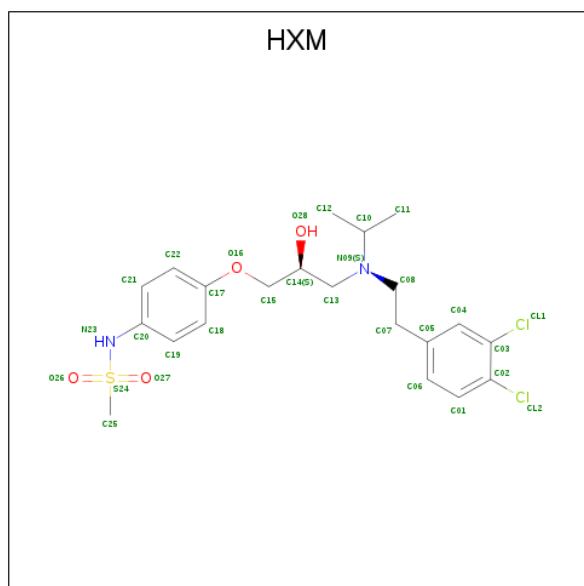
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cl	0	0
			4	4		
6	A	2	Total	Cl	0	0
			2	2		
6	D	3	Total	Cl	0	0
			3	3		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is N-{4-[(2S)-3-{[2-(3,4-dichlorophenyl)ethyl](propan-2-yl)amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: HXM) (formula: C<sub>21</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total 30	C 21	Cl 2	N 2	O 4	S 1	0	0
7	D	1	Total 30	C 21	Cl 2	N 2	O 4	S 1	0	0

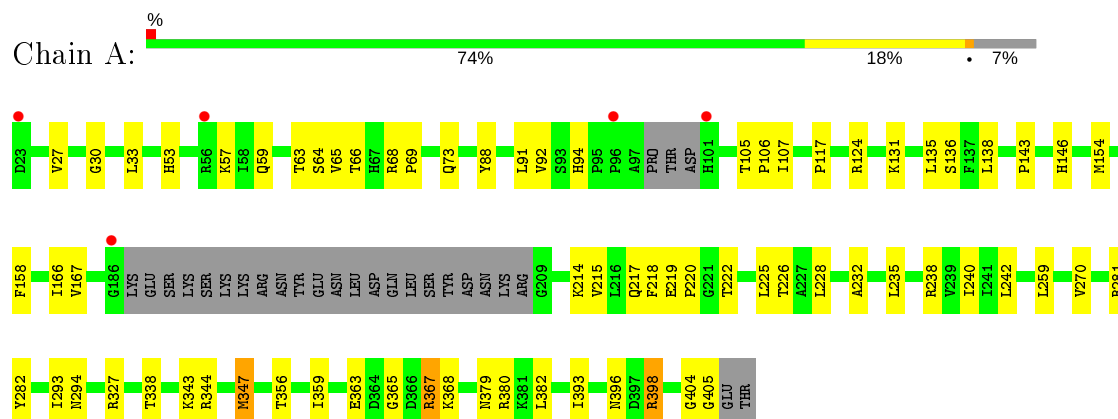
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	103	Total 103	O 103	0	0
8	B	49	Total 49	O 49	0	0
8	C	47	Total 47	O 47	0	0
8	D	33	Total 33	O 33	0	0

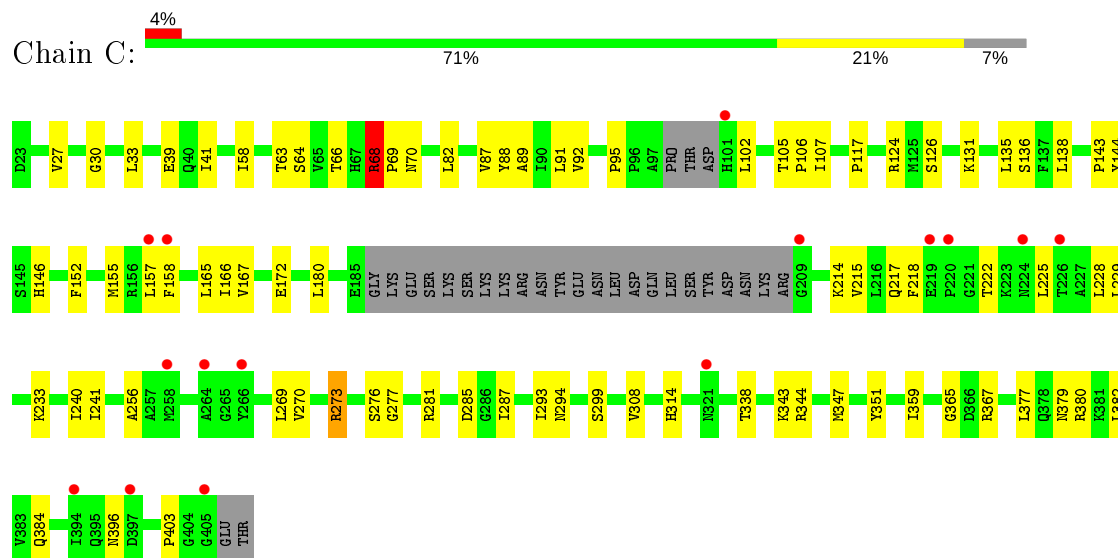
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

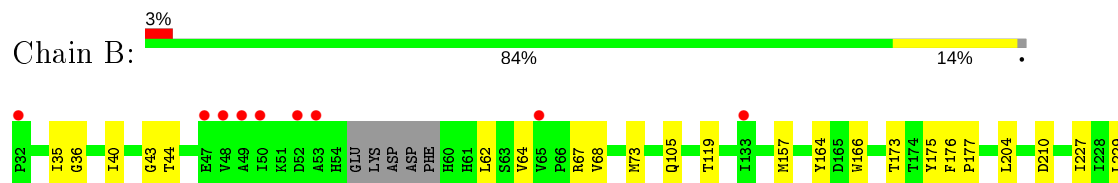
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



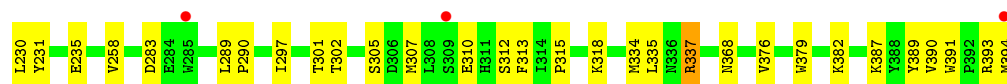
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



