Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:31 AM EDT

PDB ID	:	5EWJ
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:

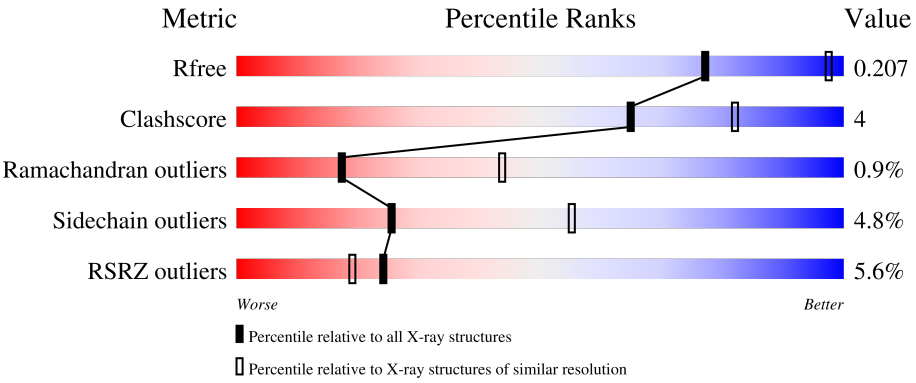
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 <=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% 80% 10% • 8%
1	C	390	7% 78% 11% • 9%
2	B	364	5% 84% 12% • •
2	D	364	7% 83% 13% • •

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	C	501	-	-	-	X
5	NAG	D	501	-	-	-	X
5	NAG	D	502	-	-	-	X

2 Entry composition (i)

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

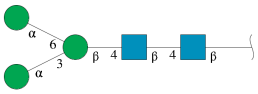
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

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.

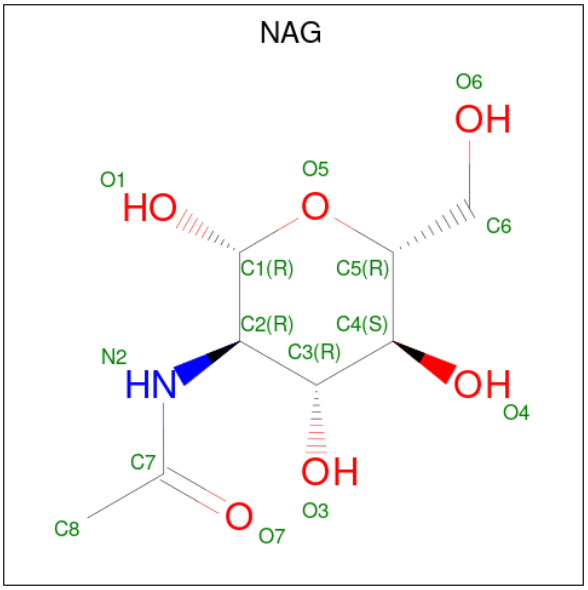


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	5	Total C N O 61 34 2 25	0	0	0

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

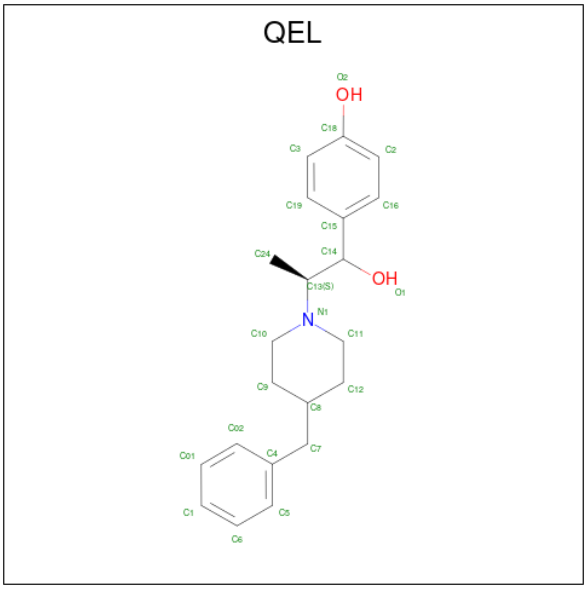
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- 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 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (three-letter code: QEL) (formula: $C_{21}H_{27}NO_2$).



