



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:00 AM UTC

PDB ID : 5EWJ / pdb_00005ewj
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX
WITH IFENPRODIL
Authors : Pandit, J.
Deposited on : 2015-11-20
Resolution : 2.77 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:

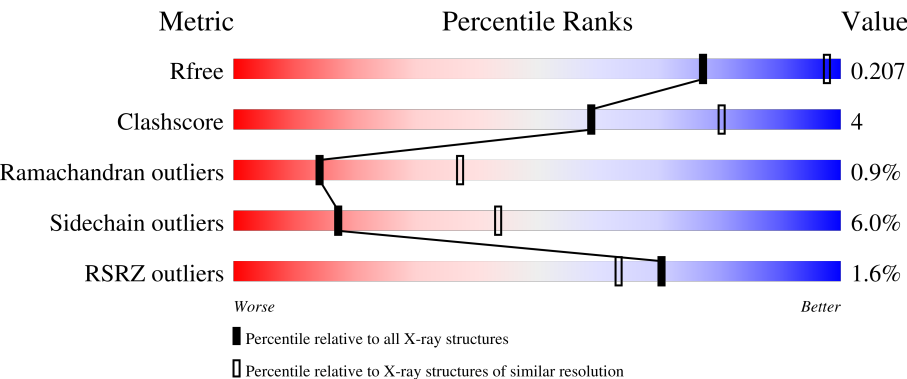
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	390	2% 76% 14% 8%
1	C	390	2% 76% 13% 9%
2	B	364	2% 82% 13% 3%
2	D	364	2% 78% 16% 4%

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Mol	Chain	Length	Quality of chain
3	E	5	 60% 40%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NMDA glutamate receptor subunit.

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

There are 12 discrepancies between the modelled and reference sequences:

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

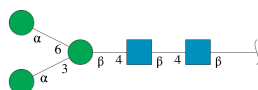
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	353	Total	C	N	O	S	0	0	0
			2750	1772	436	527	15			
2	D	355	Total	C	N	O	S	0	0	0
			2778	1791	436	535	16			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

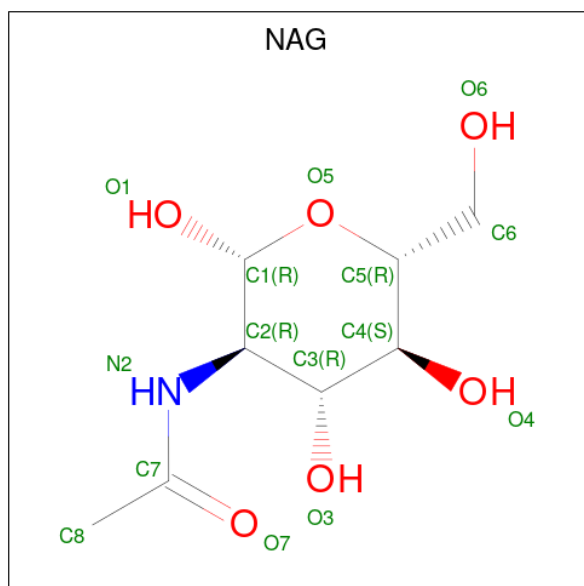


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

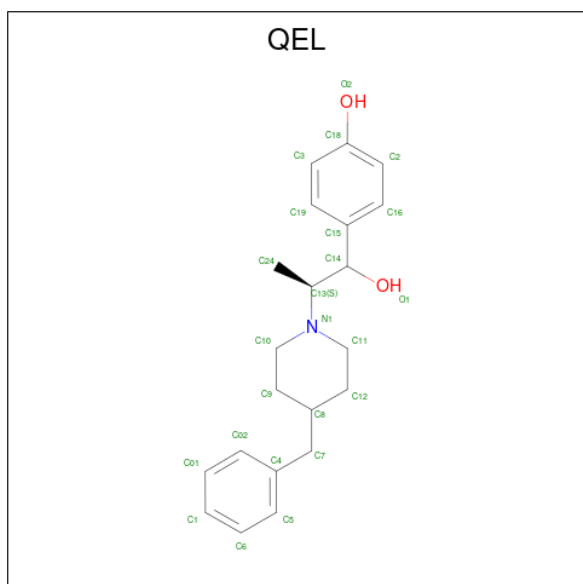
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (CCD ID: QEL) (formula: C₂₁H₂₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			24	21	1	2		
6	D	1	Total	C	N	O	0	0
			24	21	1	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	158	Total	O	0	0
			158	158		

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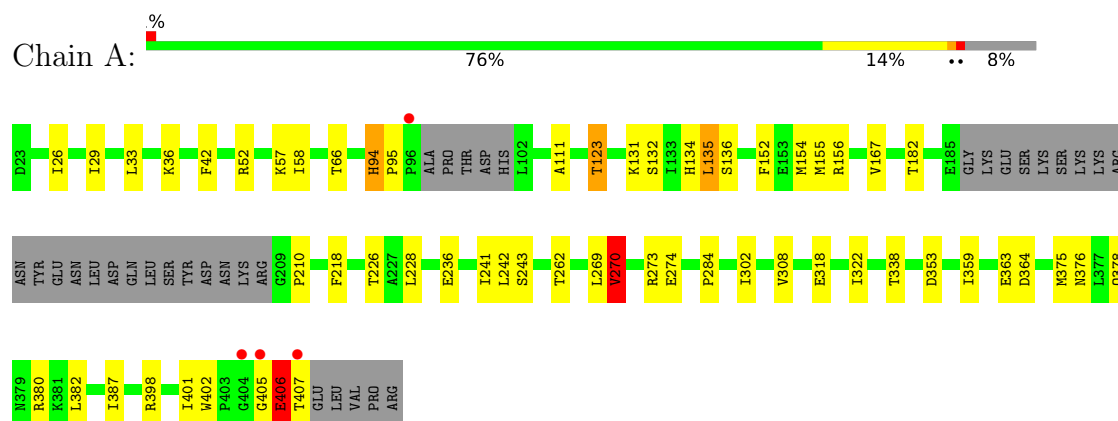
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	80	Total	O	0	0
			80	80		
7	C	53	Total	O	0	0
			53	53		
7	D	60	Total	O	0	0
			60	60		