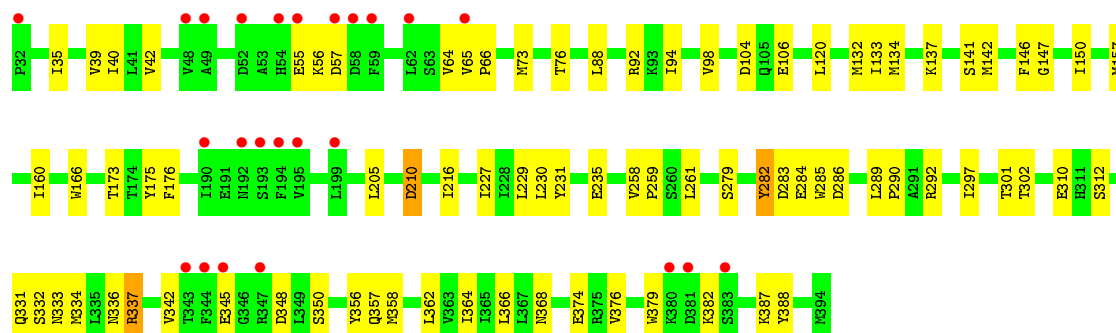
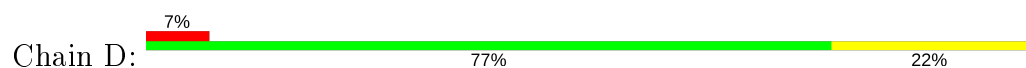
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B







- 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, $\alpha$ , $\beta$ , $\gamma$	268.13Å 59.59Å 145.50Å 90.00° 116.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.67 34.14 – 2.66	Depositor EDS
% Data completeness (in resolution range)	77.5 (25.00-2.67) 77.7 (34.14-2.66)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.190 , 0.232 0.194 , 0.230	Depositor DCC
$R_{free}$ test set	2309 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.8	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	0.94	EDS
Total number of atoms	11315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: BMA, NAG, CL, NA, HXM, 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	0.21	0/2811	0.35	0/3821
1	C	0.21	0/2747	0.35	0/3744
2	B	0.21	0/2750	0.36	0/3756
2	D	0.21	0/2762	0.36	0/3781
All	All	0.21	0/11070	0.35	0/15102

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
1	C	0	2
2	B	0	1
2	D	0	5
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	327	ARG	Sidechain
2	B	283	ASP	Peptide
1	C	273	ARG	Sidechain
1	C	68	ARG	Sidechain
2	D	279	SER	Peptide

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Mol	Chain	Res	Type	Group
2	D	282	TYR	Mainchain
2	D	333	ASN	Peptide
2	D	337	ARG	Sidechain
2	D	345	GLU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2753	0	2712	55	0
1	C	2691	0	2610	64	0
2	B	2692	0	2523	42	0
2	D	2702	0	2504	67	0
3	E	61	0	52	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
4	C	41	0	35	5	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	2	0
6	B	4	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	2	0
7	B	30	0	0	4	0
7	D	30	0	0	2	0
8	A	103	0	0	8	0
8	B	49	0	0	2	0
8	C	47	0	0	4	0
8	D	33	0	0	1	0
All	All	11315	0	10501	231	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 11.

