



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:43 PM UTC

PDB ID : 6E7U / pdb_00006e7u
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-31
Authors : Regan, M.C.; Furukawa, H.
Deposited on : 2018-07-27
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

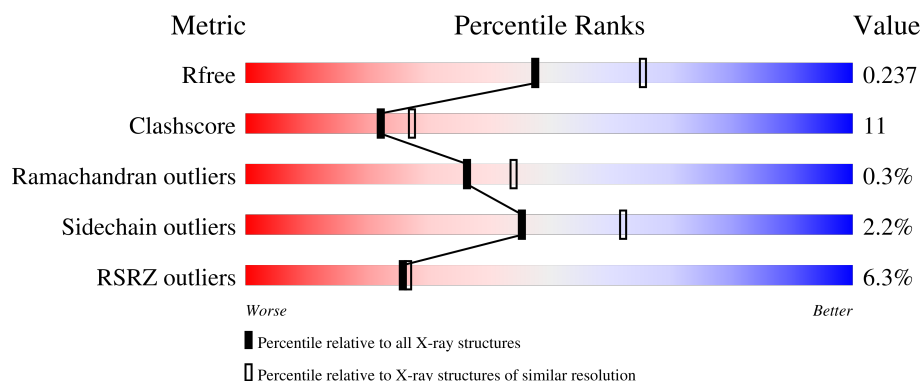
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	385	2% 77% 16% 7%
1	C	385	4% 72% 19% 7%
2	B	363	7% 84% 14% ..
2	D	363	10% 82% 17% ..
3	E	5	100%

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
6	CL	A	509	-	-	X	-
6	CL	D	406	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11538 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

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

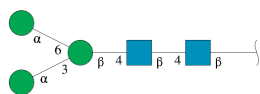
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

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

There are 2 discrepancies between the modelled and reference sequences:

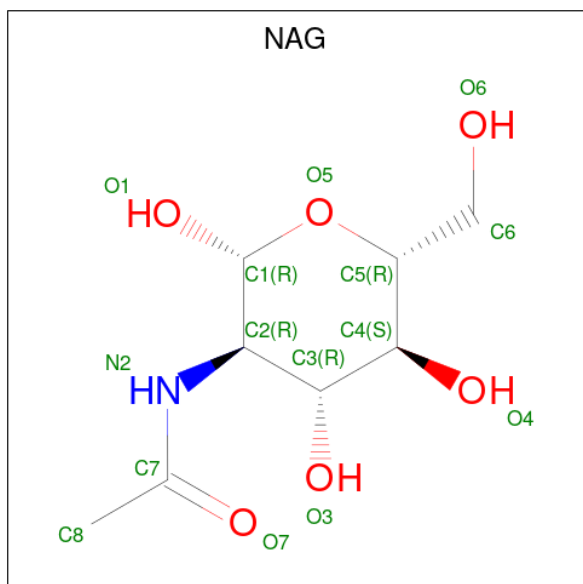
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	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
			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		

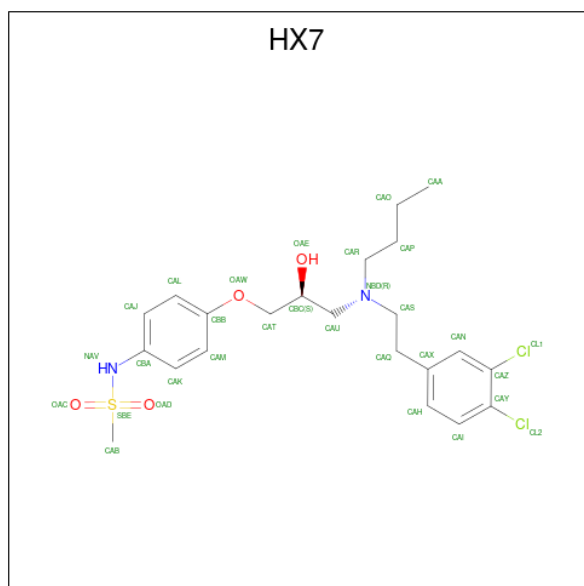
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

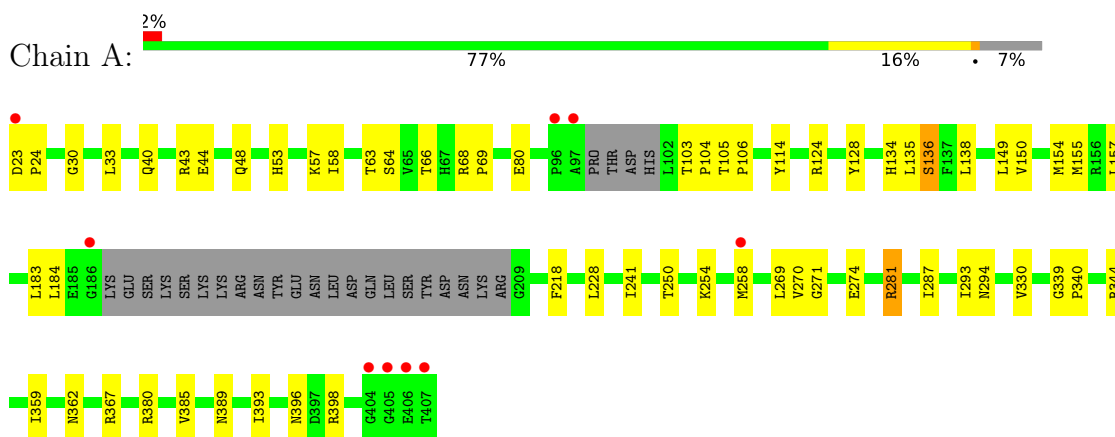
- Molecule 8 is water.

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

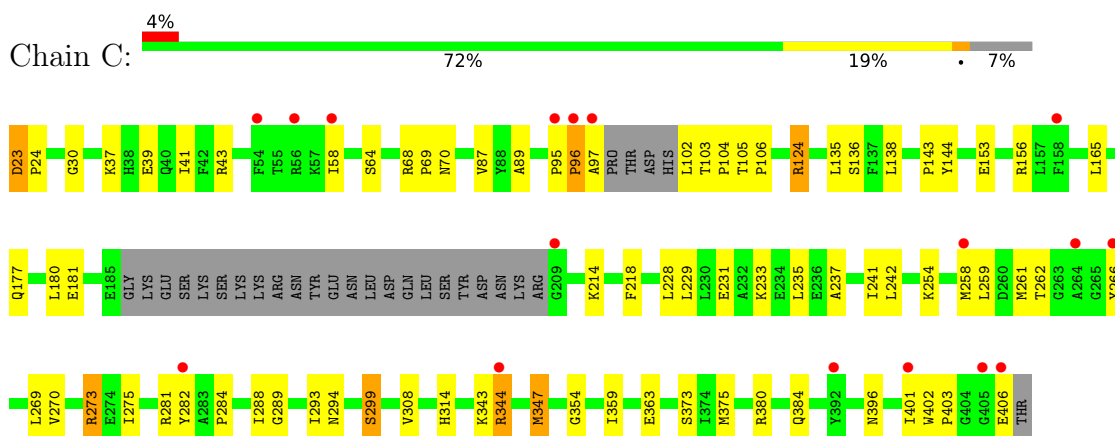
3 Residue-property plots [i](#)

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.

