



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:41 PM BST

PDB ID : 6E7S  
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-5  
Authors : Regan, M.C.; Furukawa, H.  
Deposited on : 2018-07-27  
Resolution : 2.72 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

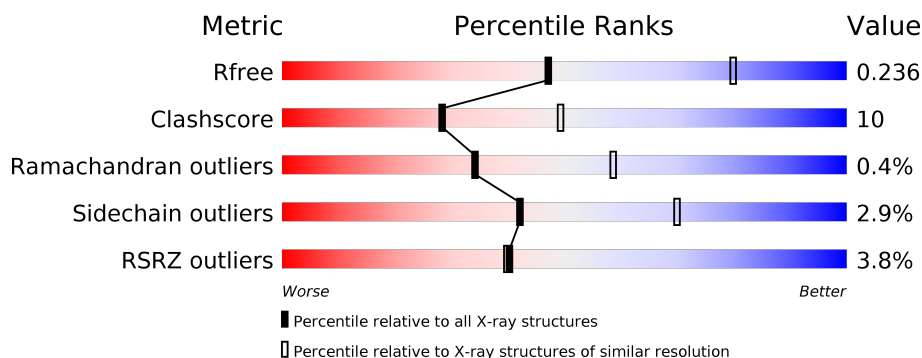
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	C	385	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>7%</div> </div> </div>
2	B	363	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div></div> </div> </div>
2	D	363	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div></div> </div> </div>
3	E	5	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>
4	F	2	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</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	A	507	-	-	-	X
5	NAG	C	504	-	-	-	X
5	NAG	D	502	-	-	-	X
7	CL	A	510	-	-	X	-
7	CL	D	504	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11392 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	507	11			
1	C	357	Total	C	N	O	S	0	0	0
			2685	1712	458	504	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

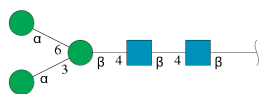
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2780	1791	445	528	16			
2	D	363	Total	C	N	O	S	0	0	0
			2725	1755	437	517	16			

There are 2 discrepancies between the modelled and reference sequences:

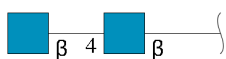
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- 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.



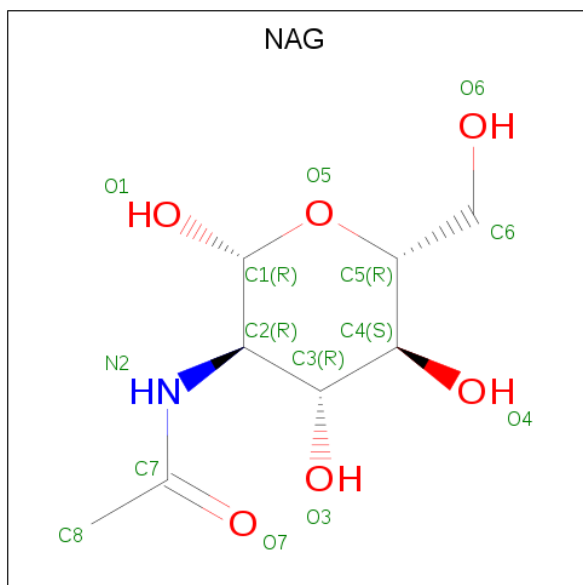
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	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		

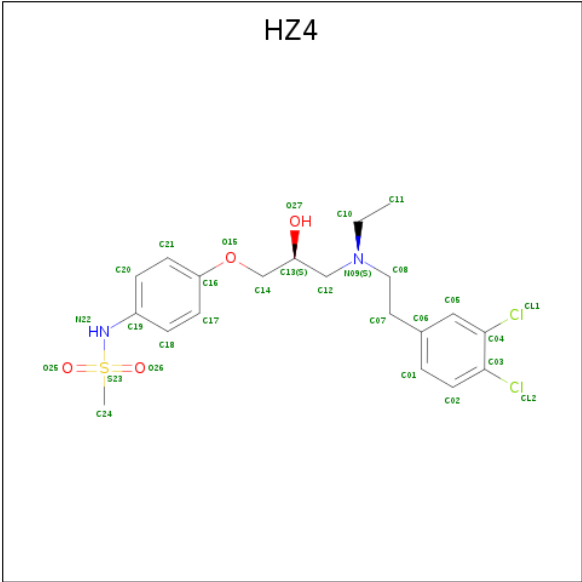
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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	3	Total	Cl	0	0
			3	3		
7	A	2	Total	Cl	0	0
			2	2		
7	D	2	Total	Cl	0	0
			2	2		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is N-{4-[(2S)-3-{[2-(3,4-dichlorophenyl)ethyl](ethyl)amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: HZ4) (formula: C<sub>20</sub>H<sub>26</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	
8	B	1	Total	C	Cl	N	O	S	0	0
			29	20	2	2	4	1		
8	D	1	Total	C	Cl	N	O	S	0	0
			29	20	2	2	4	1		

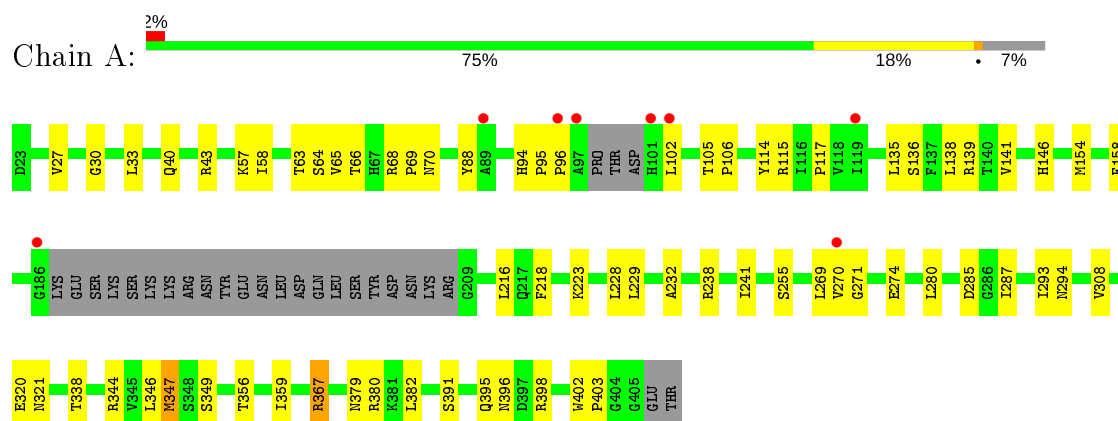
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	84	Total	O	0	0
			84	84		
9	B	42	Total	O	0	0
			42	42		
9	C	30	Total	O	0	0
			30	30		
9	D	22	Total	O	0	0
			22	22		

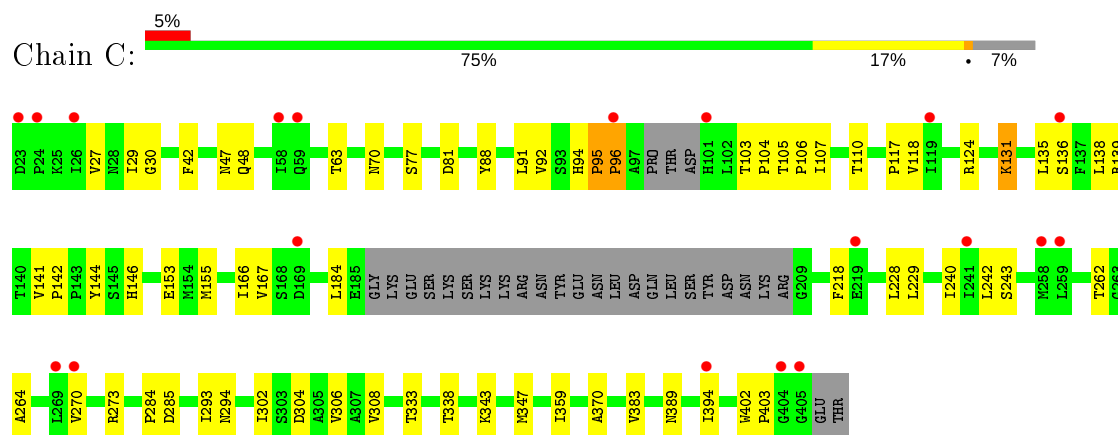
### 3 Residue-property plots [i](#)

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.