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

- Molecule 7 is water.

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

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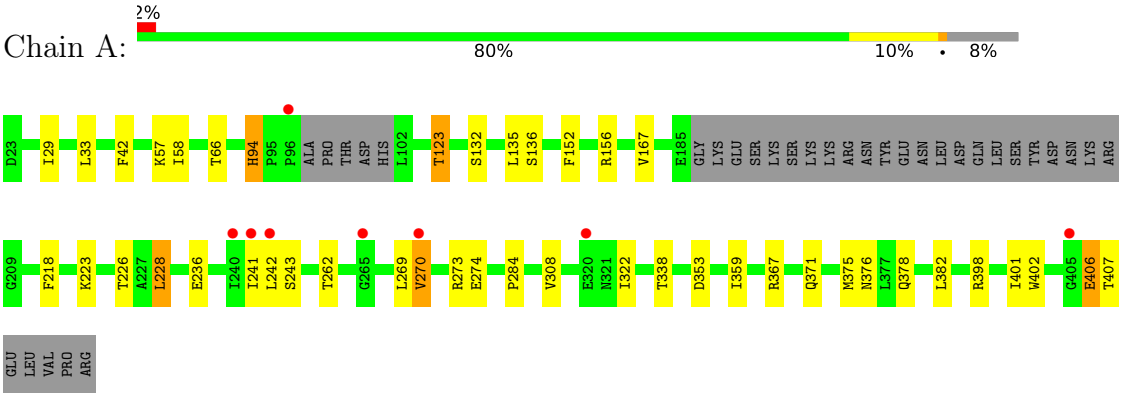
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	80	Total O 80 80	0	0
7	C	53	Total O 53 53	0	0
7	D	60	Total O 60 60	0	0

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.

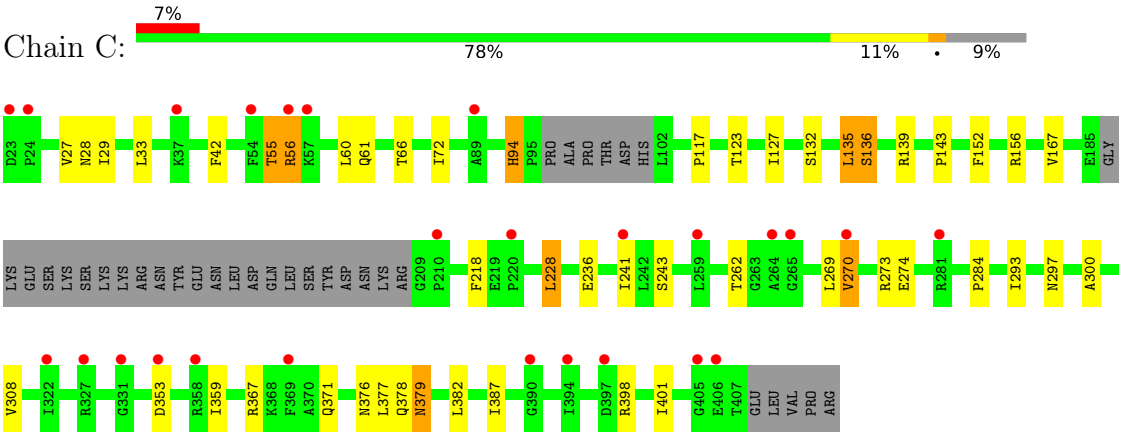
• Molecule 1: NMDA glutamate receptor subunit

Chain A:



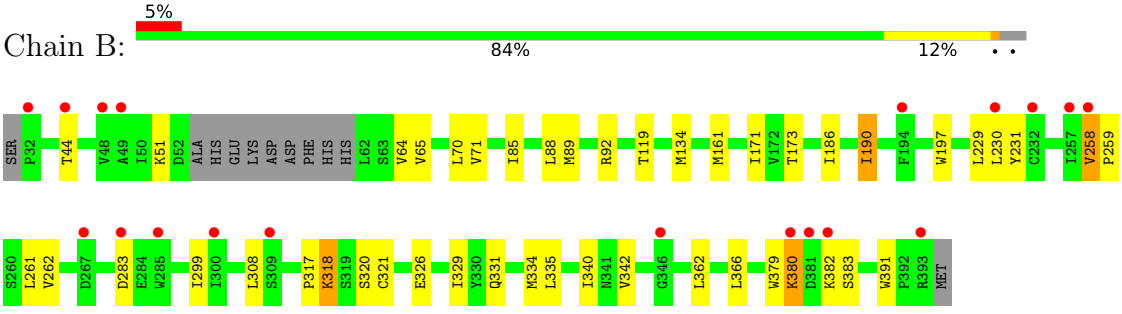
• Molecule 1: NMDA glutamate receptor subunit

Chain C:



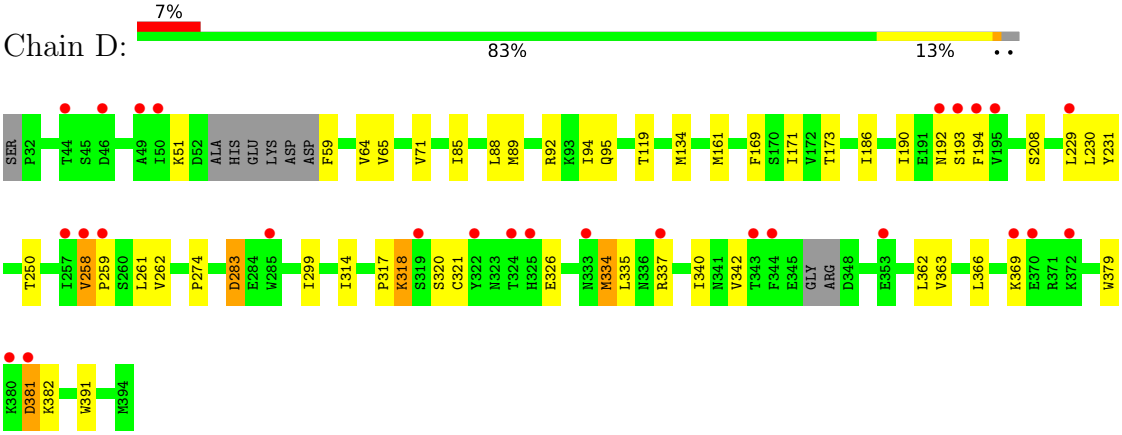
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B:



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:



• 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

Chain E:

4 Data and refinement statistics (i)

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 27.82 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.92-2.77) 98.9 (27.82-2.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.35 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA, MAN, QEL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.57	0/2809	0.73	1/3819 (0.0%)
1	C	0.47	0/2792	0.69	1/3794 (0.0%)
2	B	0.51	0/2812	0.71	0/3828
2	D	0.50	0/2841	0.74	1/3864 (0.0%)
All	All	0.51	0/11254	0.72	3/15305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	381	ASP	C-N-CA	5.53	135.52	121.70
1	C	270	VAL	N-CA-CB	-5.14	100.19	111.50
1	A	270	VAL	N-CA-CB	-5.00	100.49	111.50

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	22	0
1	C	2737	0	2705	26	0
2	B	2750	0	2662	21	0
2	D	2778	0	2691	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	91	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 (91) 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)
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
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
1:C:94:HIS:HE1	1:C:123:THR:HG23	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.89	0.54
1:C:167:VAL:HG12	1:C:243:SER:HB3	1.89	0.53
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.91	0.52
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: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
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: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
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:B:161:MET:HE2	2:B:229:LEU:HD21	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:85:ILE:HG22	2:B:89:MET:CE	2.49	0.42
2:B:89:MET:HE3	2:B:321:CYS:SG	2.59	0.42
1:C:29:ILE:HG22	1:C:42:PHE:HZ	1.84	0.42
2:D:161:MET:HE2	2:D:229:LEU:HD21	2.02	0.42
1:C:152:PHE:CE2	1:C:156:ARG:HD2	2.55	0.41
2:D:85:ILE:HG22	2:D:89:MET:CE	2.50	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:D:89:MET:HE3	2:D:321:CYS:SG	2.61	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 (i)