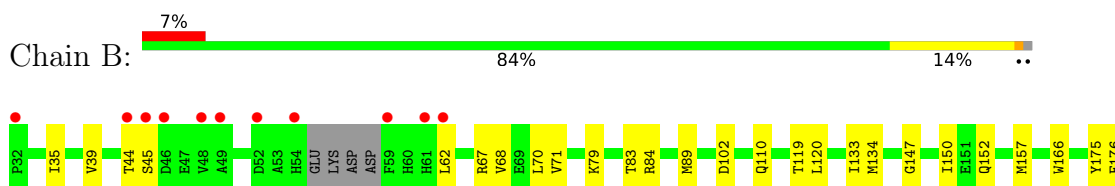
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

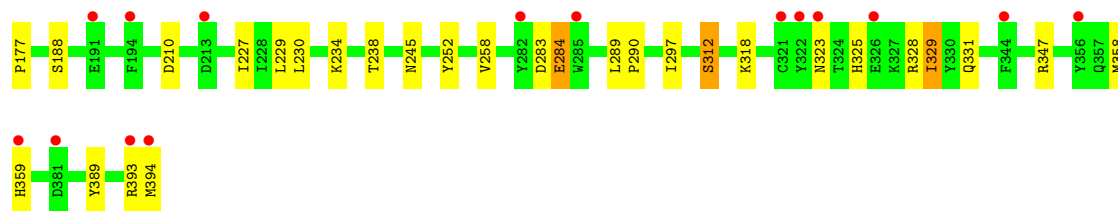


- Molecule 1: Glutamate receptor ionotropic, NMDA 1

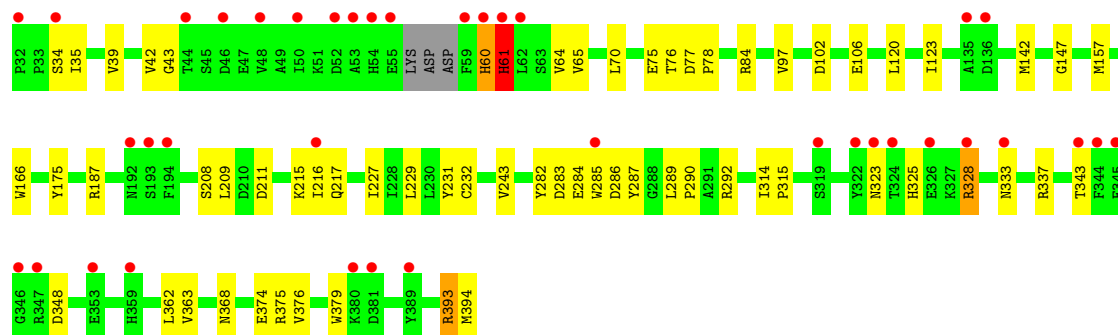
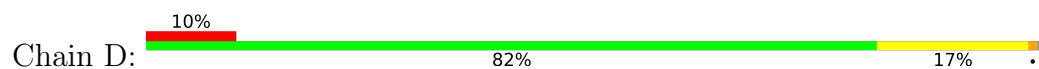


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

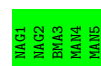




● Molecule 2: Glutamate receptor ionotropic, NMDA 2B



● 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, α , β , γ	268.62Å 59.59Å 145.91Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	25.00 – 2.27 25.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	82.0 (25.00-2.27) 82.3 (25.00-2.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.237 0.207 , 0.237	Depositor DCC
R_{free} test set	3929 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MAN, HX7, BMA, NAG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2822	0.62	0/3834
1	C	0.43	0/2783	0.63	0/3783
2	B	0.44	0/2838	0.64	0/3871
2	D	0.41	0/2781	0.65	0/3797
All	All	0.44	0/11224	0.63	0/15285