All (231) 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)
4:C:501:NAG:C8	4:C:501:NAG:O7	2.21	0.88
2:D:133:ILE:HG22	2:D:356:TYR:CZ	2.10	0.86
2:D:283:ASP:O	2:D:285:TRP:CD1	2.28	0.86
4:C:501:NAG:O7	4:C:501:NAG:N2	2.10	0.84
1:C:285:ASP:HA	1:C:377:LEU:HD23	1.59	0.83
2:D:133:ILE:HG22	2:D:356:TYR:CE1	2.15	0.81
2:D:285:TRP:CE3	2:D:286:ASP:N	2.51	0.77
1:C:135:LEU:HD12	8:C:632:HOH:O	1.85	0.76
2:D:289:LEU:HB3	2:D:290:PRO:CD	2.17	0.75
1:A:356:THR:OG1	1:A:367:ARG:NH2	2.19	0.75
1:C:233:LYS:O	8:C:601:HOH:O	2.04	0.75
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.70	0.73
1:C:95:PRO:CG	1:C:102:LEU:O	2.37	0.71
4:C:501:NAG:C8	4:C:501:NAG:H2	2.21	0.70
1:A:117:PRO:HA	1:A:136:SER:HB3	1.75	0.69
1:C:135:LEU:O	1:C:343:LYS:NZ	2.26	0.68
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.28	0.68
1:A:242:LEU:HB3	1:A:270:VAL:HG12	1.74	0.68
2:B:40:ILE:HG21	2:B:73:MET:CE	2.24	0.68
1:C:82:LEU:O	1:C:87:VAL:HG23	1.93	0.68
2:D:312:SER:O	8:D:601:HOH:O	2.13	0.67
2:D:133:ILE:CB	2:D:356:TYR:OH	2.43	0.66
1:A:135:LEU:O	1:A:343:LYS:NZ	2.26	0.66
1:A:68:ARG:HD3	8:A:622:HOH:O	1.96	0.65
1:A:68:ARG:CD	8:A:622:HOH:O	2.45	0.65
1:A:64:SER:C	1:A:65:VAL:HG23	2.19	0.63
1:C:166:ILE:HD12	1:C:240:ILE:HG23	1.79	0.63
2:D:106:GLU:HA	2:D:132:MET:HE3	1.80	0.63
2:D:106:GLU:CA	2:D:132:MET:HE3	2.30	0.62
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.81	0.62
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.81	0.61
2:D:160:ILE:HD11	2:D:364:ILE:HD12	1.82	0.61
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.35	0.61
1:C:117:PRO:HA	1:C:136:SER:HB3	1.82	0.61
2:D:133:ILE:HD12	2:D:150:ILE:HG12	1.83	0.61
2:D:366:LEU:HB3	2:D:376:VAL:HG21	1.82	0.60
1:A:135:LEU:HD12	8:A:649:HOH:O	2.00	0.60
2:B:164:TYR:CE2	2:B:391:TRP:NE1	2.69	0.60
1:C:343:LYS:O	1:C:347:MET:HG3	2.02	0.60
1:A:131:LYS:NZ	8:A:603:HOH:O	2.34	0.60
1:A:367:ARG:HD2	1:A:368:LYS:O	2.02	0.60
1:C:95:PRO:HG2	1:C:102:LEU:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:SER:O	8:B:601:HOH:O	2.17	0.59
2:D:285:TRP:HE3	2:D:286:ASP:CB	2.15	0.59
1:A:396:ASN:O	6:A:510:CL:CL	2.57	0.59
1:C:68:ARG:HB3	1:C:69:PRO:HD2	1.84	0.59
1:C:87:VAL:CG1	1:C:89:ALA:O	2.51	0.58
2:D:297:ILE:O	2:D:301:THR:HG23	2.02	0.58
1:A:398:ARG:O	6:A:510:CL:CL	2.58	0.58
2:D:106:GLU:N	2:D:132:MET:CE	2.66	0.58
2:D:285:TRP:CE3	2:D:286:ASP:CB	2.87	0.58
2:D:133:ILE:HG22	2:D:356:TYR:OH	2.04	0.58
2:B:235:GLU:OE1	2:B:235:GLU:CG	2.52	0.57
4:C:501:NAG:C8	4:C:501:NAG:N2	2.67	0.57
2:D:40:ILE:HG21	2:D:73:MET:CE	2.35	0.57
2:B:376:VAL:O	2:B:387:LYS:HB2	2.04	0.57
2:D:379:TRP:CZ2	2:D:382:LYS:HA	2.40	0.57
1:A:53:HIS:O	8:A:601:HOH:O	2.17	0.56
2:D:175:TYR:HB2	7:D:503:HXM:C25	2.35	0.56
2:D:133:ILE:HB	2:D:356:TYR:OH	2.03	0.56
1:C:135:LEU:H	1:C:135:LEU:HD12	1.71	0.56
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.88	0.55
1:C:105:THR:HB	1:C:106:PRO:HD3	1.89	0.55
2:D:205:LEU:HD22	2:D:216:ILE:HG23	1.89	0.55
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.87	0.55
1:A:135:LEU:H	1:A:135:LEU:HD12	1.72	0.55
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.88	0.55
4:C:501:NAG:C8	4:C:501:NAG:C2	2.84	0.54
1:C:379:ASN:O	1:C:380:ARG:HB2	2.06	0.54
1:C:293:ILE:O	1:C:294:ASN:HB2	2.07	0.54
2:D:120:LEU:O	2:D:142:MET:CE	2.55	0.54
2:D:88:LEU:HB3	2:D:94:ILE:CD1	2.36	0.54
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.90	0.54
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.90	0.54
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.43	0.53
1:C:41:ILE:HD13	1:C:299:SER:OG	2.08	0.53
2:B:379:TRP:CZ2	2:B:382:LYS:HA	2.44	0.53
2:B:318:LYS:N	2:B:318:LYS:HD3	2.24	0.53
1:A:57:LYS:HB3	8:A:634:HOH:O	2.09	0.52
2:B:175:TYR:HB2	7:B:503:HXM:C25	2.39	0.52
1:C:229:LEU:HD23	1:C:256:ALA:HA	1.91	0.52
2:D:302:THR:HG21	2:D:342:VAL:HG13	1.92	0.52
2:B:307:MET:SD	2:B:315:PRO:HD3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NE	2:B:210:ASP:OD1	2.36	0.52
1:C:95:PRO:HG3	1:C:102:LEU:O	2.09	0.52
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.92	0.52
1:A:33:LEU:O	1:A:66:THR:HA	2.10	0.51
2:B:389:TYR:HD1	2:B:390:VAL:HG23	1.73	0.51
1:C:152:PHE:HA	1:C:155:MET:CE	2.40	0.51
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.92	0.51
2:D:88:LEU:HB3	2:D:94:ILE:HD11	1.92	0.51
1:A:154:MET:HG2	1:A:393:ILE:HD11	1.93	0.51
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.92	0.51
2:B:289:LEU:HB3	2:B:290:PRO:CD	2.41	0.50
2:B:235:GLU:CG	2:B:235:GLU:OE2	2.59	0.50
1:C:58:ILE:HD11	1:C:314:HIS:CD2	2.46	0.50
2:D:39:VAL:HG22	2:D:98:VAL:HB	1.93	0.50
1:A:30:GLY:HA2	1:A:63:THR:O	2.12	0.50
2:D:133:ILE:CA	2:D:356:TYR:OH	2.60	0.50
2:D:66:PRO:HB3	2:D:301:THR:HG21	1.93	0.50
2:D:285:TRP:HE3	2:D:286:ASP:N	2.09	0.50
2:B:313:PHE:HE1	2:D:334:MET:HE1	1.77	0.50
2:D:348:ASP:OD1	2:D:350:SER:OG	2.20	0.49
1:C:131:LYS:HE3	8:C:647:HOH:O	2.13	0.49
2:B:157:MET:HE3	2:B:229:LEU:HD22	1.94	0.49
1:C:124:ARG:O	1:C:143:PRO:HA	2.12	0.49
2:B:393:ARG:O	2:B:394:MET:CB	2.61	0.49
1:A:293:ILE:O	1:A:294:ASN:HB2	2.13	0.49
2:B:105:GLN:NE2	8:B:603:HOH:O	2.26	0.49
2:D:133:ILE:CD1	2:D:150:ILE:HG12	2.42	0.49
2:B:68:VAL:HG11	2:B:297:ILE:HD13	1.95	0.49
2:D:133:ILE:CG2	2:D:356:TYR:OH	2.61	0.49
1:A:136:SER:HB2	8:A:662:HOH:O	2.11	0.48
1:A:68:ARG:HD2	8:A:622:HOH:O	2.12	0.48
1:C:403:PRO:HA	8:C:612:HOH:O	2.12	0.48
1:A:232:ALA:HA	1:A:235:LEU:HD12	1.96	0.48
1:C:222:THR:HB	1:C:225:LEU:HD21	1.96	0.48
2:D:289:LEU:O	2:D:292:ARG:N	2.44	0.48
1:A:281:ARG:NH2	1:A:282:TYR:CE2	2.81	0.48
2:B:119:THR:O	2:B:318:LYS:HE3	2.13	0.48
1:C:285:ASP:HA	1:C:377:LEU:CD2	2.38	0.47
1:C:308:VAL:HG11	1:C:359:ILE:HG21	1.96	0.47