5.3.1 Protein backbone (i)

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%)	14	38
2	B	349/364 (96%)	329 (94%)	18 (5%)	2 (1%)	25	54
2	D	349/364 (96%)	327 (94%)	16 (5%)	6 (2%)	9	27
All	All	1399/1508 (93%)	1325 (95%)	62 (4%)	12 (1%)	17	44

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 (i)

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%)	278 (95%)	14 (5%)	25	55
1	C	289/336 (86%)	277 (96%)	12 (4%)	30	60
2	B	298/326 (91%)	282 (95%)	16 (5%)	22	50
2	D	305/326 (94%)	290 (95%)	15 (5%)	25	54
All	All	1184/1324 (89%)	1127 (95%)	57 (5%)	25	55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	123	THR
1	A	136	SER
1	A	223	LYS
1	A	226	THR
1	A	228	LEU
1	A	236	GLU
1	A	273	ARG
1	A	353	ASP
1	A	367	ARG
1	A	371	GLN
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	92	ARG
2	B	134	MET
2	B	190	ILE
2	B	258	VAL
2	B	261	LEU
2	B	308	LEU
2	B	318	LYS
2	B	320	SER
2	B	326	GLU
2	B	335	LEU
2	B	340	ILE
2	B	380	LYS
2	B	382	LYS
1	C	94	HIS
1	C	127	ILE
1	C	136	SER
1	C	228	LEU
1	C	236	GLU
1	C	273	ARG
1	C	353	ASP
1	C	367	ARG
1	C	371	GLN
1	C	377	LEU
1	C	379	ASN
1	C	398	ARG

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Mol	Chain	Res	Type
2	D	59	PHE
2	D	64	VAL
2	D	65	VAL
2	D	92	ARG
2	D	134	MET
2	D	192	ASN
2	D	194	PHE
2	D	258	VAL
2	D	261	LEU
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	376	ASN
2	B	105	GLN
2	B	311	HIS
1	C	28	ASN
1	C	94	HIS
1	C	376	ASN
1	C	379	ASN
2	D	95	GLN
2	D	105	GLN
2	D	118	GLN
2	D	219	GLN
2	D	311	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.30	0	17,19,21	0.59	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.99	1 (5%)
3	BMA	E	3	3	11,11,12	0.28	0	15,15,17	0.94	1 (6%)
3	MAN	E	4	3	11,11,12	0.41	0	15,15,17	0.70	0
3	MAN	E	5	3	11,11,12	0.42	0	15,15,17	0.92	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	-	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(^{o})	Ideal(^{o})
3	E	2	NAG	C1-C2-N2	-3.25	104.94	110.49
3	E	3	BMA	C1-O5-C5	2.94	116.17	112.19

There are no chirality outliers.