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

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

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2765	0	2731	52	0
1	C	2728	0	2694	65	2
2	B	2771	0	2637	51	2
2	D	2720	0	2563	60	0
3	E	61	0	52	0	0
4	A	14	0	13	0	0
4	B	28	0	26	3	0
4	C	28	0	26	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	3	0
6	B	4	0	0	2	0
6	C	2	0	0	0	0
6	D	4	0	0	3	0
7	B	31	0	0	4	0
7	D	31	0	0	5	0
8	A	135	0	0	5	0
8	B	76	0	0	8	0
8	C	75	0	0	4	0
8	D	47	0	0	3	0
All	All	11538	0	10755	233	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:ASP:O	2:D:285:TRP:HD1	1.12	1.30
2:D:283:ASP:O	2:D:285:TRP:CD1	1.93	1.21
1:C:237:ALA:O	8:C:601:HOH:O	1.70	1.07
1:C:229:LEU:HB3	1:C:261:MET:HE1	1.38	1.05
1:A:270:VAL:CG1	1:A:274:GLU:HB2	1.89	1.02
1:C:41:ILE:HD13	1:C:299:SER:OG	1.73	0.88
6:D:406:CL:CL	8:D:513:HOH:O	2.32	0.84
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.60	0.83
2:B:157:MET:HE3	2:B:229:LEU:HD22	1.63	0.80
2:D:120:LEU:C	2:D:142:MET:HE2	2.08	0.78
1:A:270:VAL:CG1	1:A:274:GLU:CB	2.62	0.77
2:D:120:LEU:C	2:D:142:MET:CE	2.59	0.76
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.66	0.75
2:B:312:SER:O	8:B:601:HOH:O	2.03	0.75
2:D:314:ILE:HB	2:D:315:PRO:HD2	1.69	0.74
6:B:507:CL:CL	8:B:669:HOH:O	2.42	0.74
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.23	0.74
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.69	0.73
1:C:23:ASP:N	1:C:24:PRO:CD	2.52	0.72
1:A:270:VAL:HG11	1:A:274:GLU:HB2	1.72	0.72
2:B:234:LYS:O	2:B:238:THR:HG23	1.90	0.71
6:D:406:CL:CL	8:D:533:HOH:O	2.45	0.71
1:C:262:THR:HB	1:C:284:PRO:HB3	1.72	0.71
1:A:44:GLU:O	1:A:48:GLN:HG3	1.90	0.71
2:D:60:HIS:O	2:D:61:HIS:CB	2.38	0.71
2:B:133:ILE:HD12	2:B:150:ILE:CG1	2.20	0.70
7:B:503:HX7:OAE	7:B:503:HX7:CAR	2.39	0.70
4:B:502:NAG:H2	4:B:502:NAG:H61	1.73	0.70
2:D:343:THR:HG22	2:D:348:ASP:HA	1.72	0.70
7:D:402:HX7:OAE	7:D:402:HX7:CAR	2.39	0.70
1:A:135:LEU:C	1:A:135:LEU:HD12	2.16	0.70
2:B:157:MET:CE	2:B:229:LEU:HD22	2.22	0.69
1:A:136:SER:HB3	8:A:626:HOH:O	1.93	0.69
2:D:285:TRP:CZ3	2:D:286:ASP:HB2	2.27	0.69
1:A:57:LYS:HG2	1:A:58:ILE:HG23	1.73	0.69
2:B:318:LYS:HD2	2:B:331:GLN:OE1	1.93	0.69
1:A:270:VAL:HG12	1:A:274:GLU:HB2	1.74	0.68
2:B:331:GLN:O	8:B:602:HOH:O	2.13	0.67
7:D:402:HX7:CAQ	7:D:402:HX7:CBC	2.73	0.65
7:B:503:HX7:CAQ	7:B:503:HX7:CBC	2.72	0.65
1:A:398:ARG:O	6:A:509:CL:CL	2.52	0.65
1:C:96:PRO:O	1:C:97:ALA:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:368:ASN:HA	2:D:394:MET:HE2	1.80	0.64
1:A:80:GLU:HG3	2:B:79:LYS:HE2	1.79	0.64
1:C:135:LEU:C	1:C:135:LEU:HD12	2.21	0.64
2:D:285:TRP:CE3	2:D:286:ASP:HB2	2.33	0.64
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.79	0.63
1:A:218:PHE:HB3	1:A:228:LEU:CD1	2.28	0.63
2:D:75:GLU:OE2	2:D:75:GLU:HA	1.98	0.63
2:D:368:ASN:HA	2:D:394:MET:CE	2.30	0.62
2:D:35:ILE:HG13	2:D:35:ILE:O	1.99	0.61
1:A:270:VAL:HG11	1:A:274:GLU:CB	2.26	0.61
2:B:283:ASP:O	2:B:284:GLU:C	2.42	0.61
1:A:270:VAL:HG21	1:A:287:ILE:HD11	1.84	0.60
1:A:270:VAL:HG12	1:A:271:GLY:N	2.15	0.60
1:A:157:LEU:O	8:A:601:HOH:O	2.17	0.60
1:A:396:ASN:O	6:A:509:CL:CL	2.57	0.60
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.83	0.60
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.33	0.60
2:B:79:LYS:O	2:B:83:THR:HG23	2.02	0.59
2:B:39:VAL:HB	2:B:70:LEU:HD23	1.83	0.59
2:D:286:ASP:OD1	2:D:375:ARG:NH2	2.36	0.59
1:C:136:SER:HB3	8:C:650:HOH:O	2.02	0.59
2:D:328:ARG:CZ	2:D:328:ARG:HB3	2.32	0.59
1:C:23:ASP:N	1:C:24:PRO:HD2	2.18	0.58
1:A:103:THR:HB	1:A:104:PRO:HD2	1.84	0.58
2:D:216:ILE:HD11	2:D:243:VAL:HG21	1.86	0.57
2:B:133:ILE:HD12	2:B:150:ILE:HG12	1.85	0.57
1:C:259:LEU:HD12	1:C:261:MET:CE	2.35	0.57
2:D:39:VAL:HB	2:D:70:LEU:HD23	1.85	0.57
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.86	0.56
1:C:68:ARG:HB3	1:C:69:PRO:HD2	1.87	0.56
1:C:135:LEU:HD23	7:D:402:HX7:CAM	2.35	0.56
2:D:157:MET:CE	2:D:229:LEU:HD22	2.33	0.56
2:D:285:TRP:CD1	2:D:285:TRP:N	2.72	0.56
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.40	0.56
2:D:285:TRP:CG	2:D:286:ASP:H	2.23	0.56
1:C:41:ILE:CD1	1:C:299:SER:OG	2.52	0.56
1:C:229:LEU:HB3	1:C:261:MET:CE	2.26	0.56
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.88	0.55
2:D:376:VAL:HG12	2:D:376:VAL:O	2.06	0.55
2:B:133:ILE:HG23	6:B:504:CL:CL	2.43	0.55
1:C:344:ARG:HG3	1:C:344:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:MET:HE1	2:D:229:LEU:HB3	1.88	0.55
2:B:133:ILE:CD1	2:B:150:ILE:HG12	2.37	0.54
1:C:396:ASN:C	1:C:396:ASN:OD1	2.50	0.54
2:B:89:MET:HE3	2:B:318:LYS:HB2	1.90	0.54
1:C:344:ARG:HG3	1:C:344:ARG:NH1	2.21	0.54
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.23	0.54
2:B:120:LEU:O	2:B:318:LYS:HE3	2.08	0.54
1:A:103:THR:HB	1:A:104:PRO:CD	2.38	0.53
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.73	0.53
1:C:135:LEU:HD23	7:D:402:HX7:CBB	2.39	0.53
1:C:58:ILE:HD11	1:C:314:HIS:CD2	2.44	0.53
1:C:254:LYS:HE2	1:C:282:TYR:CE2	2.44	0.53
2:D:289:LEU:N	2:D:290:PRO:CD	2.72	0.53
2:D:157:MET:CE	2:D:229:LEU:HD13	2.39	0.52
1:C:30:GLY:N	1:C:87:VAL:CG2	2.72	0.52
1:A:105:THR:N	1:A:106:PRO:CD	2.72	0.52
1:A:149:LEU:HD23	1:A:183:LEU:HD11	1.90	0.52
2:D:157:MET:HE2	2:D:229:LEU:HD13	1.91	0.52
2:B:67:ARG:O	2:B:67:ARG:HG2	2.09	0.52
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.91	0.52
2:B:323:ASN:HA	2:B:325:HIS:CE1	2.44	0.52
2:B:157:MET:HE1	2:B:229:LEU:HB3	1.92	0.51
1:C:95:PRO:HG2	1:C:102:LEU:HD12	1.91	0.51
1:C:105:THR:N	1:C:106:PRO:CD	2.72	0.51
1:C:293:ILE:O	1:C:294:ASN:HB2	2.10	0.51
1:C:373:SER:HB3	1:C:375:MET:SD	2.50	0.51