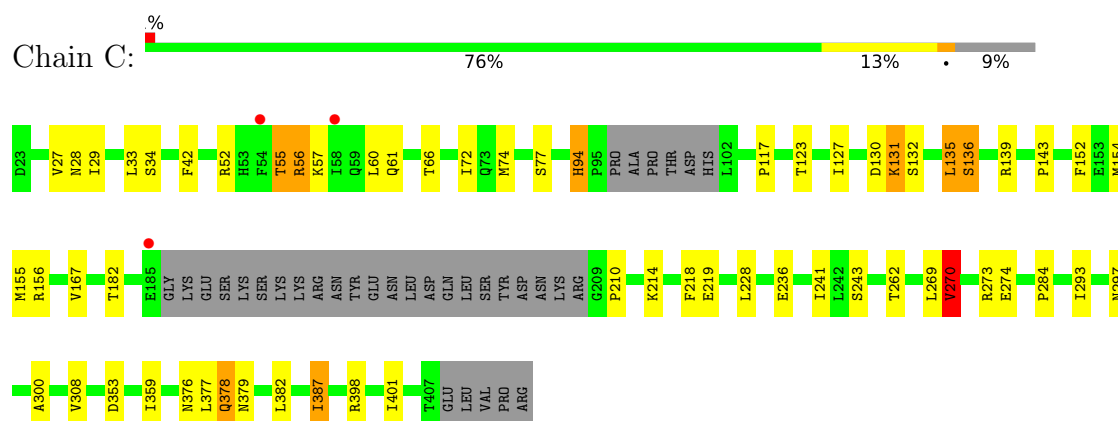
3 Residue-property plots [i](#)

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.

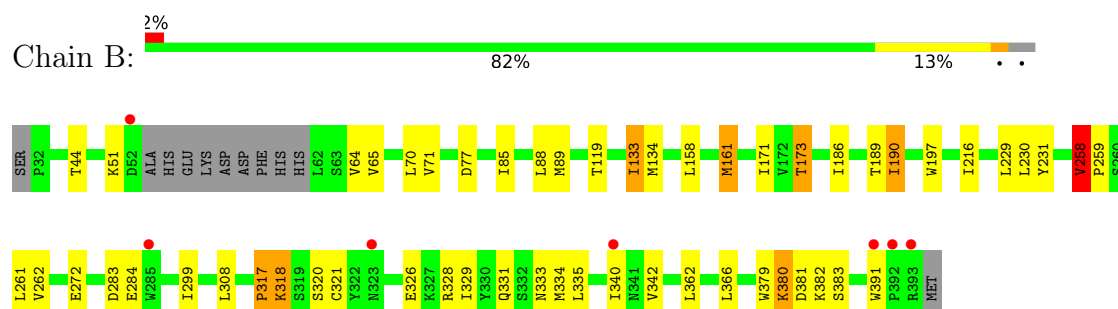
• Molecule 1: NMDA glutamate receptor subunit



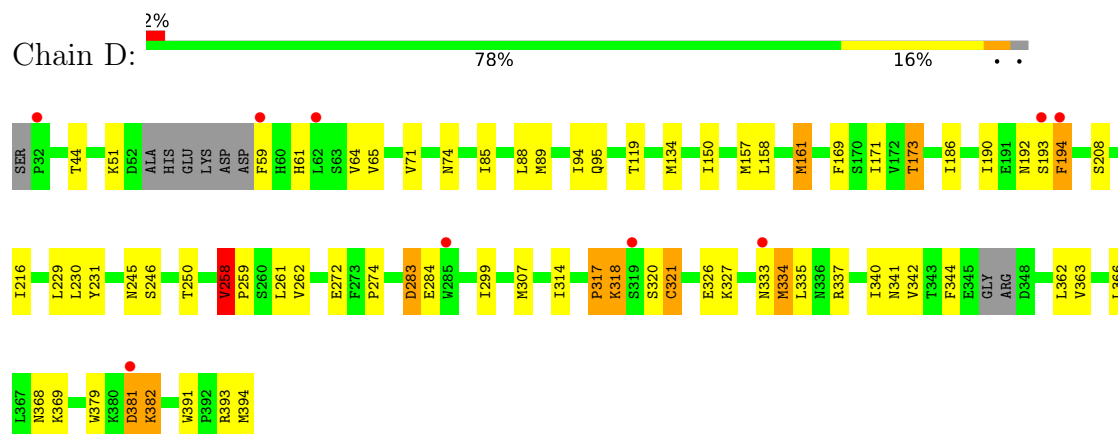
• Molecule 1: NMDA glutamate receptor subunit