1:C:87:VAL:HG12	1:C:89:ALA:O	2.13	0.47
1:C:41:ILE:CD1	1:C:299:SER:OG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:OE1	1:C:64:SER:OG	2.26	0.47
1:A:105:THR:N	1:A:106:PRO:CD	2.77	0.47
1:A:105:THR:HB	1:A:106:PRO:HD3	1.94	0.47
2:D:374:GLU:O	2:D:376:VAL:HG23	2.14	0.47
1:C:30:GLY:HA2	1:C:63:THR:O	2.14	0.47
1:C:68:ARG:N	1:C:68:ARG:HD2	2.29	0.47
2:B:175:TYR:CE1	2:B:204:LEU:HD21	2.49	0.47
1:C:359:ILE:HD13	1:C:367:ARG:CZ	2.44	0.47
2:D:147:GLY:HA2	2:D:282:TYR:CD2	2.49	0.47
1:A:154:MET:CE	1:A:158:PHE:HE2	2.28	0.47
2:B:230:LEU:HB3	2:B:258:VAL:HG12	1.97	0.47
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.49	0.47
1:A:138:LEU:N	1:A:138:LEU:HD12	2.30	0.46
2:D:230:LEU:HB3	2:D:258:VAL:HG12	1.97	0.46
2:B:40:ILE:HG21	2:B:73:MET:HE3	1.95	0.46
2:D:40:ILE:HG21	2:D:73:MET:HE2	1.98	0.46
2:B:289:LEU:N	2:B:290:PRO:HD2	2.31	0.46
1:A:214:LYS:HG3	1:A:215:VAL:N	2.30	0.46
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.98	0.46
2:B:337:ARG:H	2:B:337:ARG:HG3	1.51	0.46
2:D:120:LEU:C	2:D:142:MET:CE	2.84	0.45
2:D:106:GLU:N	2:D:132:MET:HE1	2.30	0.45
2:D:35:ILE:HD11	2:D:301:THR:HA	1.97	0.45
1:A:64:SER:O	1:A:65:VAL:HG23	2.16	0.45
1:A:396:ASN:OD1	1:A:396:ASN:C	2.54	0.45
2:B:64:VAL:HG12	2:B:305:SER:HB2	1.99	0.45
2:D:133:ILE:HG12	6:D:504:CL:CL	2.53	0.45
1:A:135:LEU:HD21	7:B:503:HXM:C17	2.47	0.45
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.84	0.45
1:C:166:ILE:CD1	1:C:240:ILE:HG23	2.46	0.45
1:A:135:LEU:HD11	7:B:503:HXM:C15	2.47	0.45
1:C:396:ASN:C	1:C:396:ASN:OD1	2.54	0.45
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.99	0.45
2:D:387:LYS:HE3	2:D:388:TYR:CZ	2.52	0.45
1:A:359:ILE:HD13	1:A:367:ARG:CZ	2.47	0.45
1:C:152:PHE:HA	1:C:155:MET:HE3	1.97	0.45
2:D:120:LEU:HD22	2:D:332:SER:O	2.17	0.45
1:A:222:THR:HB	1:A:225:LEU:HD21	1.98	0.45
1:C:91:LEU:HD12	1:C:91:LEU:N	2.31	0.45
2:D:106:GLU:HG3	2:D:176:PHE:CE1	2.52	0.45
2:B:313:PHE:CD1	2:D:332:SER:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:HG21	1:A:107:ILE:HG21	1.99	0.44
1:C:138:LEU:HD12	1:C:138:LEU:N	2.32	0.44
1:C:126:SER:OG	1:C:172:GLU:OE1	2.31	0.44
2:D:120:LEU:HD13	2:D:331:GLN:HB3	1.98	0.44
1:A:166:ILE:HD12	1:A:240:ILE:CG2	2.47	0.44
7:D:503:HXM:C07	7:D:503:HXM:C14	2.95	0.44
1:C:105:THR:N	1:C:106:PRO:CD	2.80	0.44
2:D:134:MET:HG2	2:D:137:LYS:HG2	1.99	0.44
1:A:281:ARG:NH2	1:A:282:TYR:HE2	2.16	0.44
2:B:35:ILE:HD11	2:B:301:THR:HA	2.00	0.44
2:B:164:TYR:CD2	2:B:391:TRP:NE1	2.85	0.44
1:C:167:VAL:O	1:C:217:GLN:HA	2.17	0.44
2:B:62:LEU:HD13	2:B:302:THR:HA	2.00	0.44
1:C:70:ASN:C	1:C:70:ASN:OD1	2.55	0.44
1:C:344:ARG:NE	2:D:210:ASP:OD1	2.41	0.44
1:C:270:VAL:HG11	1:C:287:ILE:HD11	2.00	0.43
1:C:92:VAL:CG2	1:C:107:ILE:HG21	2.48	0.43
2:D:55:GLU:C	2:D:57:ASP:H	2.22	0.43
1:C:382:LEU:HD23	1:C:382:LEU:HA	1.87	0.43
1:C:157:LEU:HD23	1:C:158:PHE:CE1	2.53	0.43
1:A:363:GLU:H	1:A:363:GLU:CD	2.21	0.43
1:A:379:ASN:O	1:A:380:ARG:HB2	2.18	0.43
1:C:166:ILE:HD12	1:C:240:ILE:CG2	2.46	0.43
1:C:33:LEU:O	1:C:66:THR:HA	2.18	0.43
2:D:132:MET:O	2:D:133:ILE:C	2.57	0.43
1:A:404:GLY:O	1:A:405:GLY:C	2.57	0.43
2:B:368:ASN:OD1	2:B:368:ASN:C	2.57	0.43
1:A:347:MET:CE	1:A:365:GLY:CA	2.97	0.43
2:B:334:MET:HG3	2:B:337:ARG:HE	1.83	0.42
1:C:144:TYR:CD2	1:C:273:ARG:HD2	2.53	0.42
1:A:64:SER:C	1:A:65:VAL:CG2	2.86	0.42
2:B:40:ILE:CG2	2:B:73:MET:CE	2.96	0.42
2:D:146:PHE:HB3	2:D:282:TYR:HE2	1.84	0.42
2:D:133:ILE:HG23	6:D:504:CL:CL	2.56	0.42
1:C:58:ILE:HG13	1:C:58:ILE:O	2.19	0.42
2:D:285:TRP:CE3	2:D:286:ASP:CA	3.02	0.42
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.85	0.42
1:A:91:LEU:HD12	1:A:91:LEU:N	2.35	0.42
1:C:241:ILE:HA	1:C:269:LEU:O	2.20	0.41
2:D:368:ASN:OD1	2:D:368:ASN:C	2.58	0.41
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:O	1:A:217:GLN:HA	2.19	0.41
2:B:43:GLY:O	2:B:44:THR:C	2.58	0.41
1:A:166:ILE:HD12	1:A:240:ILE:HG23	2.01	0.41
2:B:36:GLY:HA3	2:B:67:ARG:HH11	1.85	0.41
2:D:336:ASN:O	2:D:337:ARG:C	2.59	0.41
2:D:283:ASP:CG	2:D:284:GLU:H	2.24	0.41
1:A:226:THR:HG23	1:A:259:LEU:HD21	2.02	0.41
1:C:166:ILE:CD1	1:C:240:ILE:CG2	2.99	0.41
1:C:338:THR:HG22	1:C:338:THR:O	2.21	0.41
2:D:259:PRO:HG2	2:D:261:LEU:CD2	2.51	0.41
7:B:503:HXM:C14	7:B:503:HXM:C07	2.98	0.41
1:C:276:SER:O	1:C:277:GLY:C	2.59	0.41
1:A:124:ARG:O	1:A:143:PRO:HA	2.20	0.41
2:B:389:TYR:CD1	2:B:390:VAL:HG23	2.55	0.41
1:C:229:LEU:HD23	1:C:256:ALA:CA	2.51	0.41
1:C:308:VAL:HG12	1:C:351:TYR:HB2	2.02	0.40
2:D:104:ASP:C	2:D:132:MET:HE2	2.41	0.40
2:D:64:VAL:CG1	2:D:65:VAL:N	2.84	0.40
1:A:338:THR:O	1:A:338:THR:HG22	2.21	0.40
1:C:214:LYS:HG3	1:C:215:VAL:N	2.36	0.40
1:C:347:MET:HE1	1:C:365:GLY:N	2.36	0.40
2:B:335:LEU:HG	2:B:335:LEU:O	2.21	0.40
1:C:30:GLY:N	1:C:87:VAL:HG13	2.37	0.40
1:A:219:GLU:HA	1:A:220:PRO:HD2	1.91	0.40
2:B:164:TYR:CZ	2:B:391:TRP:NE1	2.89	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	352/385 (91%)	337 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	351/385 (91%)	337 (96%)	14 (4%)	0	100	100
2	B	354/363 (98%)	336 (95%)	18 (5%)	0	100	100
2	D	361/363 (99%)	330 (91%)	29 (8%)	2 (1%)	25	47
All	All	1418/1496 (95%)	1340 (94%)	76 (5%)	2 (0%)	51	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	92	ARG
2	D	56	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	287/331 (87%)	279 (97%)	8 (3%)	43	70
1	C	277/331 (84%)	273 (99%)	4 (1%)	67	85
2	B	274/326 (84%)	272 (99%)	2 (1%)	84	93
2	D	273/326 (84%)	267 (98%)	6 (2%)	52	77
All	All	1111/1314 (85%)	1091 (98%)	20 (2%)	59	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	73	GLN
1	A	94	HIS
1	A	146	HIS
1	A	238	ARG
1	A	347	MET
1	A	367	ARG
1	A	398	ARG
2	B	310	GLU