1:A:150:VAL:O	1:A:154:MET:HG3	2.09	0.51
1:C:138:LEU:HD12	1:C:138:LEU:N	2.24	0.51
1:C:96:PRO:O	1:C:97:ALA:CB	2.59	0.51
1:C:153:GLU:OE2	1:C:156:ARG:NH1	2.44	0.51
2:B:238:THR:HG21	8:B:674:HOH:O	2.11	0.50
1:C:177:GLN:O	1:C:181:GLU:HG3	2.10	0.50
1:A:385:VAL:O	6:A:509:CL:CL	2.66	0.50
1:C:30:GLY:N	1:C:87:VAL:HG21	2.26	0.50
1:A:293:ILE:O	1:A:294:ASN:HB2	2.12	0.50
1:C:39:GLU:OE1	1:C:64:SER:OG	2.25	0.49
1:A:53:HIS:O	8:A:603:HOH:O	2.20	0.49
2:B:35:ILE:HG13	2:B:35:ILE:O	2.12	0.49
2:D:120:LEU:CA	2:D:142:MET:HE2	2.43	0.49
1:A:64:SER:O	8:A:602:HOH:O	2.19	0.49
1:C:124:ARG:O	1:C:143:PRO:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLY:HA3	1:C:359:ILE:HD11	1.93	0.49
2:D:285:TRP:CE3	2:D:286:ASP:CB	2.95	0.48
1:C:70:ASN:C	1:C:70:ASN:OD1	2.56	0.48
2:D:323:ASN:HA	2:D:325:HIS:CE1	2.47	0.48
1:A:270:VAL:CG1	1:A:271:GLY:N	2.76	0.48
2:B:329:ILE:HG12	2:B:329:ILE:O	2.13	0.48
2:D:120:LEU:O	2:D:142:MET:CE	2.61	0.48
1:C:402:TRP:HB2	1:C:406:GLU:CB	2.44	0.47
2:D:175:TYR:HB2	7:D:402:HX7:CAB	2.44	0.47
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.95	0.47
2:B:252:TYR:OH	2:B:393:ARG:HG2	2.15	0.47
1:C:273:ARG:HD3	8:C:629:HOH:O	2.15	0.47
1:C:354:GLY:HA3	1:C:359:ILE:CD1	2.45	0.47
1:C:402:TRP:HB3	1:C:403:PRO:HD2	1.97	0.47
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.95	0.47
2:B:289:LEU:N	2:B:290:PRO:CD	2.78	0.47
2:B:175:TYR:HB2	7:B:503:HX7:CAB	2.44	0.47
2:B:84:ARG:HB2	8:B:657:HOH:O	2.15	0.46
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.45	0.46
2:D:97:VAL:HB	2:D:123:ILE:HG12	1.97	0.46
2:D:282:TYR:CE1	2:D:285:TRP:HZ2	2.33	0.46
2:B:393:ARG:HG2	2:B:394:MET:N	2.31	0.46
2:D:147:GLY:HA3	8:D:504:HOH:O	2.15	0.46
2:D:283:ASP:CG	2:D:284:GLU:H	2.23	0.46
2:B:119:THR:O	2:B:318:LYS:HE3	2.16	0.46
1:A:30:GLY:HA2	1:A:63:THR:O	2.16	0.46
2:B:328:ARG:O	8:B:602:HOH:O	2.20	0.46
1:A:330:VAL:HG23	2:B:79:LYS:HD3	1.98	0.45
2:B:110:GLN:OE1	2:B:134:MET:HE2	2.15	0.45
1:C:231:GLU:O	1:C:235:LEU:HG	2.16	0.45
4:B:502:NAG:H61	4:B:502:NAG:C2	2.42	0.45
1:C:105:THR:HB	1:C:106:PRO:HD3	1.98	0.45
1:C:23:ASP:N	1:C:23:ASP:OD1	2.49	0.45
1:C:135:LEU:C	1:C:135:LEU:CD1	2.89	0.45
2:D:231:TYR:O	2:D:232:CYS:HB3	2.16	0.45
2:D:368:ASN:C	2:D:368:ASN:OD1	2.60	0.45
2:B:44:THR:HG21	2:B:289:LEU:CD2	2.46	0.45
1:A:281:ARG:NH1	1:A:281:ARG:HB2	2.32	0.45
2:D:216:ILE:HG13	2:D:217:GLN:N	2.30	0.45
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.51	0.45
1:C:275:ILE:HD13	1:C:289:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:C	1:A:396:ASN:OD1	2.60	0.44
2:D:75:GLU:OE2	2:D:75:GLU:CA	2.65	0.44
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.99	0.44
1:A:344:ARG:HG3	1:A:344:ARG:NH1	2.33	0.44
2:D:285:TRP:CE3	2:D:363:VAL:HG21	2.52	0.44
1:A:128:TYR:HA	1:A:134:HIS:CD2	2.53	0.44
2:B:147:GLY:HA3	8:B:660:HOH:O	2.18	0.44
1:C:23:ASP:CG	1:C:24:PRO:HD3	2.43	0.44
1:A:135:LEU:C	1:A:135:LEU:CD1	2.86	0.44
2:B:102:ASP:O	2:B:102:ASP:CG	2.61	0.44
1:C:344:ARG:HH11	1:C:344:ARG:CG	2.31	0.44
2:B:133:ILE:O	2:B:133:ILE:HG13	2.17	0.44
2:D:374:GLU:O	2:D:376:VAL:HG23	2.18	0.44
2:D:285:TRP:CE3	2:D:363:VAL:CG2	3.00	0.44
2:D:285:TRP:CE3	2:D:286:ASP:CG	2.96	0.44
1:C:102:LEU:HD12	1:C:102:LEU:C	2.43	0.43
2:B:133:ILE:CD1	2:B:150:ILE:CG1	2.92	0.43
1:C:87:VAL:CG2	1:C:89:ALA:O	2.65	0.43
1:C:233:LYS:O	8:C:602:HOH:O	2.21	0.43
2:D:285:TRP:CG	2:D:286:ASP:N	2.86	0.43
1:A:57:LYS:HB3	8:A:667:HOH:O	2.18	0.43
1:A:362:ASN:C	1:A:362:ASN:OD1	2.62	0.43
1:C:37:LYS:HA	1:C:37:LYS:HD2	1.89	0.43
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.00	0.43
1:A:270:VAL:HG11	1:A:274:GLU:HB3	2.01	0.43
1:C:347:MET:HE3	1:C:347:MET:HB3	1.75	0.43
1:C:30:GLY:HA3	1:C:87:VAL:HG21	2.00	0.43
2:D:77:ASP:HB2	2:D:78:PRO:HD2	2.01	0.43
2:D:43:GLY:HA3	2:D:102:ASP:CG	2.43	0.43
2:B:71:VAL:HG13	2:B:84:ARG:HH21	1.82	0.42
2:D:35:ILE:HG23	2:D:64:VAL:CG1	2.49	0.42
1:A:23:ASP:N	1:A:24:PRO:CD	2.82	0.42
1:C:103:THR:HB	1:C:104:PRO:HD2	2.01	0.42
2:D:285:TRP:CD2	2:D:286:ASP:N	2.81	0.42
1:C:87:VAL:HG22	1:C:89:ALA:O	2.20	0.42
2:D:362:LEU:HB2	2:D:379:TRP:HB3	2.01	0.42
1:A:155:MET:HE1	1:A:184:LEU:HD21	2.01	0.42
1:A:359:ILE:HD13	1:A:367:ARG:CZ	2.49	0.42
2:D:106:GLU:OE2	6:D:406:CL:CL	2.75	0.42
2:D:289:LEU:N	2:D:290:PRO:HD2	2.36	0.41
1:C:241:ILE:HA	1:C:269:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:THR:HG21	2:B:289:LEU:HD21	2.01	0.41
1:C:343:LYS:NZ	2:D:208:SER:OG	2.48	0.41
1:A:241:ILE:HA	1:A:269:LEU:O	2.21	0.41
1:A:250:THR:HG22	1:A:254:LYS:HE3	2.01	0.41
1:A:339:GLY:N	1:A:340:PRO:CD	2.83	0.41
4:B:502:NAG:C2	4:B:502:NAG:C6	2.99	0.41
1:A:138:LEU:HD12	1:A:138:LEU:N	2.36	0.41
1:A:389:ASN:OD1	1:A:389:ASN:C	2.63	0.41
1:C:259:LEU:CD1	1:C:261:MET:CE	2.99	0.41
2:B:245:ASN:OD1	2:B:245:ASN:C	2.64	0.41
2:B:289:LEU:N	2:B:290:PRO:HD2	2.36	0.41
1:C:233:LYS:HG3	1:C:266:TYR:OH	2.21	0.41
1:C:242:LEU:HB3	1:C:270:VAL:HG12	2.03	0.41
2:D:34:SER:HA	2:D:65:VAL:O	2.21	0.41
2:D:211:ASP:OD2	2:D:216:ILE:HG12	2.21	0.41
1:C:214:LYS:NZ	1:C:231:GLU:OE2	2.54	0.41
1:A:135:LEU:HD23	7:B:503:HX7:CBB	2.51	0.40
1:A:154:MET:HG2	1:A:393:ILE:HD11	2.03	0.40
2:B:120:LEU:HD13	2:B:331:GLN:HB3	2.04	0.40
2:B:318:LYS:HE2	8:B:658:HOH:O	2.20	0.40
1:A:344:ARG:NE	2:B:210:ASP:OD1	2.50	0.40
2:B:68:VAL:HG11	2:B:297:ILE:HD13	2.04	0.40
1:C:343:LYS:HD3	2:D:209:LEU:HD23	2.02	0.40
2:B:318:LYS:N	2:B:318:LYS:HD3	2.35	0.40
1:C:95:PRO:HA	1:C:96:PRO:HD3	1.88	0.40
1:A:33:LEU:O	1:A:66:THR:HA	2.21	0.40
2:D:376:VAL:O	2:D:376:VAL:CG1	2.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ARG:NH2	1:C:384:GLN:OE1[4_7510]	1.92	0.28
2:B:389:TYR:O	1:C:380:ARG:NH1[4_7510]	2.18	0.02