• 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	268.46Å 60.10Å 145.00Å 90.00° 116.22° 90.00°	Depositor
Resolution (Å)	27.92 – 2.77 27.92 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.92-2.77) 98.8 (27.92-2.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.76Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6	Depositor
R, R_{free}	0.174 , 0.211 0.175 , 0.207	Depositor DCC
R_{free} test set	2685 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.4	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	0.96	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.95	2/2809 (0.1%)	1.34	13/3819 (0.3%)
1	C	0.83	0/2792	1.33	8/3794 (0.2%)
2	B	0.89	3/2812 (0.1%)	1.34	10/3828 (0.3%)
2	D	0.88	2/2841 (0.1%)	1.40	29/3864 (0.8%)
All	All	0.89	7/11254 (0.1%)	1.35	60/15305 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	LYS	CA-C	6.24	1.60	1.52
2	D	161	MET	SD-CE	-6.24	1.64	1.79
2	B	161	MET	SD-CE	-5.65	1.65	1.79
2	B	77	ASP	CA-C	5.33	1.60	1.53
1	A	405	GLY	C-N	5.32	1.40	1.33
2	B	133	ILE	CG1-CD1	5.17	1.72	1.51
2	D	157	MET	SD-CE	-5.04	1.67	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	VAL	N-CA-CB	-10.95	100.19	112.45
1	A	270	VAL	N-CA-CB	-10.68	100.49	112.45
2	D	333	ASN	CA-CB-CG	8.52	121.11	112.60
2	B	321	CYS	N-CA-C	-7.72	104.01	113.50
2	D	321	CYS	N-CA-C	-7.63	104.11	113.50
2	D	381	ASP	CA-C-N	7.32	135.52	121.54
2	D	381	ASP	C-N-CA	7.32	135.52	121.54
2	D	317	PRO	CA-C-N	6.99	131.04	121.05
2	D	317	PRO	C-N-CA	6.99	131.04	121.05
2	B	317	PRO	CA-C-N	6.92	130.94	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	317	PRO	C-N-CA	6.92	130.94	121.05
1	A	95	PRO	N-CA-C	6.89	119.11	110.70
1	A	406	GLU	N-CA-C	6.54	118.28	110.44
2	D	341	ASN	CA-CB-CG	6.22	118.82	112.60
2	B	258	VAL	N-CA-CB	-6.19	102.54	111.21
2	B	189	THR	CA-C-N	6.02	128.71	120.46
2	B	189	THR	C-N-CA	6.02	128.71	120.46
2	D	258	VAL	N-CA-CB	-5.88	102.98	111.21
2	D	284	GLU	N-CA-C	-5.87	105.38	112.54
2	B	333	ASN	CA-CB-CG	5.86	118.46	112.60
2	D	61	HIS	CA-C-N	5.80	132.62	121.54
2	D	61	HIS	C-N-CA	5.80	132.62	121.54
1	A	364	ASP	CA-CB-CG	5.76	118.36	112.60
2	D	61	HIS	N-CA-C	-5.71	107.31	114.56
2	D	344	PHE	CA-CB-CG	5.69	119.49	113.80
1	C	130	ASP	CA-C-N	5.60	128.56	120.38
1	C	130	ASP	C-N-CA	5.60	128.56	120.38
2	D	307	MET	CA-C-N	5.59	127.77	120.28
2	D	307	MET	C-N-CA	5.59	127.77	120.28
2	D	194	PHE	CA-C-N	5.57	129.43	121.02
2	D	194	PHE	C-N-CA	5.57	129.43	121.02
2	D	245	ASN	CA-C-N	5.52	127.68	120.28
2	D	245	ASN	C-N-CA	5.52	127.68	120.28
1	C	131	LYS	CA-C-N	5.51	128.12	120.29
1	C	131	LYS	C-N-CA	5.51	128.12	120.29
2	D	333	ASN	N-CA-C	-5.50	106.62	113.38
2	D	74	ASN	CA-CB-CG	5.45	118.05	112.60
1	C	34	SER	N-CA-C	5.43	117.01	111.14
1	C	378	GLN	CA-C-N	5.39	131.83	121.54
1	C	378	GLN	C-N-CA	5.39	131.83	121.54
2	B	284	GLU	N-CA-C	-5.38	105.97	112.54
1	A	363	GLU	CB-CG-CD	5.34	121.68	112.60
2	B	381	ASP	CA-C-N	5.31	130.89	122.61
2	B	381	ASP	C-N-CA	5.31	130.89	122.61
1	A	135	LEU	N-CA-C	5.25	117.08	111.36
2	D	246	SER	CA-C-N	5.17	128.97	121.52
2	D	246	SER	C-N-CA	5.17	128.97	121.52
2	D	150	ILE	CA-C-N	5.16	127.19	120.28
2	D	150	ILE	C-N-CA	5.16	127.19	120.28
2	D	327	LYS	CA-C-N	5.16	127.44	120.38
2	D	327	LYS	C-N-CA	5.16	127.44	120.38
1	A	318	GLU	N-CA-C	-5.15	106.50	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	GLU	CA-C-N	5.14	130.95	121.70
1	A	406	GLU	C-N-CA	5.14	130.95	121.70
1	A	111	ALA	CA-C-N	5.12	125.66	119.98
1	A	111	ALA	C-N-CA	5.12	125.66	119.98
2	D	393	ARG	N-CA-C	5.10	116.58	108.67
1	A	302	ILE	N-CA-C	-5.10	105.52	110.42
1	A	134	HIS	CA-CB-CG	-5.09	108.71	113.80
2	D	382	LYS	N-CA-C	-5.08	99.97	110.80

There are no chirality outliers.

There are no planarity outliers.

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	2752	0	2717	24	0
1	C	2737	0	2705	29	0
2	B	2750	0	2662	21	0
2	D	2778	0	2691	26	0
3	E	61	0	52	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	14	0	13	0	0
5	B	28	0	26	0	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
6	B	24	0	27	2	0
6	D	24	0	27	1	0
7	A	158	0	0	0	0
7	B	80	0	0	0	0
7	C	53	0	0	0	0
7	D	60	0	0	0	0
All	All	11563	0	10959	97	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 4.