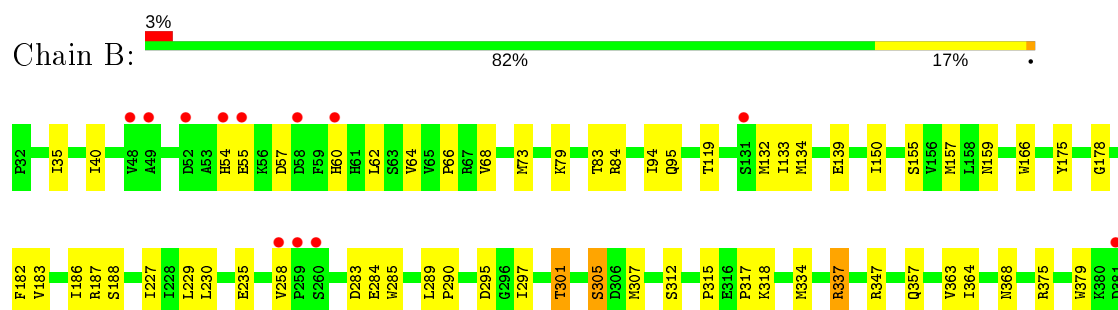
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Glutamate receptor ionotropic, NMDA 1



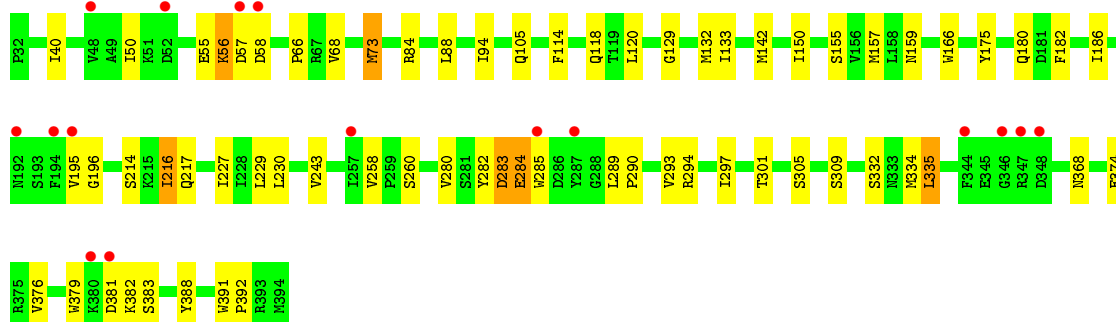
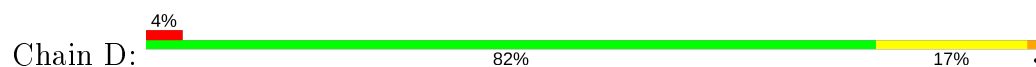
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



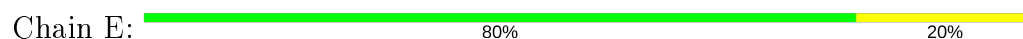




- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- 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



- 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, $\alpha$ , $\beta$ , $\gamma$	268.43Å 60.63Å 145.39Å 90.00° 116.42° 90.00°	Depositor
Resolution (Å)	25.00 – 2.72 29.88 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.72) 98.3 (29.88-2.72)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.234 0.192 , 0.236	Depositor DCC
$R_{free}$ test set	2763 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, HZ4, 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	0/2814	0.35	0/3825
1	C	0.20	0/2741	0.35	0/3738
2	B	0.21	0/2843	0.35	0/3879
2	D	0.21	0/2789	0.35	0/3816
All	All	0.21	0/11187	0.35	0/15258

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	2756	0	2721	55	0
1	C	2685	0	2588	53	0
2	B	2780	0	2626	49	0
2	D	2725	0	2532	53	0
3	E	61	0	52	0	0
4	F	28	0	25	2	0
5	A	28	0	26	1	0
5	B	28	0	26	0	0
5	C	27	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	26	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	2	0	0	2	0
7	B	3	0	0	1	0
7	C	1	0	0	0	0
7	D	2	0	0	2	0
8	B	29	0	0	2	0
8	D	29	0	0	2	0
9	A	84	0	0	6	0
9	B	42	0	0	2	0
9	C	30	0	0	5	0
9	D	22	0	0	3	0
All	All	11392	0	10644	214	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 10.