5.3 Torsion angles ⓘ

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	353/385 (92%)	338 (96%)	15 (4%)	0	100	100
1	C	351/385 (91%)	339 (97%)	11 (3%)	1 (0%)	36	44
2	B	356/363 (98%)	337 (95%)	18 (5%)	1 (0%)	36	44
2	D	356/363 (98%)	341 (96%)	13 (4%)	2 (1%)	21	25
All	All	1416/1496 (95%)	1355 (96%)	57 (4%)	4 (0%)	36	44

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/331 (87%)	285 (99%)	4 (1%)	59	74
1	C	287/331 (87%)	278 (97%)	9 (3%)	35	50
2	B	293/326 (90%)	285 (97%)	8 (3%)	39	55
2	D	281/326 (86%)	276 (98%)	5 (2%)	51	68
All	All	1150/1314 (88%)	1124 (98%)	26 (2%)	45	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	258	MET
1	A	281	ARG
1	A	380	ARG
2	B	62	LEU
2	B	152	GLN
2	B	188	SER
2	B	312	SER
2	B	329	ILE
2	B	358	MET
2	B	359[A]	HIS
2	B	359[B]	HIS
1	C	23	ASP
1	C	258	MET
1	C	281	ARG
1	C	288	ILE
1	C	299	SER
1	C	344	ARG
1	C	347	MET
1	C	363	GLU
1	C	401	ILE
2	D	84	ARG
2	D	215	LYS
2	D	328	ARG
2	D	337	ARG
2	D	393	ARG

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

Mol	Chain	Res	Type
1	A	28	ASN
1	A	61	GLN
1	A	171	HIS
1	A	217	GLN
1	A	321	ASN
2	B	105	GLN
2	B	192	ASN
1	C	73	GLN
1	C	217	GLN
1	C	314	HIS
1	C	334	ASN

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Mol	Chain	Res	Type
1	C	371	GLN
2	D	118	GLN
2	D	359	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	3,1	14,14,15	0.38	0	17,19,21	0.57	0
3	NAG	E	2	3	14,14,15	0.37	0	17,19,21	0.71	0
3	BMA	E	3	3	11,11,12	0.38	0	15,15,17	0.47	0
3	MAN	E	4	3	11,11,12	0.39	0	15,15,17	0.68	0
3	MAN	E	5	3	11,11,12	0.29	0	15,15,17	0.48	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	3,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