All (97) 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:85:ILE:HG22	2:D:89:MET:HE2	1.55	0.88
2:B:85:ILE:HG22	2:B:89:MET:HE2	1.54	0.88
1:A:376:ASN:HD22	1:A:378:GLN:HE21	1.27	0.82
1:C:55:THR:HG22	1:C:56:ARG:H	1.43	0.79
1:A:94:HIS:HE1	1:A:123:THR:HG23	1.46	0.79
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.52	0.75
1:C:28:ASN:HD21	1:C:61:GLN:HE21	1.40	0.69
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.74	0.67
1:C:376:ASN:HD21	1:C:401:ILE:H	1.44	0.66
1:A:376:ASN:ND2	1:A:378:GLN:HE21	1.93	0.64
1:A:376:ASN:HD21	1:A:401:ILE:H	1.45	0.63
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.79	0.63
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.82	0.62
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.82	0.62
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.83	0.60
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.84	0.60
2:B:51:LYS:HE3	2:B:70:LEU:HD22	1.85	0.59
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.86	0.58
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.86	0.58
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.84	0.58
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.85	0.58
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.86	0.57
2:B:258:VAL:HG13	2:B:262:VAL:HB	1.86	0.57
2:D:89:MET:HE1	2:D:119:THR:HG21	1.86	0.56
2:B:89:MET:HE1	2:B:119:THR:HG21	1.86	0.56
1:C:94:HIS:HE1	1:C:123:THR:HG23	1.69	0.56
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.88	0.55
2:B:329:ILE:HD12	2:D:314:ILE:HD11	1.88	0.54
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.73	0.54
1:A:155:MET:HE2	1:A:210:PRO:HB2	1.90	0.54
1:C:167:VAL:HG12	1:C:243:SER:HB3	1.89	0.53
1:A:322:ILE:HG23	1:A:338:THR:HG21	1.91	0.52
1:A:402:TRP:CD1	1:A:406:GLU:HA	2.41	0.52
1:C:155:MET:HE2	1:C:210:PRO:HB2	1.91	0.51
1:C:28:ASN:HD21	1:C:61:GLN:NE2	2.07	0.51
2:B:317:PRO:HA	2:B:318:LYS:HE2	1.93	0.51
1:C:262:THR:HB	1:C:284:PRO:HB3	1.93	0.51
1:C:378:GLN:HG2	1:C:401:ILE:HD12	1.93	0.50
1:C:72:ILE:HG21	2:D:321:CYS:HB3	1.93	0.50
1:C:241:ILE:HA	1:C:269:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASN:HD22	1:C:378:GLN:HE21	1.58	0.49
1:A:241:ILE:HA	1:A:269:LEU:O	2.12	0.49
2:D:95:GLN:NE2	2:D:314:ILE:HD12	2.28	0.49
2:D:317:PRO:HA	2:D:318:LYS:HE2	1.93	0.49
2:B:299:ILE:HA	2:B:342:VAL:HG11	1.94	0.49
1:A:33:LEU:O	1:A:66:THR:HA	2.13	0.49
2:D:368:ASN:HA	2:D:394:MET:HE2	1.96	0.48
2:B:318:LYS:HD2	2:B:331:GLN:OE1	2.14	0.48
2:B:119:THR:O	2:B:318:LYS:HD2	2.14	0.47
1:C:33:LEU:O	1:C:66:THR:HA	2.15	0.47
2:D:366:LEU:HD13	2:D:391:TRP:HZ2	1.79	0.47
2:D:230:LEU:O	2:D:259:PRO:HD3	2.15	0.47
2:D:169:PHE:CZ	2:D:190:ILE:HD11	2.50	0.47
2:B:230:LEU:O	2:B:259:PRO:HD3	2.15	0.46
1:A:57:LYS:HG2	1:A:58:ILE:HG23	1.98	0.46
2:B:318:LYS:H	2:B:318:LYS:CD	2.28	0.46
2:D:119:THR:O	2:D:318:LYS:HD2	2.15	0.46
1:A:262:THR:HB	1:A:284:PRO:HB3	1.97	0.46
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.98	0.46
2:D:94:ILE:O	2:D:317:PRO:HB3	2.16	0.46
1:A:132:SER:O	6:B:503:QEL:H19	2.15	0.45
2:B:366:LEU:HD13	2:B:391:TRP:HZ2	1.82	0.45
2:B:158:LEU:HA	2:B:161:MET:HE3	1.99	0.45
1:C:117:PRO:HA	1:C:136:SER:HB3	1.98	0.45
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.98	0.45
2:D:334:MET:HG3	2:D:337:ARG:HH21	1.82	0.44
1:A:135:LEU:HB2	6:B:503:QEL:H24	2.00	0.44
1:C:55:THR:HG22	1:C:56:ARG:N	2.23	0.44
2:D:318:LYS:H	2:D:318:LYS:CD	2.30	0.44
1:C:132:SER:O	6:D:503:QEL:H19	2.18	0.44
1:C:154:MET:HB2	1:C:154:MET:HE2	1.78	0.44
1:A:94:HIS:CE1	1:A:123:THR:HG23	2.37	0.44
2:D:250:THR:HB	2:D:274:PRO:HB3	2.00	0.44
1:A:152:PHE:CE2	1:A:156:ARG:HD2	2.53	0.43
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.99	0.43
2:D:283:ASP:HB3	2:D:363:VAL:HG23	2.00	0.43
1:A:29:ILE:HG22	1:A:42:PHE:HZ	1.82	0.43
2:D:173:THR:HA	2:D:231:TYR:O	2.19	0.43
2:D:158:LEU:HA	2:D:161:MET:HE3	1.99	0.42
1:C:29:ILE:HG22	1:C:42:PHE:HZ	1.84	0.42
1:A:154:MET:HB2	1:A:154:MET:HE2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:MET:HE3	1:C:77:SER:HB3	2.02	0.41
1:C:152:PHE:CE2	1:C:156:ARG:HD2	2.55	0.41
1:C:382:LEU:HD23	1:C:382:LEU:HA	1.96	0.41
1:C:297:ASN:HB3	1:C:300:ALA:HB3	2.03	0.41
2:B:71:VAL:HG11	2:B:88:LEU:HD11	2.02	0.41
2:D:362:LEU:HB2	2:D:379:TRP:HB3	2.01	0.41
2:B:173:THR:HG22	2:B:231:TYR:HB3	2.02	0.41
2:B:173:THR:HA	2:B:231:TYR:O	2.21	0.41
2:B:190:ILE:HG13	2:B:197:TRP:CG	2.56	0.41
1:C:135:LEU:HD22	2:D:208:SER:HB3	2.01	0.41
1:C:139:ARG:NH2	1:C:143:PRO:HB3	2.36	0.41
1:C:293:ILE:HD11	1:C:387:ILE:HG12	2.02	0.41
2:D:71:VAL:HG11	2:D:88:LEU:HD11	2.01	0.41
1:A:242:LEU:HB3	1:A:270:VAL:HG22	2.03	0.40
2:B:380:LYS:HD2	2:B:383:SER:HB3	2.03	0.40
1:A:375:MET:HB3	1:A:382:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/390 (90%)	336 (96%)	15 (4%)	0	100	100
1	C	350/390 (90%)	333 (95%)	13 (4%)	4 (1%)	11	32
2	B	349/364 (96%)	329 (94%)	18 (5%)	2 (1%)	21	47
2	D	349/364 (96%)	327 (94%)	16 (5%)	6 (2%)	7	22
All	All	1399/1508 (93%)	1325 (95%)	62 (4%)	12 (1%)	14	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ASP
1	C	56	ARG
1	C	135	LEU
2	D	382	LYS
1	C	55	THR
1	C	379	ASN
2	D	283	ASP
2	D	381	ASP
2	B	334	MET
2	D	334	MET
2	D	193	SER
2	D	51	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/336 (87%)	275 (94%)	17 (6%)	18	45
1	C	289/336 (86%)	273 (94%)	16 (6%)	19	47
2	B	298/326 (91%)	278 (93%)	20 (7%)	15	39
2	D	305/326 (94%)	287 (94%)	18 (6%)	18	44
All	All	1184/1324 (89%)	1113 (94%)	71 (6%)	17	43