All (214) 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:N2	2.17	1.08
1:A:270:VAL:CG1	1:A:274:GLU:HB2	1.92	1.00
2:B:235:GLU:CG	2:B:235:GLU:OE2	2.11	0.98
2:D:133:ILE:HD12	2:D:150:ILE:HG12	1.47	0.97
2:B:297:ILE:O	2:B:301:THR:OG1	1.81	0.96
2:B:312:SER:O	9:B:601:HOH:O	1.82	0.95
5:C:501:NAG:O7	5:C:501:NAG:N2	2.02	0.92
7:A:510:CL:CL	9:A:601:HOH:O	2.27	0.88
2:D:133:ILE:HD12	2:D:150:ILE:CG1	2.05	0.86
1:C:333:THR:HG21	2:D:105:GLN:NE2	1.90	0.85
2:B:285:TRP:HB3	2:B:375:ARG:HH21	1.41	0.84
2:B:235:GLU:OE1	2:B:235:GLU:CG	2.25	0.83
1:A:68:ARG:HD3	9:A:657:HOH:O	1.82	0.80
2:D:133:ILE:CD1	2:D:150:ILE:HG12	2.15	0.76
2:D:56:LYS:CB	2:D:294:ARG:NH1	2.49	0.76
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.69	0.75
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.69	0.74
1:C:95:PRO:HB2	1:C:96:PRO:HD2	1.68	0.73
1:A:270:VAL:HG21	1:A:287:ILE:HD11	1.68	0.73
2:D:283:ASP:O	2:D:285:TRP:CD1	2.42	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2:NAG:O3	4:F:2:NAG:O7	2.05	0.72
1:A:95:PRO:HB2	1:A:96:PRO:HD2	1.72	0.72
2:D:50:ILE:HG23	2:D:293:VAL:HG21	1.72	0.71
2:B:305:SER:OG	9:B:602:HOH:O	2.07	0.70
1:A:270:VAL:HG12	1:A:271:GLY:N	2.07	0.70
2:D:334:MET:O	2:D:335:LEU:CB	2.39	0.70
2:B:73:MET:HG3	2:B:84:ARG:HG2	1.73	0.69
1:C:389:ASN:OD1	1:C:389:ASN:C	2.34	0.66
2:B:235:GLU:OE1	2:B:235:GLU:OE2	2.15	0.65
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.75	0.64
1:C:117:PRO:HA	1:C:136:SER:HB3	1.78	0.64
1:A:270:VAL:HG11	1:A:274:GLU:HB2	1.78	0.64
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.79	0.64
1:C:47:ASN:HA	9:C:602:HOH:O	1.99	0.62
2:B:133:ILE:HD12	2:B:150:ILE:HG12	1.80	0.62
2:D:332:SER:HB3	9:D:621:HOH:O	1.97	0.62
1:A:105:THR:HB	1:A:106:PRO:HD3	1.81	0.62
2:B:364:ILE:HD12	2:B:364:ILE:N	2.14	0.61
2:D:66:PRO:HB3	2:D:301:THR:HG21	1.83	0.60
1:C:285:ASP:O	9:C:601:HOH:O	2.15	0.59
2:B:54:HIS:CG	2:B:54:HIS:O	2.55	0.59
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.85	0.59
2:D:282:TYR:O	2:D:283:ASP:C	2.41	0.59
1:A:270:VAL:CG1	1:A:271:GLY:N	2.66	0.59
2:D:334:MET:O	2:D:335:LEU:HB2	2.03	0.58
2:B:289:LEU:N	2:B:290:PRO:HD2	2.19	0.58
1:A:356:THR:OG1	1:A:367:ARG:NH2	2.36	0.58
1:C:105:THR:HB	1:C:106:PRO:HD3	1.86	0.57
2:B:295:ASP:OD2	2:B:347:ARG:NH2	2.38	0.57
2:B:388:TYR:CD2	2:B:392:PRO:HG3	2.39	0.57
1:C:135:LEU:HD12	1:C:135:LEU:N	2.20	0.57
2:D:283:ASP:O	2:D:284:GLU:C	2.43	0.57
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.87	0.56
1:C:95:PRO:HB2	1:C:96:PRO:CD	2.34	0.56
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.35	0.56
1:C:228:LEU:HD23	1:C:229:LEU:HD12	1.88	0.55
1:C:338:THR:HG22	1:C:338:THR:O	2.05	0.55
1:A:338:THR:O	1:A:338:THR:HG22	2.06	0.55
1:A:293:ILE:O	1:A:294:ASN:HB2	2.07	0.55
1:C:343:LYS:O	1:C:347:MET:HG3	2.07	0.54
2:B:157:MET:HE3	2:B:229:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:O	2:B:317:PRO:HB3	2.08	0.54
1:C:293:ILE:O	1:C:294:ASN:HB2	2.07	0.54
1:C:95:PRO:CB	1:C:96:PRO:HD2	2.37	0.53
2:D:289:LEU:N	2:D:290:PRO:HD2	2.24	0.53
2:D:55:GLU:C	2:D:57:ASP:H	2.12	0.53
1:C:91:LEU:HD12	1:C:91:LEU:N	2.24	0.53
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.91	0.53
2:B:79:LYS:O	2:B:83:THR:HG23	2.09	0.53
1:A:64:SER:C	1:A:65:VAL:HG23	2.30	0.52
1:A:33:LEU:O	1:A:66:THR:HA	2.10	0.52
2:D:180:GLN:HG3	9:D:618:HOH:O	2.10	0.52
2:D:129:GLY:HA2	2:D:132:MET:HE3	1.91	0.52
1:C:135:LEU:HD11	8:D:503:HZ4:C14	2.40	0.51
1:A:270:VAL:CG1	1:A:274:GLU:CB	2.77	0.51
2:D:133:ILE:HG23	7:D:504:CL:CL	2.48	0.51
1:A:321:ASN:HD22	5:A:507:NAG:C7	2.22	0.51
1:A:270:VAL:CG1	1:A:271:GLY:H	2.23	0.51
1:C:389:ASN:HD22	1:C:394:ILE:HD11	1.75	0.51
2:D:230:LEU:HB3	2:D:258:VAL:HG12	1.91	0.51
1:A:117:PRO:HA	1:A:136:SER:HB3	1.93	0.50
2:B:230:LEU:HB3	2:B:258:VAL:HG12	1.94	0.50
2:B:318:LYS:N	2:B:318:LYS:HD3	2.26	0.50
2:B:40:ILE:HG21	2:B:73:MET:HE2	1.94	0.50
2:B:73:MET:HG2	7:B:504:CL:CL	2.48	0.50
1:C:110:THR:HA	8:D:503:HZ4:CL1	2.48	0.50
2:D:289:LEU:HB3	2:D:290:PRO:CD	2.41	0.50
1:A:105:THR:N	1:A:106:PRO:CD	2.74	0.50
1:C:308:VAL:HG11	1:C:359:ILE:HG21	1.93	0.50
2:D:379:TRP:CZ2	2:D:382:LYS:HA	2.46	0.50
2:B:364:ILE:N	2:B:364:ILE:CD1	2.74	0.50
2:B:175:TYR:HB2	8:B:503:HZ4:C24	2.42	0.49
1:C:30:GLY:HA2	1:C:63:THR:O	2.13	0.49
2:D:216:ILE:HD11	2:D:243:VAL:HG21	1.94	0.49
1:A:346:LEU:O	1:A:349:SER:HB2	2.12	0.49
2:B:283:ASP:O	2:B:284:GLU:C	2.50	0.49
1:C:333:THR:HG21	2:D:105:GLN:CD	2.32	0.49
1:A:395:GLN:NE2	7:A:510:CL:CL	2.78	0.49
1:A:70:ASN:OD1	1:A:70:ASN:C	2.50	0.49
2:D:260:SER:HB3	7:D:504:CL:CL	2.49	0.49
2:D:56:LYS:CB	2:D:294:ARG:HH12	2.23	0.49
1:C:273:ARG:HD3	9:C:622:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:MET:O	2:B:337:ARG:HG3	2.13	0.49
1:C:155:MET:HE1	1:C:184:LEU:HD21	1.93	0.49
2:D:40:ILE:HG21	2:D:73:MET:HE2	1.95	0.48
1:A:30:GLY:HA2	1:A:63:THR:O	2.13	0.48
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.49	0.48
2:B:159:ASN:ND2	2:B:379:TRP:CZ3	2.82	0.48
5:D:501:NAG:O7	5:D:501:NAG:C1	2.61	0.48
1:A:396:ASN:O	9:A:601:HOH:O	2.20	0.48
1:A:402:TRP:HB3	1:A:403:PRO:HD2	1.95	0.48
1:A:379:ASN:O	1:A:380:ARG:HB2	2.13	0.47
1:A:320:GLU:O	1:A:321:ASN:HB2	2.14	0.47
2:D:159:ASN:ND2	2:D:379:TRP:CZ3	2.83	0.47
1:C:138:LEU:HD12	1:C:138:LEU:N	2.30	0.47
1:C:167:VAL:HG22	1:C:243:SER:HB3	1.96	0.47
1:C:131:LYS:HE2	2:D:175:TYR:CZ	2.50	0.47
1:A:102:LEU:HD23	9:A:640:HOH:O	2.15	0.46