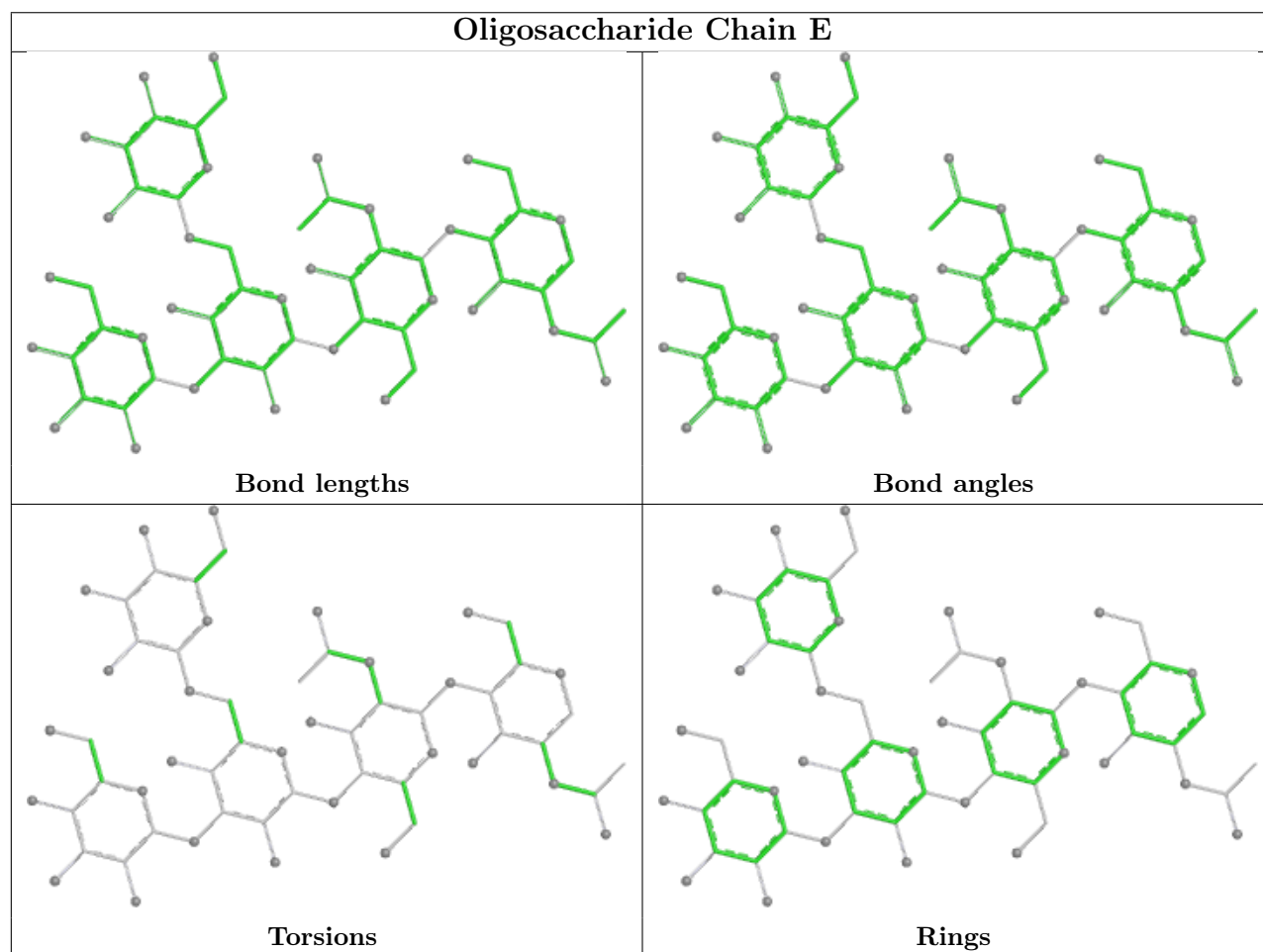
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	501	2	14,14,15	0.43	0	17,19,21	0.54	0
7	HX7	D	402	-	32,32,32	1.72	8 (25%)	43,43,43	2.23	3 (6%)
4	NAG	A	501	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	B	502	2	14,14,15	0.46	0	17,19,21	0.68	0
4	NAG	C	501	1	14,14,15	0.68	1 (7%)	17,19,21	0.56	0
4	NAG	D	401	2	14,14,15	0.86	1 (7%)	17,19,21	1.49	2 (11%)
4	NAG	C	502	1	14,14,15	0.33	0	17,19,21	0.62	0
7	HX7	B	503	-	32,32,32	1.78	7 (21%)	43,43,43	2.25	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
7	HX7	D	402	-	-	12/23/23/23	0/2/2/2
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	502	2	-	2/6/23/26	0/1/1/1
4	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	2	-	4/6/23/26	0/1/1/1
4	NAG	C	502	1	-	3/6/23/26	0/1/1/1
7	HX7	B	503	-	-	9/23/23/23	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503	HX7	SBE-NAV	6.88	1.72	1.63
7	D	402	HX7	SBE-NAV	6.37	1.71	1.63
7	B	503	HX7	OAW-CBB	3.06	1.44	1.37
7	B	503	HX7	CAB-SBE	3.02	1.82	1.75
7	D	402	HX7	CAB-SBE	2.98	1.82	1.75
7	D	402	HX7	OAW-CBB	2.93	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503	HX7	CBA-NAV	2.61	1.47	1.43
7	B	503	HX7	CAY-CL2	2.47	1.79	1.73
7	D	402	HX7	OAC-SBE	2.41	1.47	1.43
7	D	402	HX7	CAY-CL2	2.32	1.79	1.73
7	D	402	HX7	CBA-NAV	2.27	1.46	1.43
7	D	402	HX7	OAD-SBE	2.26	1.47	1.43
4	C	501	NAG	C1-C2	2.20	1.55	1.52
7	B	503	HX7	OAC-SBE	2.18	1.47	1.43
7	D	402	HX7	CAZ-CL1	2.17	1.78	1.73
7	B	503	HX7	OAD-SBE	2.14	1.47	1.43
4	D	401	NAG	O5-C1	2.07	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503	HX7	OAD-SBE-OAC	-13.12	101.29	118.87
7	D	402	HX7	OAD-SBE-OAC	-12.84	101.66	118.87
4	D	401	NAG	C1-O5-C5	4.85	118.68	112.19
7	D	402	HX7	CAB-SBE-NAV	3.60	110.61	106.56
7	B	503	HX7	CAB-SBE-NAV	3.48	110.49	106.56
4	D	401	NAG	O5-C1-C2	2.41	115.02	111.29
7	D	402	HX7	OAC-SBE-NAV	2.15	111.39	107.10
7	B	503	HX7	OAD-SBE-NAV	2.08	111.24	107.10
7	B	503	HX7	OAC-SBE-NAV	2.07	111.24	107.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	402	HX7	NBD-CAU-CBC-CAT
7	B	503	HX7	CAQ-CAS-NBD-CAU
7	D	402	HX7	CAQ-CAS-NBD-CAU
4	D	401	NAG	O5-C5-C6-O6
4	D	401	NAG	C4-C5-C6-O6
4	B	502	NAG	C8-C7-N2-C2
4	B	502	NAG	O7-C7-N2-C2
4	C	502	NAG	C8-C7-N2-C2
4	C	502	NAG	O7-C7-N2-C2
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
7	D	402	HX7	NBD-CAU-CBC-OAE
7	D	402	HX7	CAX-CAQ-CAS-NBD

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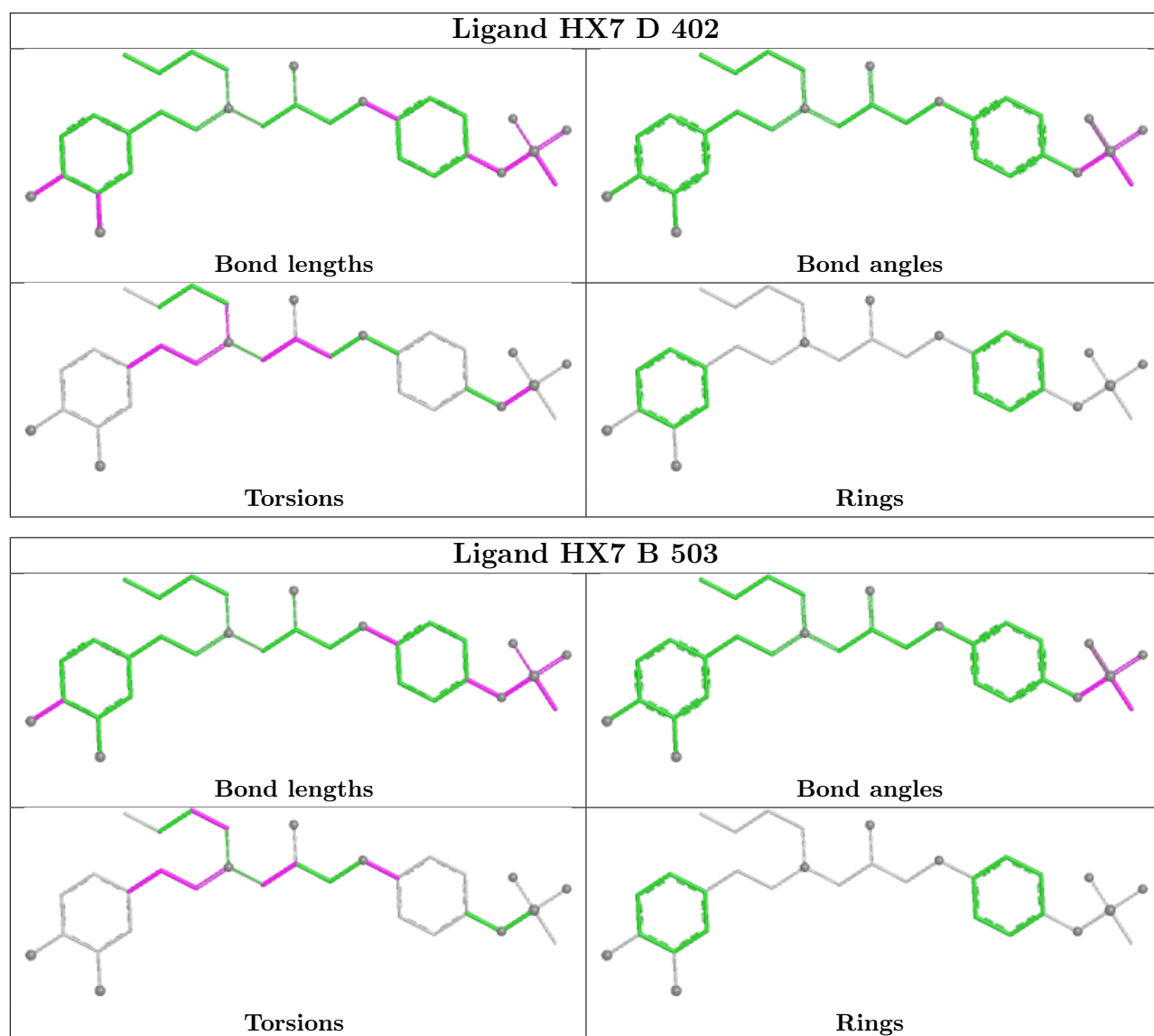
Mol	Chain	Res	Type	Atoms
7	B	503	HX7	CAS-CAQ-CAX-CAN
7	B	503	HX7	CAX-CAQ-CAS-NBD
7	B	503	HX7	CAS-CAQ-CAX-CAH
7	D	402	HX7	CAS-CAQ-CAX-CAH
7	D	402	HX7	CAS-CAQ-CAX-CAN
7	B	503	HX7	CAO-CAP-CAR-NBD
7	D	402	HX7	CBA-NAV-SBE-OAD
7	D	402	HX7	CAP-CAR-NBD-CAS
7	B	503	HX7	NBD-CAU-CBC-OAE
4	C	502	NAG	C4-C5-C6-O6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