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	52	ARG
1	A	94	HIS
1	A	123	THR
1	A	131	LYS
1	A	136	SER
1	A	182	THR
1	A	226	THR
1	A	236	GLU
1	A	270	VAL

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Mol	Chain	Res	Type
1	A	273	ARG
1	A	353	ASP
1	A	380	ARG
1	A	387	ILE
1	A	398	ARG
1	A	406	GLU
1	A	407	THR
2	B	44	THR
2	B	64	VAL
2	B	65	VAL
2	B	133	ILE
2	B	134	MET
2	B	173	THR
2	B	190	ILE
2	B	216	ILE
2	B	258	VAL
2	B	261	LEU
2	B	272	GLU
2	B	308	LEU
2	B	318	LYS
2	B	320	SER
2	B	326	GLU
2	B	328	ARG
2	B	335	LEU
2	B	340	ILE
2	B	380	LYS
2	B	382	LYS
1	C	52	ARG
1	C	57	LYS
1	C	94	HIS
1	C	127	ILE
1	C	131	LYS
1	C	136	SER
1	C	182	THR
1	C	214	LYS
1	C	219	GLU
1	C	236	GLU
1	C	270	VAL
1	C	273	ARG
1	C	353	ASP
1	C	377	LEU
1	C	387	ILE

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Mol	Chain	Res	Type
1	C	398	ARG
2	D	44	THR
2	D	59	PHE
2	D	64	VAL
2	D	65	VAL
2	D	134	MET
2	D	173	THR
2	D	192	ASN
2	D	194	PHE
2	D	216	ILE
2	D	258	VAL
2	D	261	LEU
2	D	272	GLU
2	D	318	LYS
2	D	320	SER
2	D	326	GLU
2	D	335	LEU
2	D	340	ILE
2	D	369	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	94	HIS
1	A	311	GLN
1	A	376	ASN
1	A	384	GLN
2	B	245	ASN
2	B	311	HIS
1	C	28	ASN
1	C	53	HIS
1	C	73	GLN
1	C	94	HIS
1	C	376	ASN
1	C	379	ASN
1	C	384	GLN
2	D	95	GLN
2	D	118	GLN
2	D	311	HIS
2	D	323	ASN

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	0.61	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
3	BMA	E	3	3	11,11,12	0.29	0	15,15,17	0.94	1 (6%)
3	MAN	E	4	3	11,11,12	0.40	0	15,15,17	0.67	0
3	MAN	E	5	3	11,11,12	0.41	0	15,15,17	0.88	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	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-C2-N2	-3.49	104.94	110.43
3	E	3	BMA	C1-O5-C5	2.97	116.17	112.19

There are no chirality outliers.