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.98	0.46
1:A:138:LEU:HD21	1:A:347:MET:HG2	1.97	0.46
1:C:105:THR:N	1:C:106:PRO:CD	2.79	0.46
1:C:142:PRO:HG3	1:C:370:ALA:CB	2.46	0.46
2:B:133:ILE:O	2:B:133:ILE:HG13	2.16	0.46
8:B:503:HZ4:C13	8:B:503:HZ4:C07	2.94	0.46
1:C:139:ARG:HD2	1:C:141:VAL:O	2.16	0.46
1:A:270:VAL:HG12	1:A:271:GLY:H	1.78	0.46
1:A:64:SER:O	1:A:65:VAL:HG23	2.16	0.46
4:F:2:NAG:HO3	4:F:2:NAG:C7	2.21	0.46
2:B:182:PHE:O	2:B:186:ILE:HG12	2.16	0.46
1:A:270:VAL:HG13	1:A:274:GLU:CB	2.44	0.46
2:B:289:LEU:HB3	2:B:290:PRO:CD	2.46	0.46
2:D:157:MET:HE2	2:D:229:LEU:HD13	1.97	0.46
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.96	0.45
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.51	0.45
1:A:154:MET:CE	1:A:158:PHE:HE2	2.29	0.45
2:B:119:THR:O	2:B:318:LYS:HE3	2.16	0.45
1:C:166:ILE:HD12	1:C:240:ILE:CG2	2.47	0.45
2:B:183:VAL:O	2:B:187:ARG:HG3	2.16	0.45
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.51	0.45
2:D:334:MET:O	2:D:335:LEU:HB3	2.15	0.45
2:B:363:VAL:HG11	2:B:375:ARG:HG2	1.98	0.45
1:C:262:THR:HB	1:C:284:PRO:HB3	1.97	0.45
2:D:297:ILE:O	2:D:301:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:O	2:D:142:MET:CE	2.64	0.45
2:B:307:MET:SD	2:B:315:PRO:HD3	2.57	0.45
1:A:95:PRO:CB	1:A:96:PRO:CD	2.94	0.45
1:A:139:ARG:HD2	1:A:141:VAL:O	2.17	0.44
2:D:289:LEU:HB3	2:D:290:PRO:HD3	2.00	0.44
1:C:29:ILE:HG22	1:C:42:PHE:HZ	1.82	0.44
2:B:388:TYR:CD2	2:B:392:PRO:CG	3.01	0.44
1:C:135:LEU:CD1	1:C:135:LEU:H	2.31	0.44
1:C:228:LEU:CD2	1:C:229:LEU:HD12	2.48	0.44
1:C:304:ASP:O	1:C:308:VAL:HG13	2.17	0.44
1:C:70:ASN:C	1:C:70:ASN:OD1	2.55	0.44
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.51	0.44
2:B:55:GLU:C	2:B:57:ASP:H	2.21	0.44
2:D:182:PHE:O	2:D:186:ILE:HG12	2.18	0.44
2:D:73:MET:HG3	2:D:84:ARG:HG2	1.99	0.44
2:B:95:GLN:NE2	2:B:315:PRO:O	2.51	0.43
2:B:66:PRO:HD3	2:B:301:THR:HG21	2.00	0.43
1:C:135:LEU:CD1	1:C:135:LEU:N	2.82	0.43
1:C:302:ILE:O	1:C:306:VAL:HG23	2.19	0.43
1:C:135:LEU:HD12	1:C:135:LEU:H	1.84	0.43
2:B:379:TRP:CZ2	2:B:382:LYS:HA	2.53	0.43
1:C:402:TRP:HB3	1:C:403:PRO:HD2	2.00	0.43
2:B:150:ILE:HD13	2:B:178:GLY:HA3	2.00	0.43
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.79	0.43
2:D:133:ILE:HG13	2:D:133:ILE:O	2.19	0.43
2:B:60:HIS:CE1	2:B:66:PRO:HG3	2.54	0.43
2:D:129:GLY:HA2	2:D:132:MET:CE	2.49	0.43
2:B:368:ASN:OD1	2:B:368:ASN:C	2.57	0.42
2:D:260:SER:HA	2:D:280:VAL:O	2.19	0.42
1:C:124:ARG:NH2	9:C:604:HOH:O	2.41	0.42
1:C:47:ASN:OD1	9:C:602:HOH:O	2.21	0.42
2:D:114:PHE:O	2:D:118:GLN:HG2	2.19	0.42
1:C:103:THR:HB	1:C:104:PRO:HD2	2.02	0.42
2:D:68:VAL:HG21	2:D:297:ILE:HD13	2.02	0.42
2:D:388:TYR:CE2	2:D:392:PRO:HG2	2.55	0.42
1:A:57:LYS:HG2	1:A:58:ILE:HG23	2.00	0.42
1:A:68:ARG:CD	9:A:657:HOH:O	2.52	0.42
1:C:92:VAL:HG21	1:C:107:ILE:HG21	2.02	0.42
1:C:138:LEU:HD21	1:C:347:MET:HG2	2.02	0.42
1:A:114:TYR:O	1:A:115:ARG:HB2	2.20	0.42
2:B:133:ILE:CD1	2:B:150:ILE:HG12	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:O	1:C:81:ASP:HB2	2.20	0.42
2:D:376:VAL:O	2:D:376:VAL:CG1	2.67	0.41
1:A:270:VAL:HG11	1:A:274:GLU:CB	2.49	0.41
2:B:285:TRP:HB3	2:B:375:ARG:NH2	2.22	0.41
2:D:84:ARG:O	2:D:88:LEU:HG	2.20	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.86	0.41
1:C:144:TYR:CD2	1:C:273:ARG:HD2	2.56	0.41
2:D:391:TRP:HA	2:D:392:PRO:HD3	1.81	0.41
1:A:223:LYS:NZ	9:A:608:HOH:O	2.49	0.41
2:D:214:SER:HA	9:D:604:HOH:O	2.19	0.41
1:A:396:ASN:OD1	1:A:396:ASN:C	2.59	0.41
2:D:132:MET:O	2:D:133:ILE:C	2.58	0.41
2:D:88:LEU:O	2:D:94:ILE:HD13	2.21	0.41
1:A:241:ILE:HA	1:A:269:LEU:O	2.20	0.41
1:A:65:VAL:HG13	1:A:68:ARG:HH12	1.86	0.41
2:B:35:ILE:HG23	2:B:64:VAL:HG11	2.03	0.41
2:B:391:TRP:CD2	2:B:392:PRO:HD2	2.56	0.41
2:D:216:ILE:HG13	2:D:217:GLN:N	2.36	0.41
2:D:368:ASN:OD1	2:D:368:ASN:C	2.59	0.41
1:A:229:LEU:CD1	1:A:255:SER:HB2	2.50	0.41
1:A:344:ARG:NH1	1:A:344:ARG:HG3	2.36	0.41
1:C:333:THR:CG2	1:C:333:THR:O	2.69	0.41
2:D:195:VAL:HG12	2:D:196:GLY:N	2.36	0.41
1:C:242:LEU:HB3	1:C:270:VAL:HG12	2.03	0.40
1:A:216:LEU:CD1	1:A:232:ALA:HB2	2.50	0.40
1:A:65:VAL:HG12	1:A:66:THR:O	2.22	0.40
2:B:68:VAL:HG11	2:B:297:ILE:HD13	2.03	0.40
2:B:132:MET:O	2:B:133:ILE:C	2.60	0.40
1:C:264:ALA:HA	1:C:403:PRO:O	2.22	0.40
2:D:381:ASP:C	2:D:383:SER:H	2.25	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
1	C	351/385 (91%)	334 (95%)	15 (4%)	2 (1%)	25	48
2	B	361/363 (99%)	340 (94%)	21 (6%)	0	100	100
2	D	361/363 (99%)	337 (93%)	20 (6%)	4 (1%)	14	32
All	All	1425/1496 (95%)	1348 (95%)	71 (5%)	6 (0%)	34	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	283	ASP
2	D	284	GLU
2	D	335	LEU
2	D	56	LYS
1	C	96	PRO
1	C	95	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	289/331 (87%)	280 (97%)	9 (3%)	40	68
1	C	276/331 (83%)	269 (98%)	7 (2%)	47	75
2	B	288/326 (88%)	278 (96%)	10 (4%)	36	63
2	D	277/326 (85%)	270 (98%)	7 (2%)	47	75
All	All	1130/1314 (86%)	1097 (97%)	33 (3%)	42	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	146	HIS
1	A	238	ARG
1	A	285	ASP
1	A	347	MET
1	A	367	ARG
1	A	391	SER
1	A	398	ARG
2	B	62	LEU
2	B	134	MET
2	B	139	GLU
2	B	155	SER
2	B	188	SER
2	B	301	THR
2	B	305	SER
2	B	337	ARG
2	B	357	GLN
2	B	393	ARG
1	C	48	GLN
1	C	94	HIS
1	C	118	VAL
1	C	131	LYS
1	C	146	HIS
1	C	153	GLU
1	C	383	VAL
2	D	58	ASP
2	D	73	MET
2	D	155	SER
2	D	216	ILE
2	D	305	SER
2	D	309	SER
2	D	374	GLU