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	402	HX7	5	0
4	B	502	NAG	3	0
7	B	503	HX7	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/385 (93%)	0.01	9 (2%) 58 60	17, 30, 60, 74	0
1	C	357/385 (92%)	0.35	17 (4%) 35 36	22, 42, 69, 83	0
2	B	359/363 (98%)	0.44	26 (7%) 21 22	17, 43, 70, 83	1 (0%)
2	D	360/363 (99%)	0.49	38 (10%) 11 12	22, 43, 77, 93	0
All	All	1435/1496 (95%)	0.32	90 (6%) 26 27	17, 39, 69, 93	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	59	PHE	5.6
2	B	61	HIS	5.6
2	B	48	VAL	5.5
1	C	97	ALA	5.5
2	D	61	HIS	5.4
1	A	407	THR	4.9
1	A	97	ALA	4.7
2	D	285	TRP	4.6
2	B	59	PHE	4.6
2	D	345	GLU	4.4
2	D	344	PHE	4.4
2	B	46	ASP	4.3
2	D	44	THR	4.2
2	B	393	ARG	3.9
2	B	194	PHE	3.9
2	B	44	THR	3.8
2	D	48	VAL	3.7
1	C	406	GLU	3.7
2	D	359	HIS	3.7
1	C	266	TYR	3.6
2	D	322	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	192	ASN	3.4
2	D	216	ILE	3.4
2	D	389	TYR	3.4
2	D	32	PRO	3.3
2	B	45	SER	3.3
2	B	381	ASP	3.3
2	D	381	ASP	3.3
1	A	23	ASP	3.3
1	A	96	PRO	3.2
1	C	392	TYR	3.2
1	A	186	GLY	3.1
2	B	52	ASP	3.1
2	B	213	ASP	3.1
1	C	96	PRO	3.1
2	D	62	LEU	3.1
2	D	50	ILE	3.0
2	D	193	SER	3.0
2	D	326	GLU	3.0
2	D	353	GLU	2.9
2	B	32	PRO	2.9
2	B	54	HIS	2.9
1	A	406	GLU	2.9
1	C	54	PHE	2.8
2	B	344	PHE	2.8
2	B	62	LEU	2.8
2	B	359[A]	HIS	2.8
2	D	60	HIS	2.8
2	D	52	ASP	2.8
1	A	258	MET	2.8
2	D	53	ALA	2.8
2	D	328	ARG	2.7
2	D	55	GLU	2.7
1	A	405	GLY	2.7
1	C	405	GLY	2.6
2	D	136	ASP	2.6
2	D	323	ASN	2.6
2	D	347	ARG	2.6
2	D	324	THR	2.6
2	D	346	GLY	2.6
1	A	404	GLY	2.5
1	C	209	GLY	2.5
1	C	264	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	135	ALA	2.4
1	C	158	PHE	2.4
2	B	285	TRP	2.4
1	C	56	ARG	2.4
2	B	321	CYS	2.4
2	B	356	TYR	2.3
2	D	46	ASP	2.3
2	B	282	TYR	2.3
2	D	333	ASN	2.3
1	C	58	ILE	2.3
2	D	380	LYS	2.3
2	D	194	PHE	2.2
2	B	49	ALA	2.2
2	D	54	HIS	2.2
2	D	34	SER	2.2
2	B	394	MET	2.2
1	C	95	PRO	2.2
2	D	319	SER	2.2
2	B	322	TYR	2.1
2	D	343	THR	2.1
1	C	282	TYR	2.1
2	B	191	GLU	2.1
1	C	401	ILE	2.1
1	C	344	ARG	2.1
2	B	326	GLU	2.1
2	B	323	ASN	2.1
1	C	258	MET	2.0