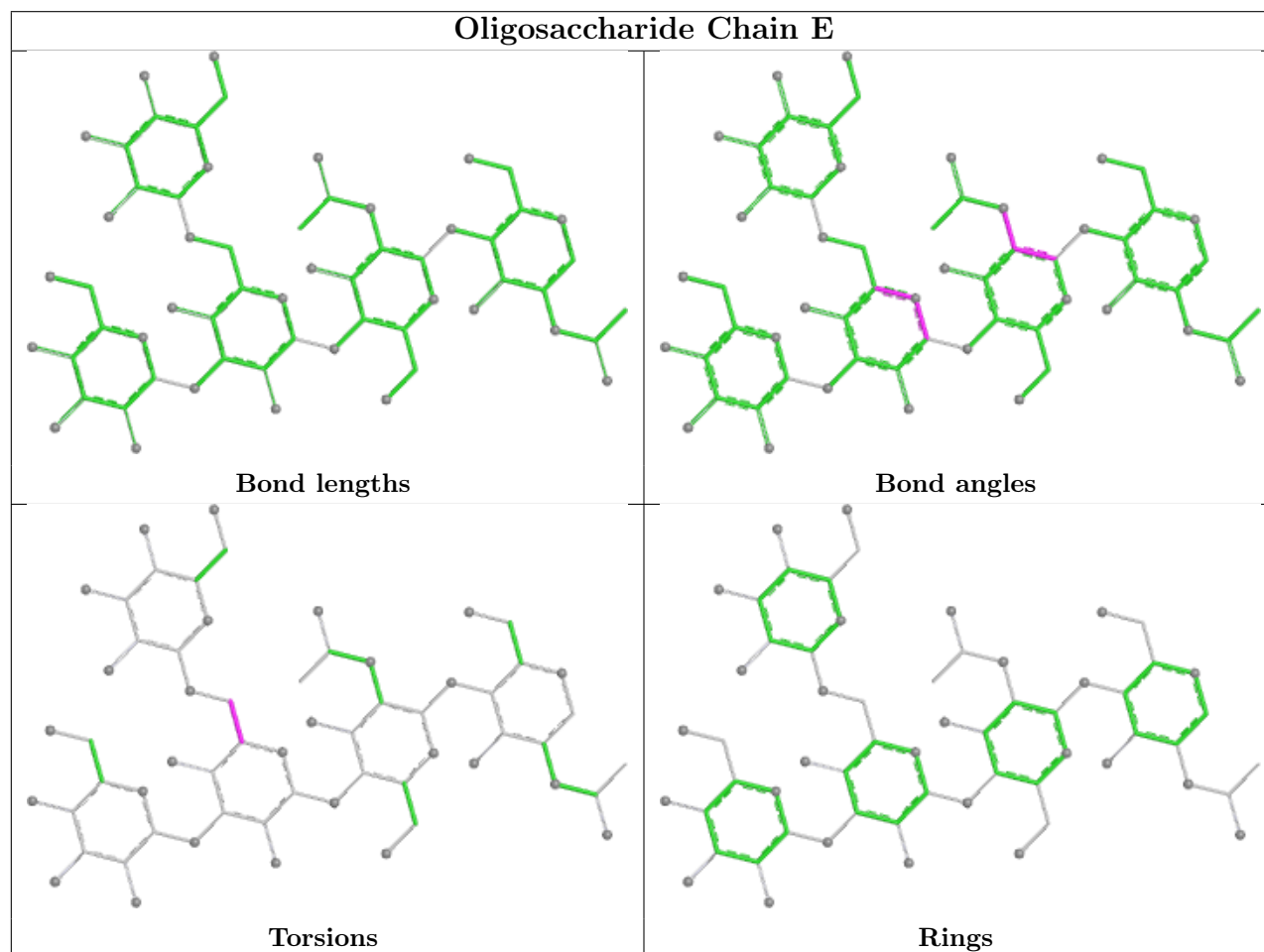
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	QEL	D	503	-	26,26,26	0.30	0	35,35,35	0.55	1 (2%)
5	NAG	D	501	2	14,14,15	0.34	0	17,19,21	0.55	0
5	NAG	B	501	2	14,14,15	0.33	0	17,19,21	0.65	0
6	QEL	B	503	-	26,26,26	0.38	0	35,35,35	0.57	1 (2%)
5	NAG	A	502	1	14,14,15	0.29	0	17,19,21	1.06	1 (5%)
5	NAG	D	502	2	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	B	502	2	14,14,15	0.27	0	17,19,21	1.90	2 (11%)
5	NAG	C	502	1	14,14,15	0.40	0	17,19,21	0.81	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	QEL	D	503	-	-	3/16/26/26	0/3/3/3
5	NAG	D	501	2	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	1/6/23/26	0/1/1/1
6	QEL	B	503	-	-	4/16/26/26	0/3/3/3
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	502	2	-	1/6/23/26	0/1/1/1
5	NAG	B	502	2	-	1/6/23/26	0/1/1/1
5	NAG	C	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	NAG	O5-C1-C2	5.68	120.08	111.29
5	B	502	NAG	C1-O5-C5	5.10	119.02	112.19
5	A	502	NAG	C1-O5-C5	4.01	117.56	112.19
6	D	503	QEL	C10-N1-C13	2.47	122.08	114.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	NAG	C1-C2-N2	2.47	114.32	110.43
6	B	503	QEL	C10-N1-C13	2.34	121.66	114.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

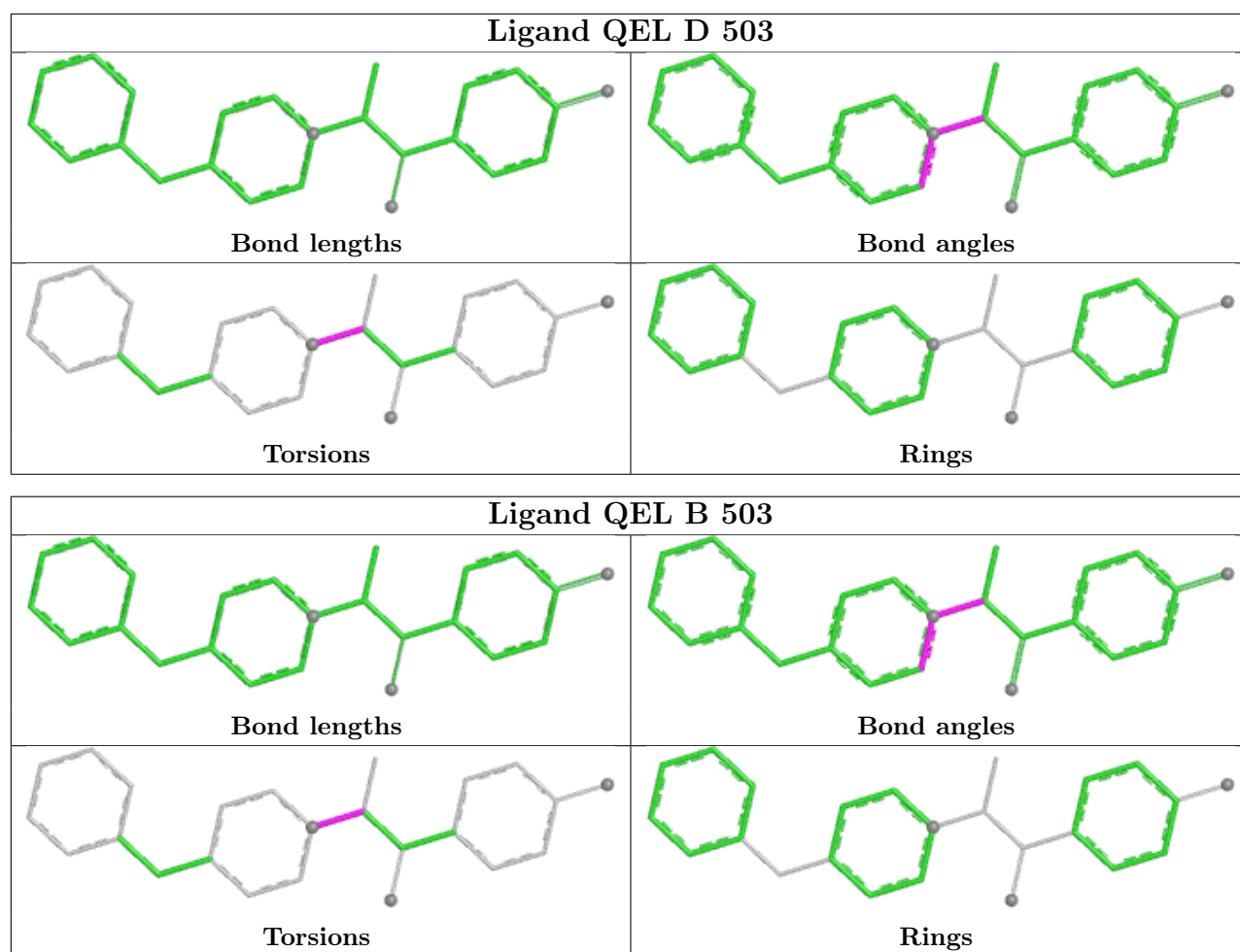
Mol	Chain	Res	Type	Atoms
6	B	503	QEL	C24-C13-N1-C10
6	B	503	QEL	C14-C13-N1-C11
6	B	503	QEL	C24-C13-N1-C11
6	D	503	QEL	C24-C13-N1-C10
6	D	503	QEL	C24-C13-N1-C11
5	A	502	NAG	C4-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	D	502	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
6	B	503	QEL	C14-C13-N1-C10
6	D	503	QEL	C14-C13-N1-C10