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Mol	Chain	Res	Type
2	B	337	ARG
1	C	68	ARG
1	C	146	HIS
1	C	281	ARG
1	C	384	GLN
2	D	141	SER
2	D	210	ASP
2	D	235	GLU
2	D	310	GLU
2	D	357	GLN
2	D	358	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	314	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	0.31	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	2	3	14,14,15	0.32	0	17,19,21	0.78	0
3	BMA	E	3	3	11,11,12	0.26	0	15,15,17	0.64	0
3	MAN	E	4	3	11,11,12	0.25	0	15,15,17	0.73	0
3	MAN	E	5	3	11,11,12	0.25	0	15,15,17	0.61	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	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

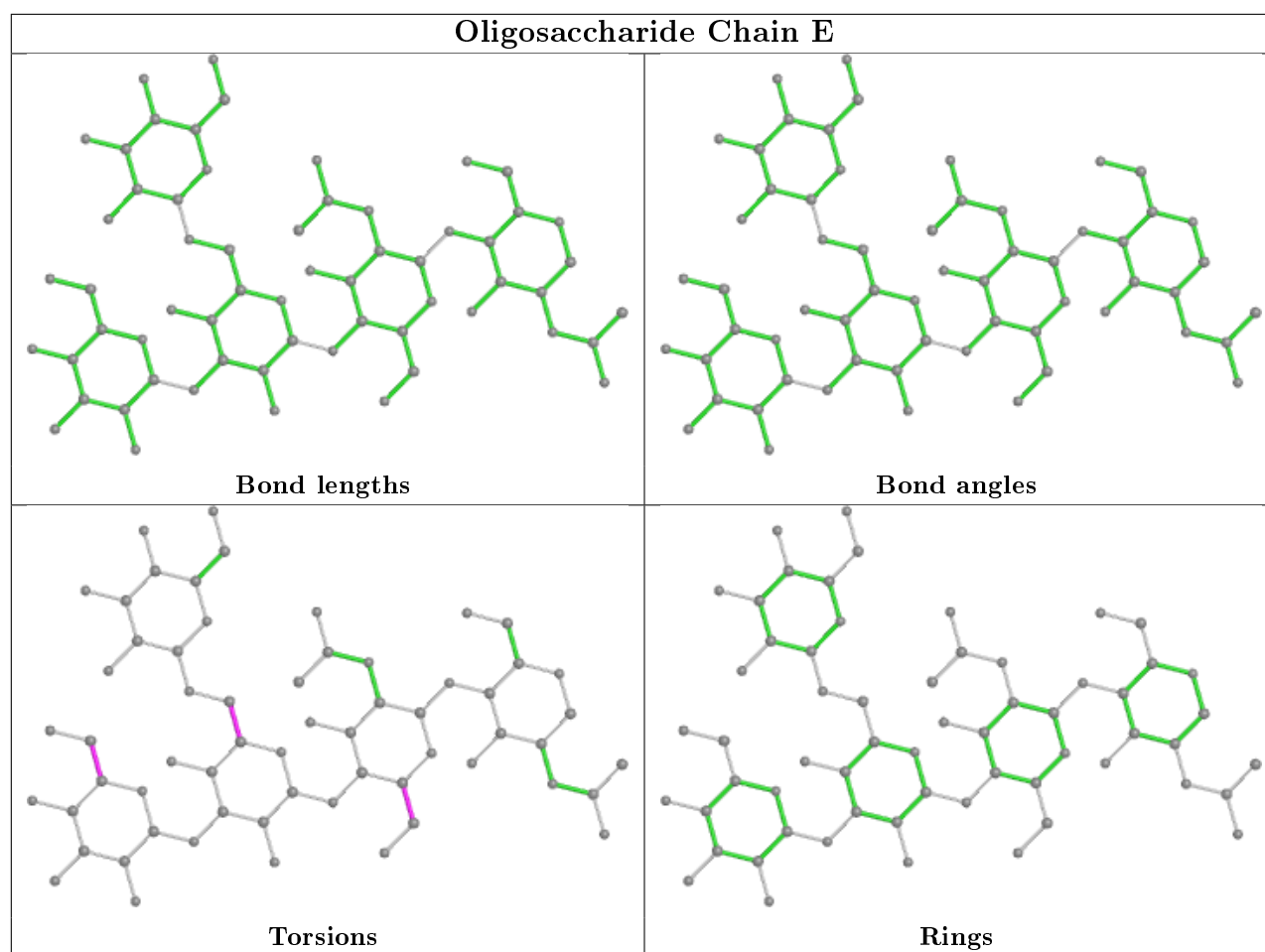
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	MAN	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	C	502	1	14,14,15	0.31	0	17,19,21	0.73	0
4	NAG	A	501	1	14,14,15	0.26	0	17,19,21	0.84	1 (5%)
4	NAG	A	507	1	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	C	503	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	D	502	2	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	B	501	2	14,14,15	0.30	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	HXM	B	503	-	31,31,31	1.57	4 (12%)	43,43,43	2.18	3 (6%)
4	NAG	C	501	1	11,11,15	0.42	0	12,15,21	0.63	0
4	NAG	B	502	2	14,14,15	0.36	0	17,19,21	0.79	0
7	HXM	D	503	-	31,31,31	1.59	4 (12%)	43,43,43	2.19	5 (11%)