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

Mol	Chain	Res	Type
2	B	192	ASN
1	C	28	ASN
1	C	86	GLN
1	C	334	ASN
2	D	54	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 ⓘ

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	0.31	0	17,19,21	0.74	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.80	0
3	BMA	E	3	3	11,11,12	0.24	0	15,15,17	0.93	2 (13%)
3	MAN	E	4	3	11,11,12	0.26	0	15,15,17	0.70	0
3	MAN	E	5	3	11,11,12	0.27	0	15,15,17	0.82	0
4	NAG	F	1	1,4	14,14,15	0.33	0	17,19,21	0.70	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.73	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	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	E	3	BMA	C1-C2-C3	2.19	112.36	109.67
3	E	3	BMA	O5-C5-C6	2.15	110.57	107.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

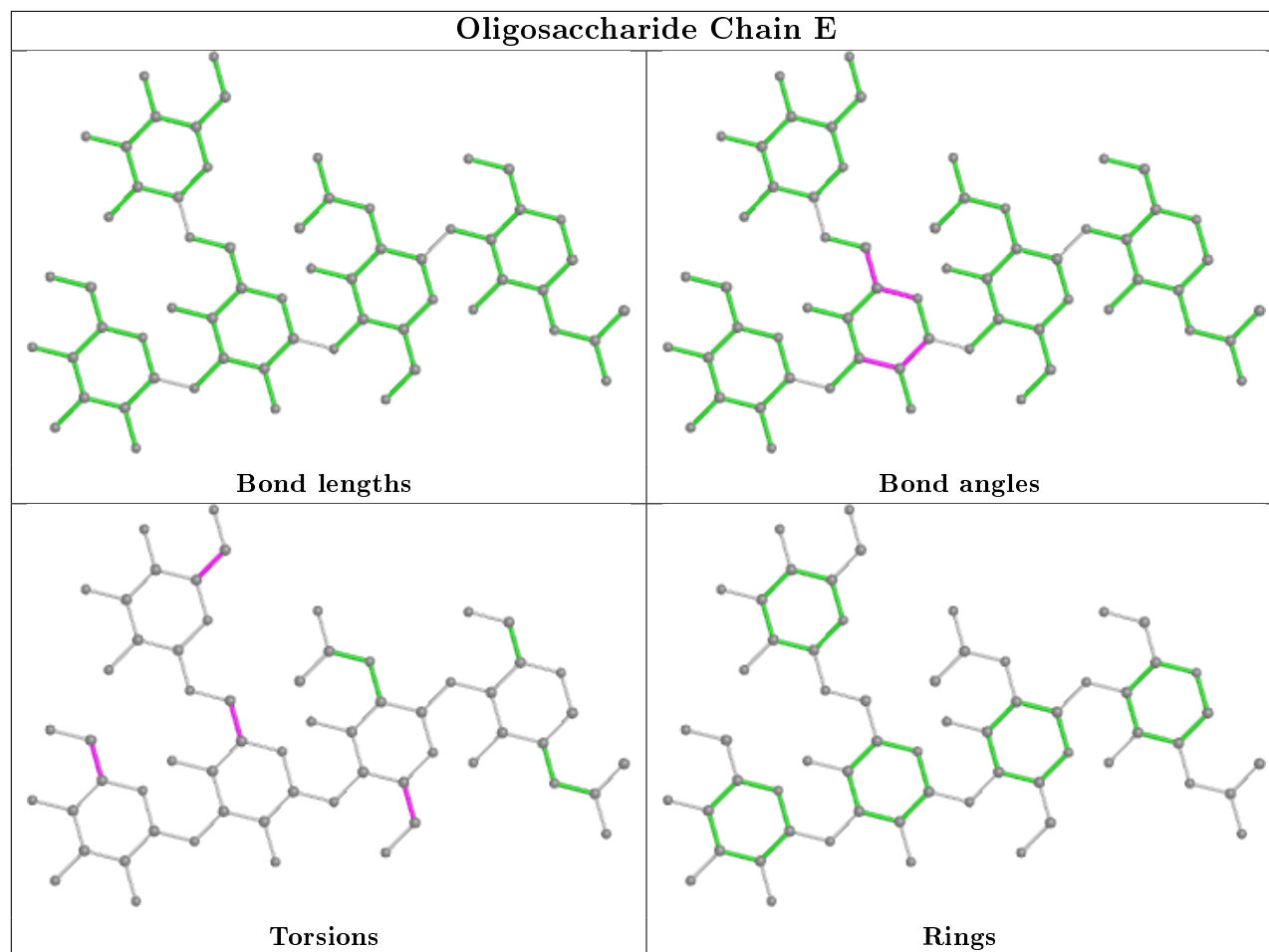
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7

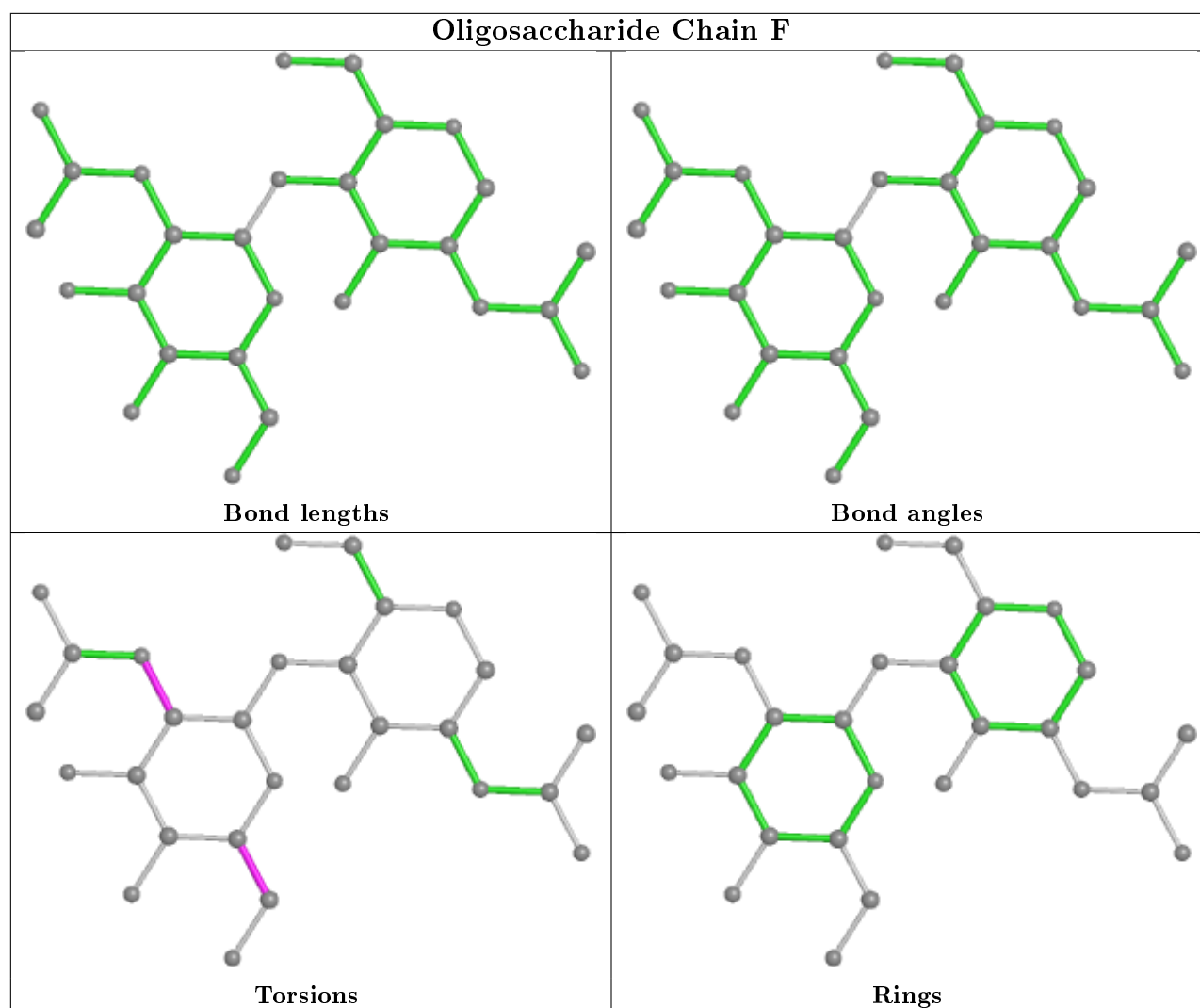
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	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 oligosaccharide.





## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 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	$\# Z  > 2$
5	NAG	A	507	1	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
5	NAG	C	504	1	14,14,15	0.29	0	17,19,21	0.60	0
5	NAG	B	502	2	14,14,15	0.30	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	502	2	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	B	501	2	14,14,15	0.26	0	17,19,21	0.69	0
5	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.67	0
5	NAG	D	501	2	14,14,15	0.63	0	17,19,21	2.38	3 (17%)
8	HZ4	D	503	-	30,30,30	2.23	7 (23%)	41,41,41	2.12	4 (9%)
8	HZ4	B	503	-	30,30,30	2.20	7 (23%)	41,41,41	2.11	3 (7%)
5	NAG	C	501	1	11,11,15	0.37	0	12,15,21	0.56	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	507	1	-	0/6/23/26	0/1/1/1
5	NAG	C	504	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	502	2	-	4/6/23/26	0/1/1/1
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	2	-	1/6/23/26	0/1/1/1
8	HZ4	D	503	-	-	6/21/21/21	0/2/2/2
8	HZ4	B	503	-	-	3/21/21/21	0/2/2/2
5	NAG	C	501	1	-	2/2/19/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	HZ4	S23-N22	8.20	1.74	1.63
8	B	503	HZ4	S23-N22	8.00	1.74	1.63
8	B	503	HZ4	C24-S23	3.65	1.84	1.75
8	D	503	HZ4	C24-S23	3.61	1.83	1.75
8	D	503	HZ4	C04-CL1	3.07	1.80	1.73
8	D	503	HZ4	C19-N22	3.03	1.48	1.43
8	B	503	HZ4	C19-N22	2.99	1.47	1.43
8	B	503	HZ4	C04-CL1	2.98	1.80	1.73
8	B	503	HZ4	O25-S23	2.92	1.48	1.43
8	D	503	HZ4	O25-S23	2.84	1.48	1.43
8	D	503	HZ4	C03-CL2	2.43	1.79	1.73
8	B	503	HZ4	C03-CL2	2.41	1.79	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	HZ4	O27-C13	-2.08	1.37	1.43
8	D	503	HZ4	O27-C13	-2.03	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	HZ4	O26-S23-O25	-12.02	101.57	118.85
8	B	503	HZ4	O26-S23-O25	-11.80	101.89	118.85
5	D	501	NAG	C1-O5-C5	8.39	123.56	112.19
8	B	503	HZ4	C24-S23-N22	3.37	110.47	106.63
8	D	503	HZ4	C24-S23-N22	3.23	110.31	106.63
5	D	501	NAG	C1-C2-N2	3.17	115.90	110.49
5	A	507	NAG	C1-O5-C5	-2.10	109.35	112.19
8	B	503	HZ4	C14-O15-C16	-2.09	113.49	117.93
8	D	503	HZ4	O26-S23-N22	2.03	111.23	107.10
8	D	503	HZ4	O25-S23-N22	2.01	111.20	107.10
5	D	501	NAG	O5-C1-C2	2.00	114.45	111.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	NAG	C1-C2-N2-C7
8	D	503	HZ4	N09-C12-C13-C14
5	C	501	NAG	O5-C5-C6-O6
5	D	502	NAG	O5-C5-C6-O6
5	C	501	NAG	C4-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6
5	B	502	NAG	C8-C7-N2-C2
5	B	502	NAG	O7-C7-N2-C2
5	D	502	NAG	C8-C7-N2-C2
5	D	502	NAG	O7-C7-N2-C2
5	C	504	NAG	O5-C5-C6-O6
8	D	503	HZ4	N09-C12-C13-O27
8	B	503	HZ4	O27-C13-C14-O15
5	C	504	NAG	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
8	B	503	HZ4	C06-C07-C08-N09
8	D	503	HZ4	C11-C10-N09-C12
8	D	503	HZ4	C05-C06-C07-C08
8	D	503	HZ4	C01-C06-C07-C08
5	A	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	D	503	HZ4	C11-C10-N09-C08
8	B	503	HZ4	C13-C12-N09-C10

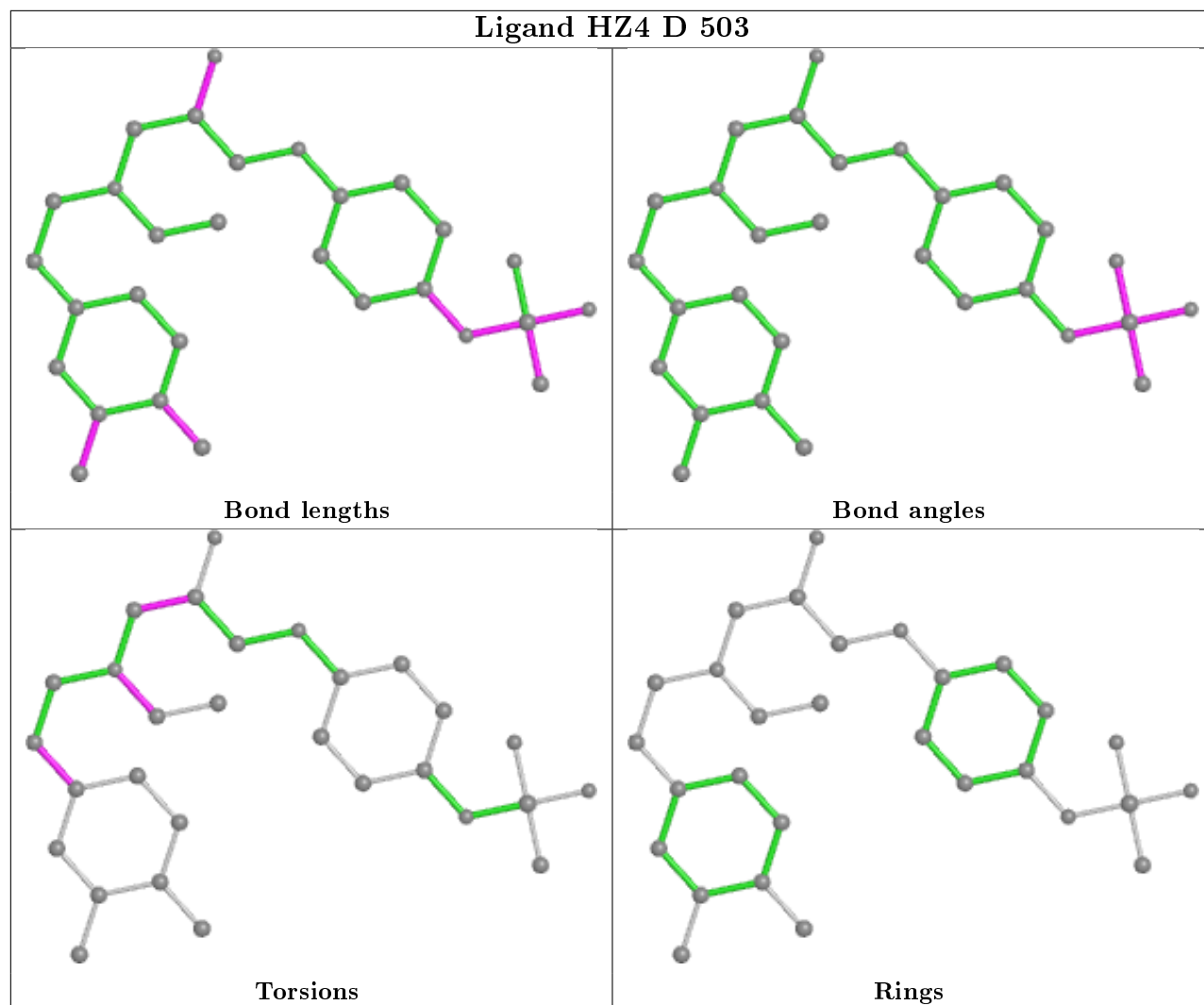
There are no ring outliers.

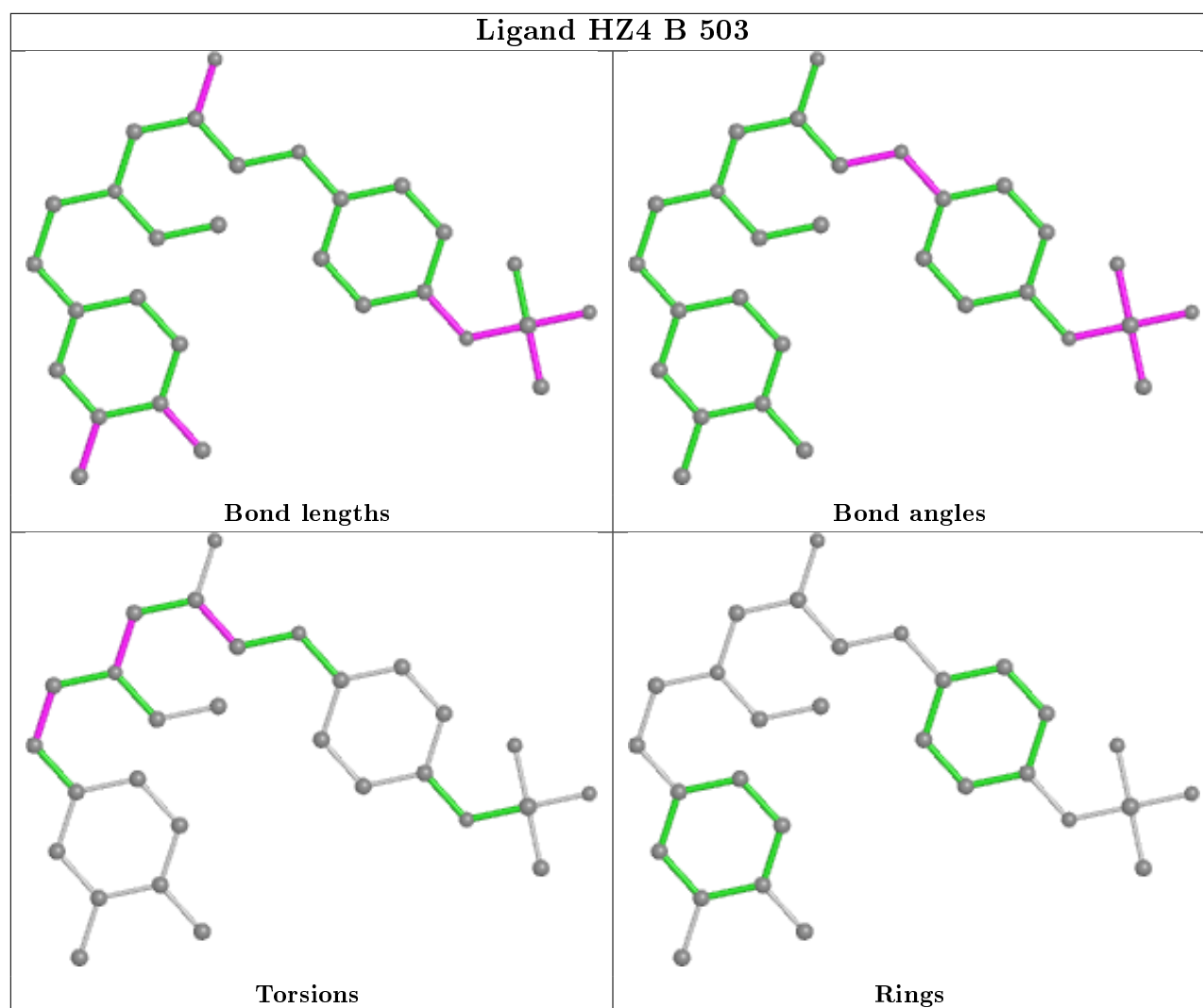
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	NAG	1	0
5	D	501	NAG	1	0
8	D	503	HZ4	2	0
8	B	503	HZ4	2	0
5	C	501	NAG	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.