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	503	QEL	1	0
6	B	503	QEL	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, 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	357/390 (91%)	-0.53	4 (1%) 78 72	34, 52, 82, 101	0
1	C	356/390 (91%)	-0.06	3 (0%) 82 77	55, 82, 111, 145	0
2	B	353/364 (96%)	-0.22	7 (1%) 65 58	38, 72, 108, 125	0
2	D	355/364 (97%)	-0.05	9 (2%) 58 50	55, 80, 121, 144	0
All	All	1421/1508 (94%)	-0.22	23 (1%) 70 63	34, 73, 111, 145	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	GLY	4.2
2	B	285	TRP	3.2
2	D	333	ASN	3.1
1	C	185	GLU	3.1
2	B	392	PRO	3.0
2	D	32	PRO	3.0
2	D	59	PHE	2.8
2	D	285	TRP	2.8
1	C	54	PHE	2.7
1	A	407	THR	2.7
2	B	52	ASP	2.7
1	A	404	GLY	2.6
2	D	194	PHE	2.4
2	D	381	ASP	2.4
1	C	58	ILE	2.4
2	B	393	ARG	2.4
1	A	96	PRO	2.2
2	D	193	SER	2.2
2	D	62	LEU	2.2
2	D	319	SER	2.2
2	B	391	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	340	ILE	2.1
2	B	323	ASN	2.1

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

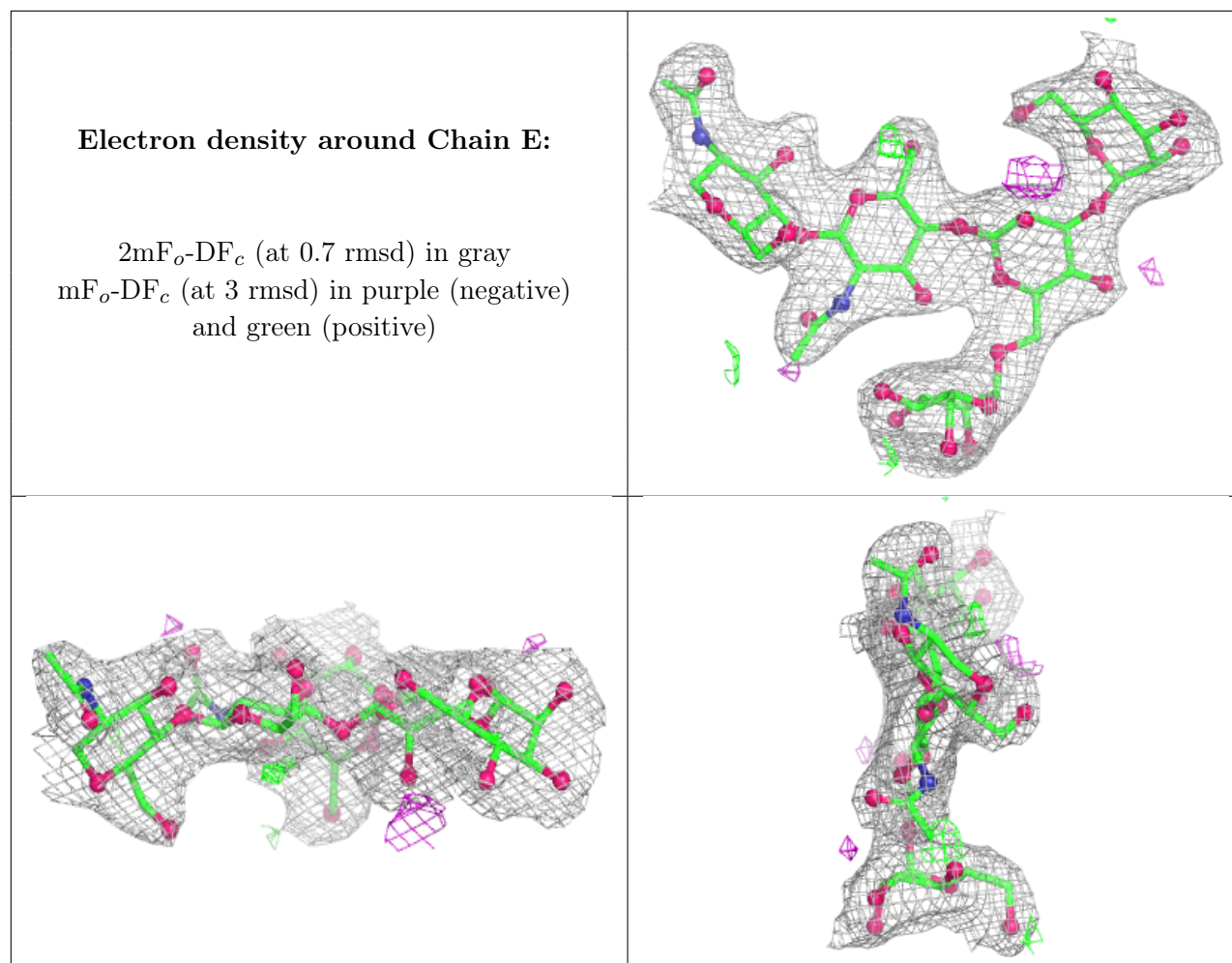
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	MAN	E	4	11/12	0.84	0.10	80,81,85,85	0
3	NAG	E	2	14/15	0.94	0.07	62,63,71,73	0
3	BMA	E	3	11/12	0.95	0.07	62,69,77,78	0
3	NAG	E	1	14/15	0.96	0.07	50,57,64,70	0
3	MAN	E	5	11/12	0.97	0.06	55,62,68,70	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.