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	C	502	1	-	1/6/23/26	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1
4	NAG	C	503	1	-	1/6/23/26	0/1/1/1
4	NAG	D	502	2	-	4/6/23/26	0/1/1/1
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
7	HXM	B	503	-	-	9/23/23/23	0/2/2/2
4	NAG	C	501	1	-	2/2/19/26	0/1/1/1
4	NAG	B	502	2	-	4/6/23/26	0/1/1/1
7	HXM	D	503	-	-	10/23/23/23	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	503	HXM	S24-N23	6.31	1.71	1.63
7	B	503	HXM	S24-N23	6.24	1.71	1.63
7	D	503	HXM	C25-S24	2.92	1.82	1.75
7	B	503	HXM	C25-S24	2.90	1.82	1.75
7	D	503	HXM	C02-CL2	2.27	1.79	1.73
7	B	503	HXM	C02-CL2	2.25	1.79	1.73
7	D	503	HXM	C03-CL1	2.20	1.78	1.73
7	B	503	HXM	C03-CL1	2.13	1.78	1.73

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	HXM	O27-S24-O26	-12.29	101.17	118.85
7	B	503	HXM	O27-S24-O26	-12.15	101.39	118.85
7	B	503	HXM	C25-S24-N23	3.40	110.51	106.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	503	HXM	C25-S24-N23	3.16	110.24	106.63
7	B	503	HXM	C08-N09-C10	-2.33	110.10	113.33
4	A	501	NAG	O5-C1-C2	-2.23	107.77	111.29
7	D	503	HXM	C08-N09-C10	-2.20	110.29	113.33
7	D	503	HXM	O27-S24-N23	2.17	111.53	107.10
4	D	502	NAG	O5-C5-C6	2.11	110.50	107.20
7	D	503	HXM	C13-N09-C10	-2.02	109.28	113.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	503	HXM	N09-C13-C14-C15
7	D	503	HXM	O28-C14-C15-O16
7	D	503	HXM	C20-N23-S24-O26
7	B	503	HXM	C13-C14-C15-O16
7	B	503	HXM	O28-C14-C15-O16
4	C	501	NAG	C4-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	B	502	NAG	C4-C5-C6-O6
4	D	502	NAG	C8-C7-N2-C2
4	D	502	NAG	O7-C7-N2-C2
4	B	502	NAG	C8-C7-N2-C2
4	B	502	NAG	O7-C7-N2-C2
4	B	502	NAG	O5-C5-C6-O6
7	B	503	HXM	C20-N23-S24-O26
7	D	503	HXM	C13-C14-C15-O16
7	D	503	HXM	N09-C13-C14-O28
4	D	502	NAG	O5-C5-C6-O6
7	B	503	HXM	C22-C17-O16-C15
4	D	502	NAG	C4-C5-C6-O6
4	C	502	NAG	O5-C5-C6-O6
7	D	503	HXM	C22-C17-O16-C15
7	B	503	HXM	C18-C17-O16-C15
4	C	503	NAG	O5-C5-C6-O6
7	D	503	HXM	C18-C17-O16-C15
7	B	503	HXM	C06-C05-C07-C08
7	B	503	HXM	N09-C13-C14-O28
7	B	503	HXM	N09-C13-C14-C15
7	D	503	HXM	C04-C05-C07-C08
7	B	503	HXM	C04-C05-C07-C08
7	D	503	HXM	C20-N23-S24-C25

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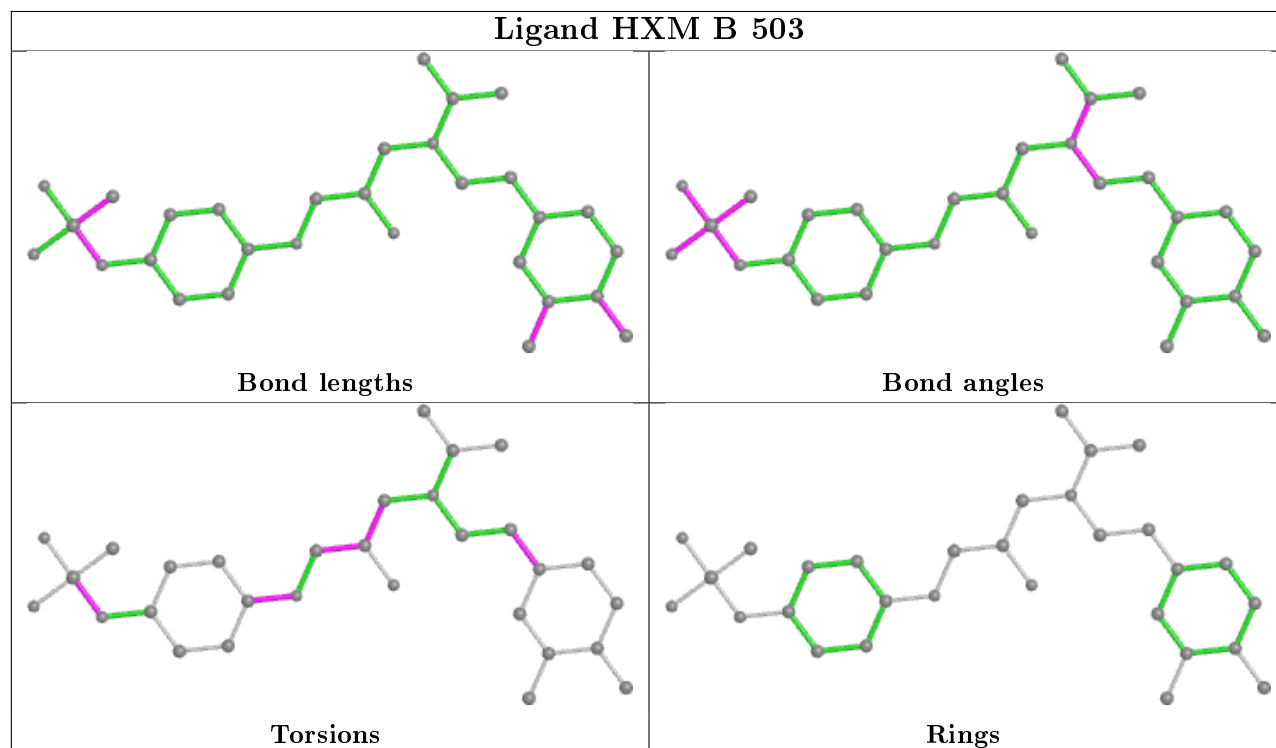
Mol	Chain	Res	Type	Atoms
7	D	503	HXM	C06-C05-C07-C08