## Ligand HZ4 D 503





## 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%)	-0.15	8 (2%) 62 63	37, 54, 92, 153	0
1	C	357/385 (92%)	0.18	19 (5%) 26 25	57, 85, 119, 164	0
2	B	363/363 (100%)	0.07	12 (3%) 46 47	39, 72, 123, 169	0
2	D	363/363 (100%)	0.09	16 (4%) 34 33	56, 81, 139, 181	0
All	All	1441/1496 (96%)	0.05	55 (3%) 40 40	37, 75, 121, 181	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	GLY	5.5
1	A	101	HIS	4.0
2	B	54	HIS	3.6
1	C	101	HIS	3.6
2	D	381	ASP	3.6
2	B	48	VAL	3.6
2	D	194	PHE	3.5
1	A	102	LEU	3.4
1	A	96	PRO	3.3
2	D	346	GLY	3.2
1	C	96	PRO	3.2
2	D	344	PHE	3.0
1	C	259	LEU	2.9
2	D	58	ASP	2.8
2	D	52	ASP	2.8
2	D	195	VAL	2.7
2	D	348	ASP	2.7
1	A	119	ILE	2.7
2	B	58	ASP	2.7
2	D	287	TYR	2.6
1	A	97	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	259	PRO	2.6
1	C	58	ILE	2.6
2	B	49	ALA	2.6
1	C	59	GLN	2.6
1	C	404	GLY	2.6
2	D	380	LYS	2.5
2	D	192	ASN	2.5
1	C	394	ILE	2.5
1	C	169	ASP	2.5
2	D	347	ARG	2.5
1	C	258	MET	2.5
2	B	131	SER	2.4
1	C	405	GLY	2.4
2	B	60	HIS	2.4
2	B	258	VAL	2.4
2	D	285	TRP	2.4
1	C	219	GLU	2.3
1	C	241	ILE	2.3
1	C	24	PRO	2.3
1	C	270	VAL	2.3
2	B	260	SER	2.3
1	C	269	LEU	2.3
2	B	55	GLU	2.2
2	D	48	VAL	2.2
1	C	119	ILE	2.2
1	A	89	ALA	2.2
1	A	270	VAL	2.1
1	C	136	SER	2.1
1	C	23	ASP	2.1
2	D	257	ILE	2.1
2	B	52	ASP	2.1
2	D	57	ASP	2.0
1	C	26	ILE	2.0
2	B	381	ASP	2.0

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

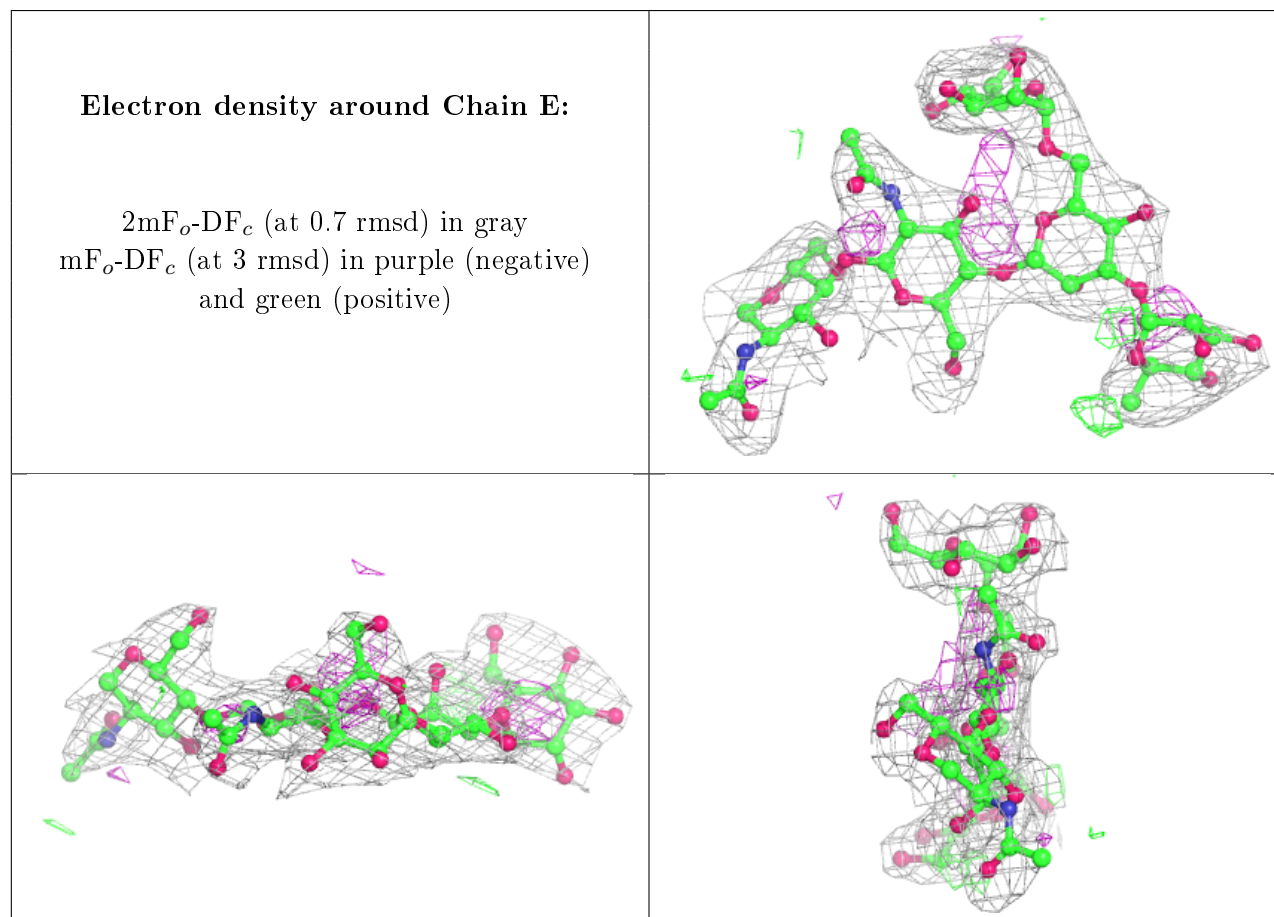
There are no non-standard protein/DNA/RNA residues in this entry.