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

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

6.3 Carbohydrates [i](#)

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

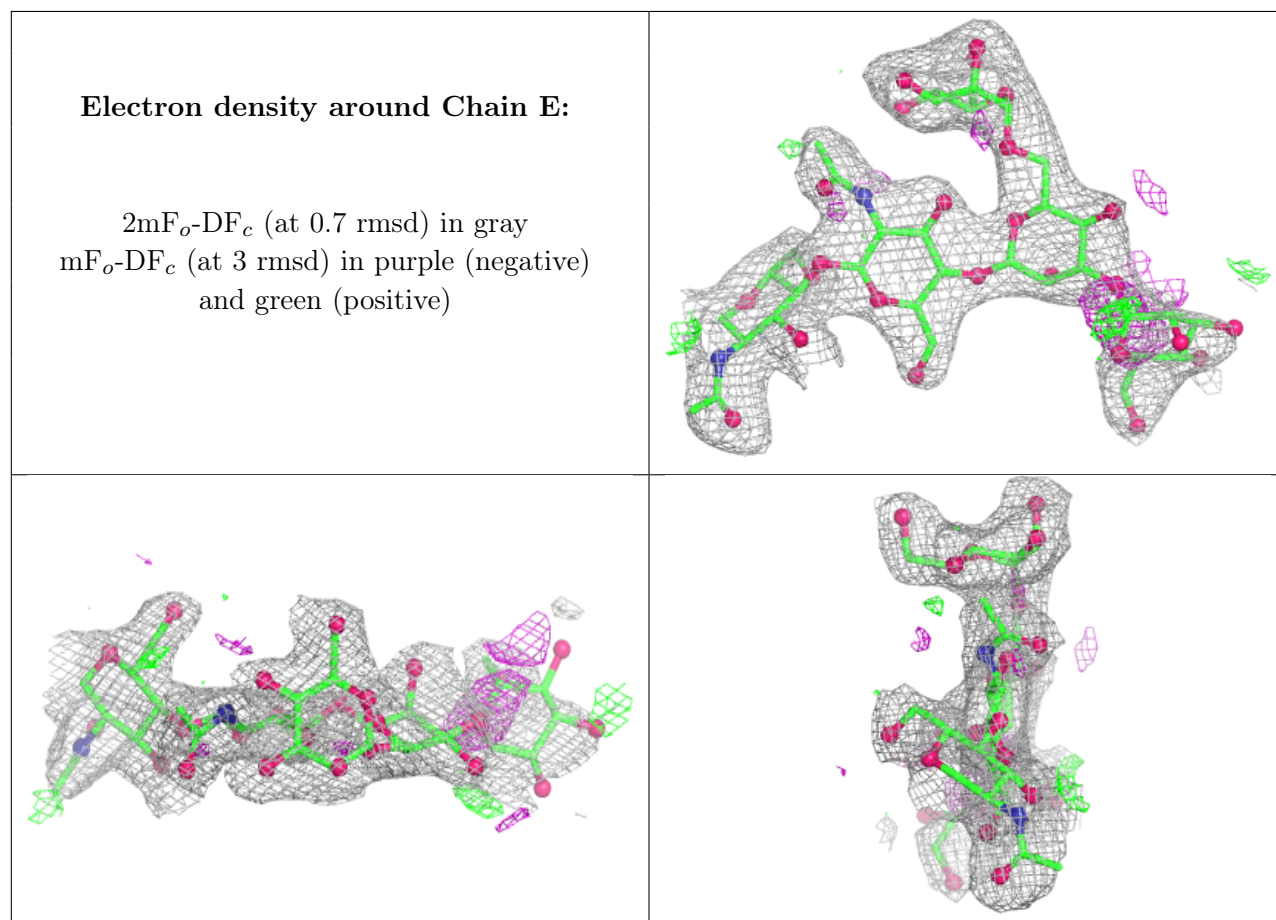
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	E	4	11/12	0.50	0.22	82,85,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	E	3	11/12	0.87	0.12	69,73,79,81	0
3	NAG	E	2	14/15	0.89	0.11	56,58,64,66	0
3	MAN	E	5	11/12	0.89	0.14	63,68,71,71	0
3	NAG	E	1	14/15	0.90	0.10	41,46,51,52	0

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	502	14/15	0.41	0.22	72,76,81,84	0
4	NAG	D	401	14/15	0.49	0.18	74,77,82,84	0

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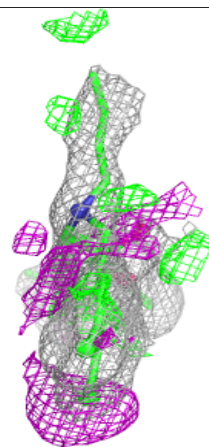
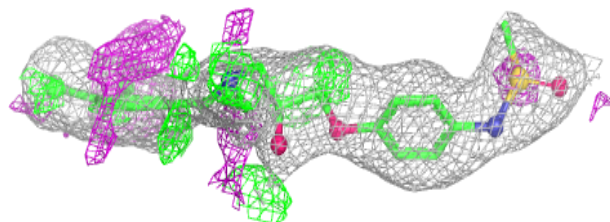
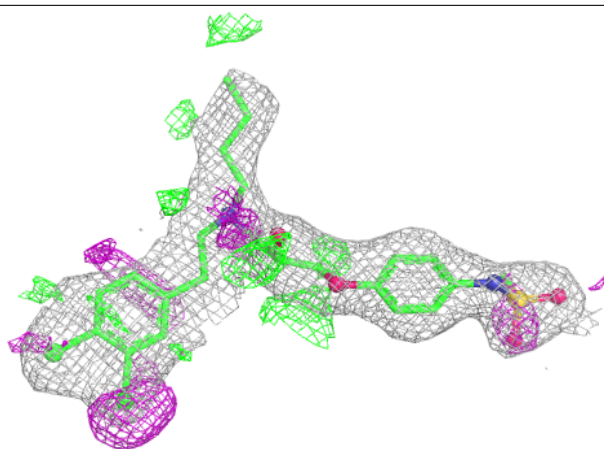
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	501	14/15	0.50	0.20	61,66,70,71	0
4	NAG	C	501	14/15	0.70	0.16	65,74,81,81	0
4	NAG	C	502	14/15	0.82	0.12	44,47,51,52	0
4	NAG	A	501	14/15	0.85	0.10	35,38,40,41	0
6	CL	B	505	1/1	0.88	0.13	72,72,72,72	0
7	HX7	B	503	31/31	0.88	0.14	34,38,42,43	0
6	CL	D	403	1/1	0.89	0.13	57,57,57,57	0
6	CL	B	506	1/1	0.89	0.10	53,53,53,53	0
6	CL	A	509	1/1	0.90	0.11	48,48,48,48	0
6	CL	D	405	1/1	0.90	0.18	66,66,66,66	0
6	CL	B	507	1/1	0.90	0.11	61,61,61,61	0
7	HX7	D	402	31/31	0.90	0.13	34,40,46,52	0
6	CL	D	404	1/1	0.91	0.14	77,77,77,77	0
6	CL	B	504	1/1	0.91	0.11	53,53,53,53	0
6	CL	C	504	1/1	0.93	0.12	69,69,69,69	0
6	CL	A	508	1/1	0.93	0.10	57,57,57,57	0
6	CL	C	505	1/1	0.96	0.05	43,43,43,43	0
5	NA	C	503	1/1	0.97	0.04	28,28,28,28	0
6	CL	D	406	1/1	0.97	0.11	70,70,70,70	0
5	NA	A	507	1/1	0.98	0.03	19,19,19,19	0

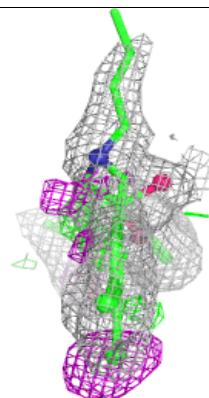
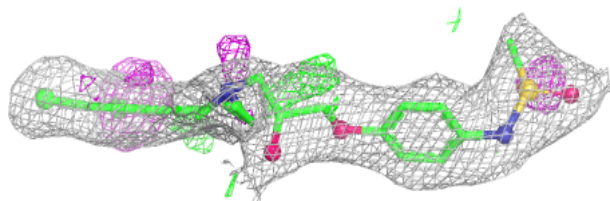
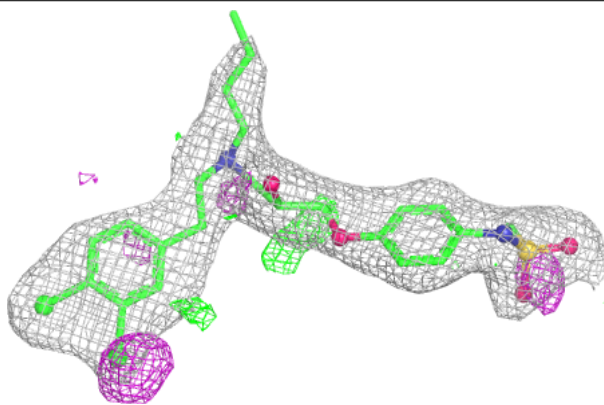
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HX7 B 503:

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

**Electron density around HX7 D 402:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.