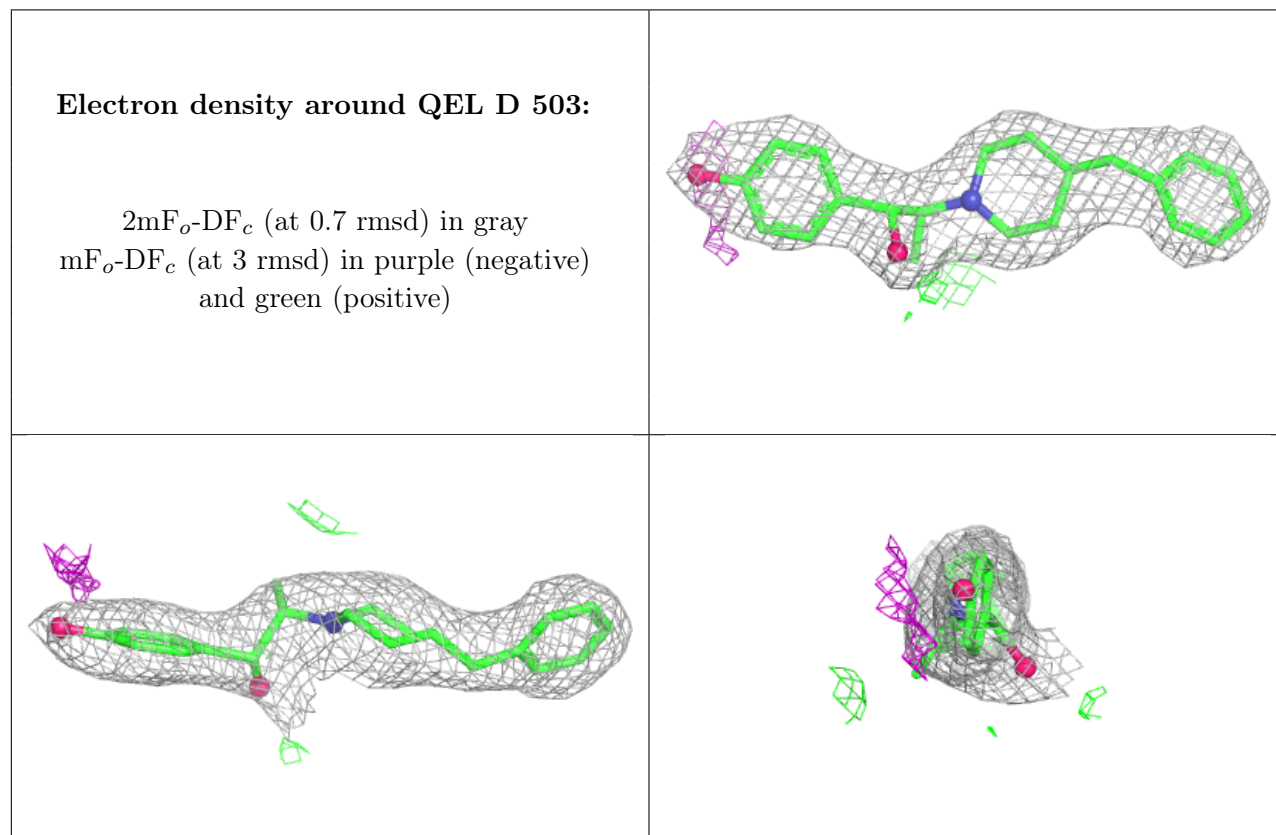


6.4 Ligands ⓘ

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.

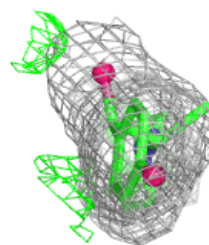
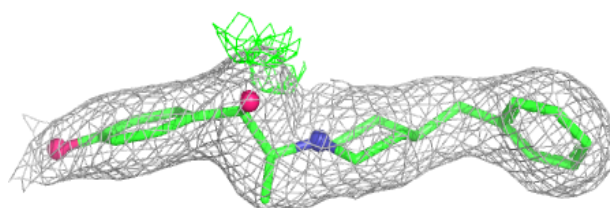
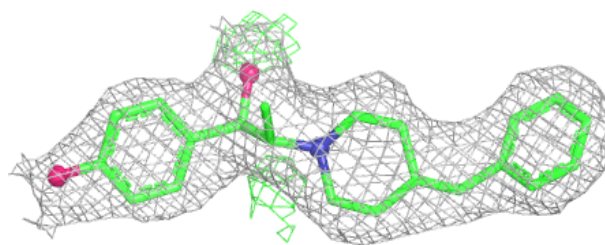
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	D	501	14/15	0.31	0.12	154,160,163,164	0
5	NAG	D	502	14/15	0.38	0.14	164,170,173,174	0
5	NAG	B	502	14/15	0.43	0.12	142,147,153,153	0
5	NAG	B	501	14/15	0.44	0.14	140,145,148,149	0
4	NA	C	501	1/1	0.72	0.38	100,100,100,100	0
5	NAG	C	502	14/15	0.83	0.12	88,94,97,100	0
5	NAG	A	502	14/15	0.94	0.07	58,69,76,77	0
4	NA	A	501	1/1	0.94	0.07	65,65,65,65	0
6	QEL	D	503	24/24	0.94	0.10	64,69,73,77	0
6	QEL	B	503	24/24	0.96	0.07	36,45,60,60	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 QEL 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.