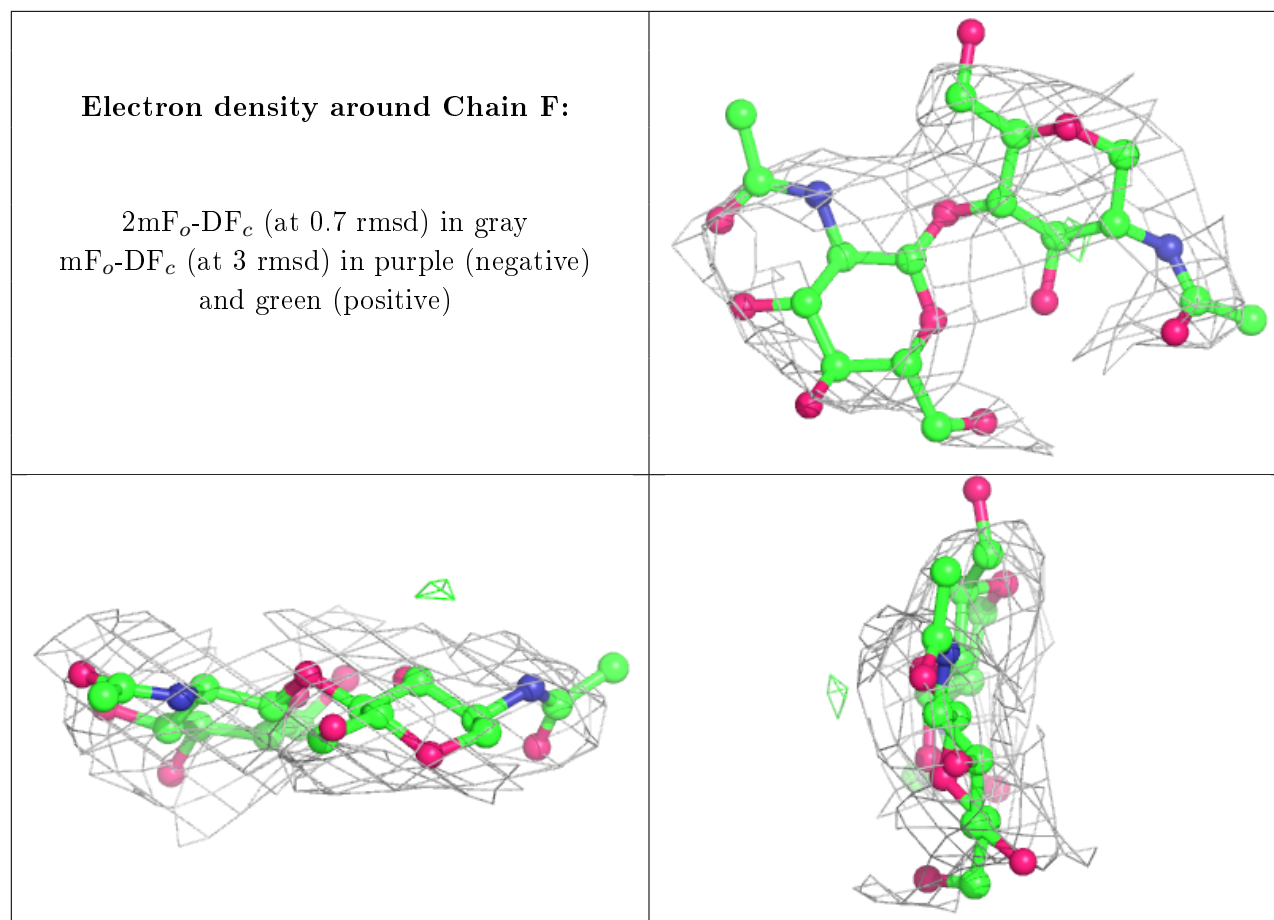
## 6.3 Carbohydrates ⓘ

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	0.71	0.33	119,135,144,145	0
4	NAG	F	2	14/15	0.78	0.38	142,156,165,169	0
4	NAG	F	1	14/15	0.90	0.31	120,136,152,155	0
3	NAG	E	2	14/15	0.92	0.29	69,75,94,104	0
3	MAN	E	5	11/12	0.94	0.29	75,81,92,93	0
3	BMA	E	3	11/12	0.94	0.27	84,91,105,129	0
3	NAG	E	1	14/15	0.94	0.23	67,69,76,81	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	D	501	14/15	0.57	0.34	131,150,167,171	0
5	NAG	A	507	14/15	0.61	0.46	111,153,174,181	0
5	NAG	C	504	14/15	0.64	0.41	140,153,166,169	0
5	NAG	D	502	14/15	0.73	0.40	125,143,153,154	0
5	NAG	B	501	14/15	0.74	0.27	104,125,129,134	0
5	NAG	B	502	14/15	0.80	0.27	145,158,172,179	0
7	CL	D	505	1/1	0.84	0.78	113,113,113,113	0
7	CL	B	505	1/1	0.88	0.71	82,82,82,82	0
7	CL	D	504	1/1	0.89	0.25	100,100,100,100	0
7	CL	C	506	1/1	0.91	0.16	84,84,84,84	0
7	CL	A	509	1/1	0.91	0.21	91,91,91,91	0
7	CL	B	504	1/1	0.92	0.27	98,98,98,98	0

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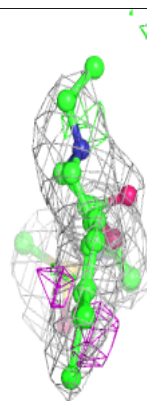
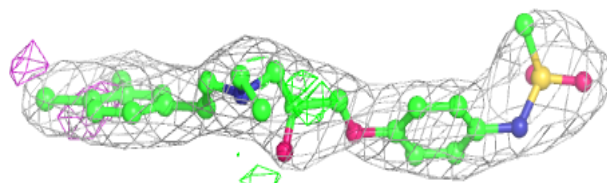
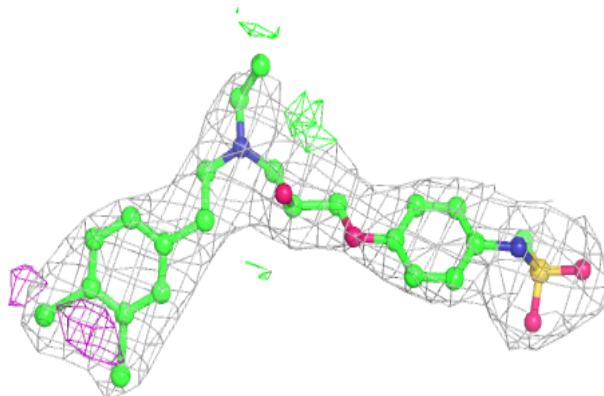
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	501	13/15	0.92	0.24	78,99,114,135	0
5	NAG	A	501	14/15	0.93	0.24	54,78,92,94	0
7	CL	B	506	1/1	0.95	0.14	101,101,101,101	0
8	HZ4	D	503	29/29	0.96	0.16	44,66,96,98	0
6	NA	C	505	1/1	0.97	0.09	60,60,60,60	0
6	NA	A	508	1/1	0.98	0.19	48,48,48,48	0
8	HZ4	B	503	29/29	0.98	0.15	38,50,63,83	0
7	CL	A	510	1/1	0.98	0.10	81,81,81,81	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.

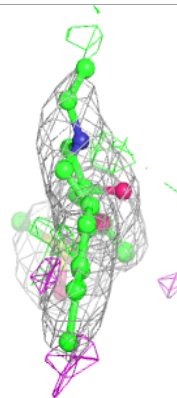
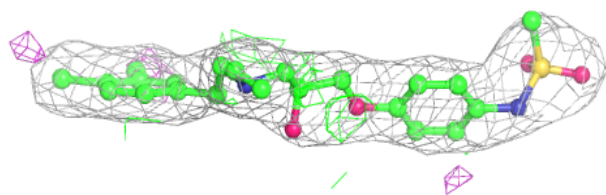
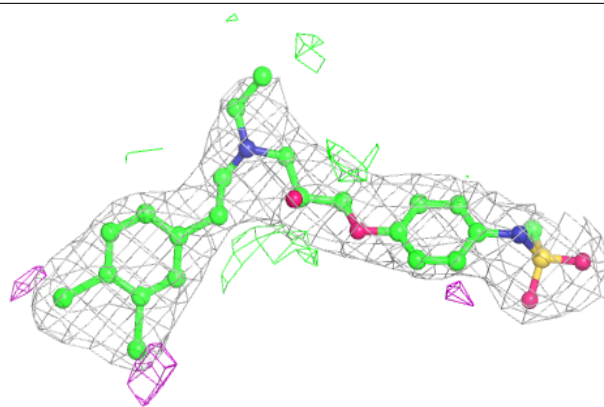
**Electron density around HZ4 D 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HZ4 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.