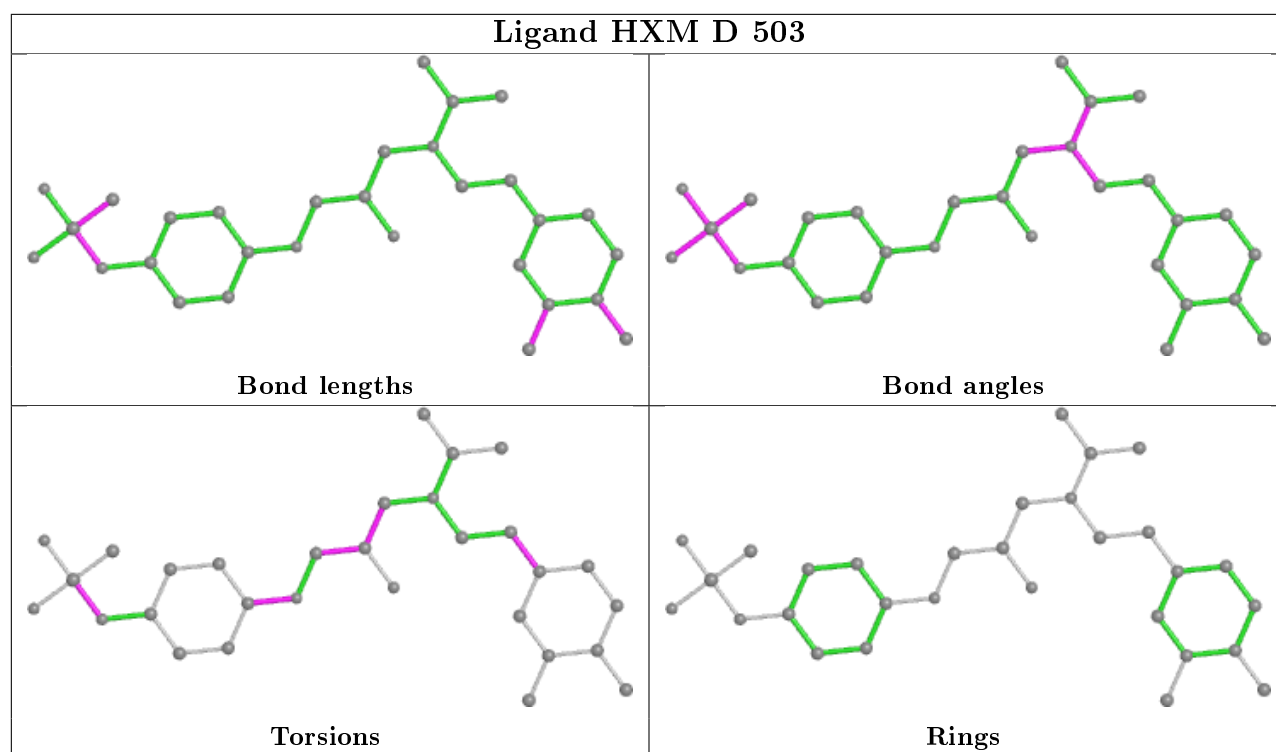
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	HXM	4	0
4	C	501	NAG	5	0
7	D	503	HXM	2	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, 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	358/385 (92%)	-0.30	5 (1%) 75 76	20, 37, 72, 108	0
1	C	357/385 (92%)	-0.11	15 (4%) 36 34	30, 52, 91, 109	0
2	B	358/363 (98%)	0.02	12 (3%) 45 44	22, 50, 88, 107	0
2	D	363/363 (100%)	0.05	24 (6%) 18 16	28, 54, 102, 142	0
All	All	1436/1496 (95%)	-0.08	56 (3%) 39 37	20, 49, 90, 142	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	VAL	5.2
2	D	59	PHE	4.5
2	D	194	PHE	4.4
2	D	57	ASP	4.0
2	B	49	ALA	3.9
2	D	192	ASN	3.8
2	D	347	ARG	3.6
2	D	48	VAL	3.6
2	B	52	ASP	3.5
2	B	50	ILE	3.5
2	D	343	THR	3.4
1	C	258	MET	3.3
1	C	101	HIS	3.3
2	D	381	ASP	3.3
2	D	58	ASP	3.3
1	C	397	ASP	3.2
2	D	345	GLU	3.2
2	D	195	VAL	3.1
2	B	32	PRO	3.1
2	B	53	ALA	3.0
2	B	47	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	32	PRO	2.9
2	D	193	SER	2.8
1	A	186	GLY	2.8
1	C	394	ILE	2.7
1	C	226	THR	2.7
2	D	62	LEU	2.7
1	A	96	PRO	2.6
1	C	220	PRO	2.6
1	C	219	GLU	2.6
1	C	266	TYR	2.6
2	B	65	VAL	2.5
1	C	264	ALA	2.5
1	C	158	PHE	2.5
2	D	49	ALA	2.5
1	C	224	ASN	2.4
2	D	52	ASP	2.4
2	B	309	SER	2.3
2	B	133	ILE	2.3
2	D	54	HIS	2.3
2	D	344	PHE	2.3
2	D	65	VAL	2.3
2	B	394	MET	2.2
1	C	321	ASN	2.2
1	A	101	HIS	2.2
2	D	55	GLU	2.2
2	B	285	TRP	2.1
2	D	383	SER	2.1
2	D	380	LYS	2.1
2	D	190	ILE	2.1
1	C	209	GLY	2.1
1	C	157	LEU	2.1
1	A	56	ARG	2.1
1	A	23	ASP	2.1
1	C	405	GLY	2.0
2	D	199	LEU	2.0

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

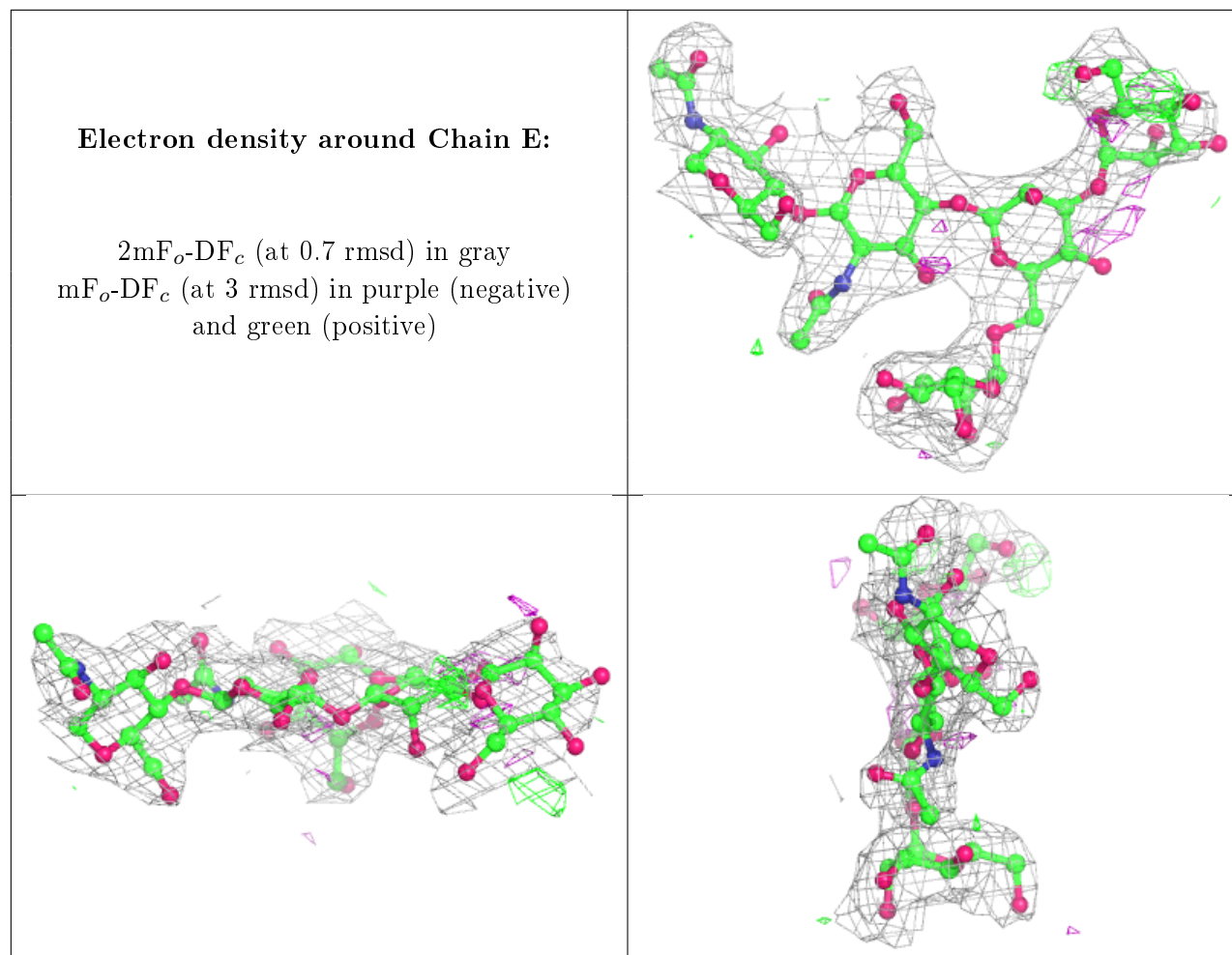
There are no non-standard protein/DNA/RNA residues in this entry.

### 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	0.77	0.29	96,113,118,130	0
3	NAG	E	2	14/15	0.93	0.18	61,68,76,84	0
3	NAG	E	1	14/15	0.94	0.16	49,56,59,63	0
3	BMA	E	3	11/12	0.95	0.23	66,74,93,101	0
3	MAN	E	5	11/12	0.97	0.12	54,59,64,65	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 ⓘ

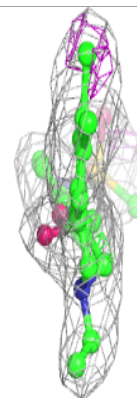
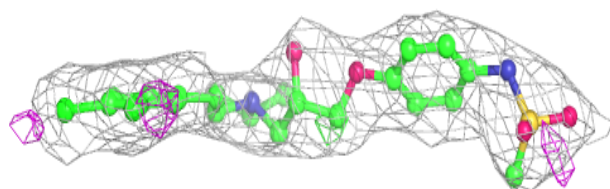
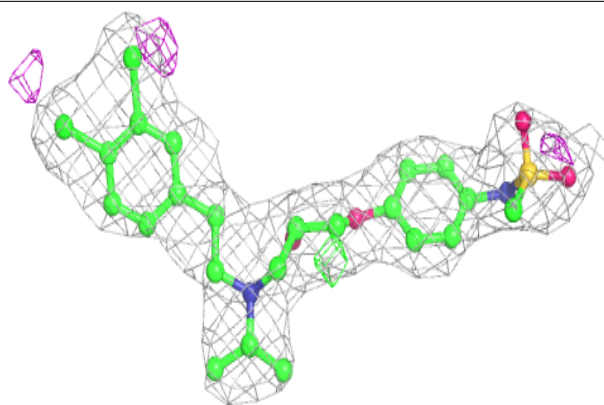
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NAG	C	503	14/15	0.48	0.46	115,126,140,148	0
4	NAG	A	507	14/15	0.68	0.48	93,117,136,143	0
4	NAG	B	501	14/15	0.76	0.33	85,100,114,118	0
4	NAG	B	502	14/15	0.76	0.49	111,128,137,140	0
4	NAG	D	502	14/15	0.78	0.39	101,110,115,119	0
4	NAG	C	502	14/15	0.80	0.41	99,115,133,140	0
6	CL	B	505	1/1	0.87	0.19	67,67,67,67	0
6	CL	D	506	1/1	0.87	0.36	81,81,81,81	0
6	CL	D	505	1/1	0.92	0.11	79,79,79,79	0
4	NAG	C	501	13/15	0.92	0.12	51,57,64,68	0
6	CL	C	506	1/1	0.92	0.14	63,63,63,63	0
6	CL	B	504	1/1	0.93	0.36	79,79,79,79	0
6	CL	A	510	1/1	0.94	0.06	54,54,54,54	0
4	NAG	A	501	14/15	0.94	0.20	40,47,57,59	0
6	CL	B	507	1/1	0.96	0.19	77,77,77,77	0
7	HXM	B	503	30/30	0.96	0.16	30,44,54,64	0
6	CL	C	505	1/1	0.97	0.40	73,73,73,73	0
7	HXM	D	503	30/30	0.97	0.12	32,41,54,60	0
6	CL	B	506	1/1	0.98	0.08	53,53,53,53	0
5	NA	C	504	1/1	0.98	0.06	42,42,42,42	0
6	CL	A	509	1/1	0.98	0.23	67,67,67,67	0
5	NA	A	508	1/1	0.98	0.07	24,24,24,24	0
6	CL	D	504	1/1	0.98	0.17	71,71,71,71	0

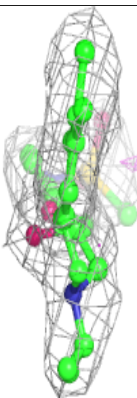
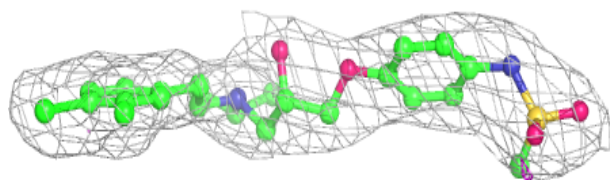
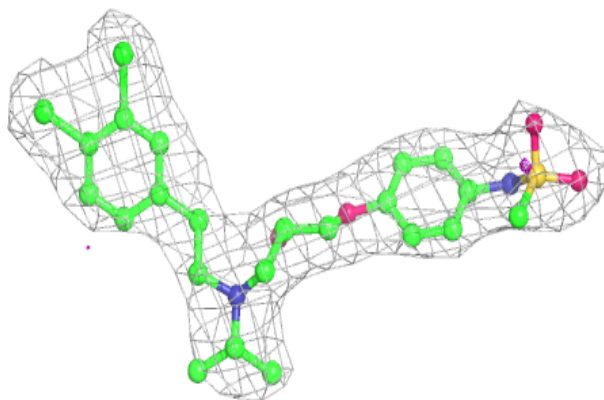
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HXM 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 HXM D 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.