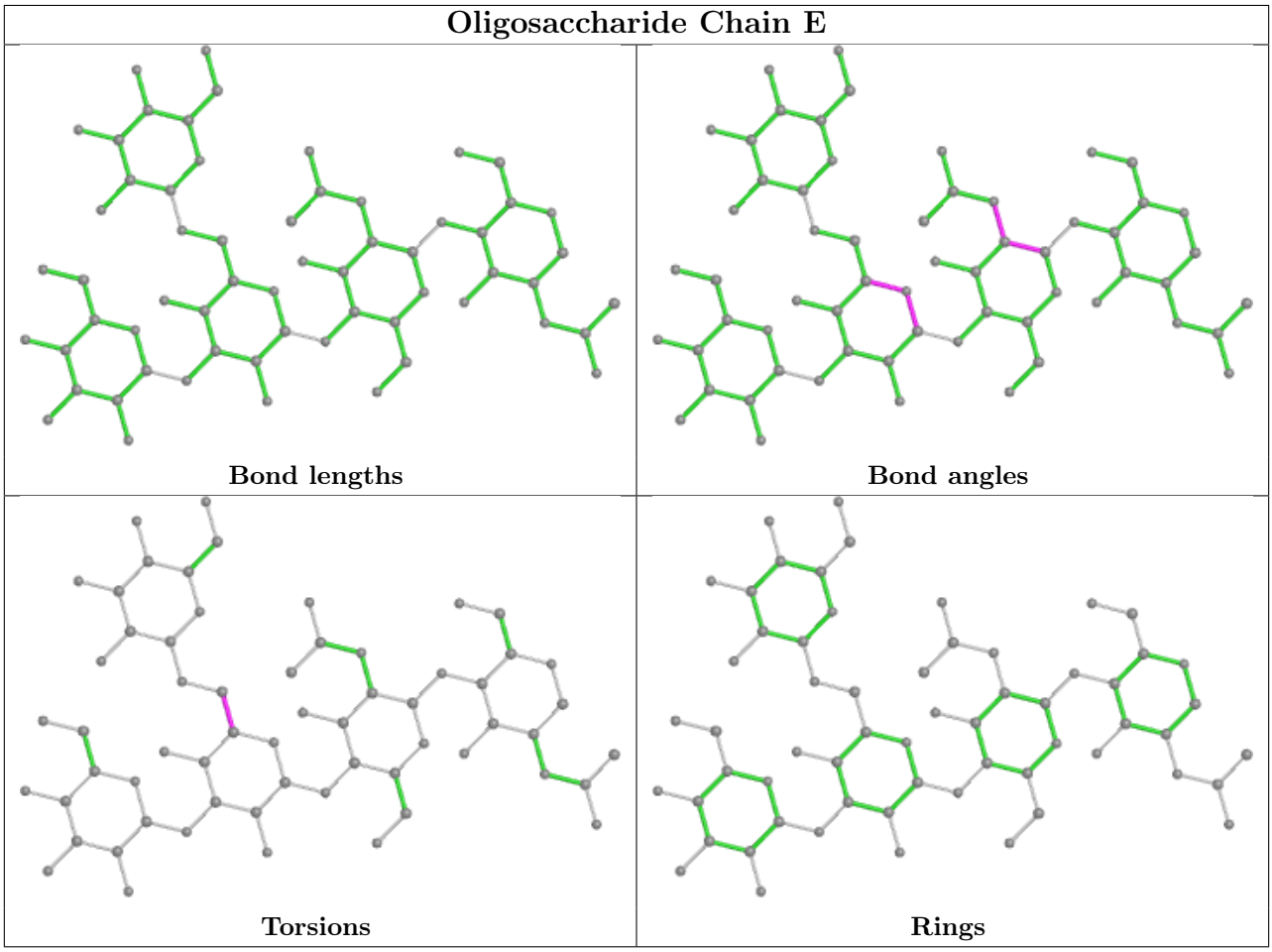
All (1) torsion outliers are listed below:

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	$\#\|Z\| > 2$
5	NAG	A	502	1	14,14,15	0.28	0	17,19,21	1.05	1 (5%)

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	0.59	1 (2%)
5	NAG	D	501	2	14,14,15	0.33	0	17,19,21	0.52	0
5	NAG	C	502	1	14,14,15	0.38	0	17,19,21	0.77	1 (5%)
5	NAG	B	501	2	14,14,15	0.32	0	17,19,21	0.63	0
5	NAG	D	502	2	14,14,15	0.36	0	17,19,21	0.55	0
5	NAG	B	502	2	14,14,15	0.25	0	17,19,21	1.87	2 (11%)
6	QEL	B	503	-	26,26,26	0.38	0	35,35,35	0.59	1 (2%)

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	502	1	-	2/6/23/26	0/1/1/1
6	QEL	D	503	-	-	4/16/26/26	0/3/3/3
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	C	502	1	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	1/6/23/26	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
6	QEL	B	503	-	-	3/16/26/26	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	502	NAG	O5-C1-C2	5.57	120.08	111.29
5	B	502	NAG	C1-O5-C5	5.04	119.02	112.19
5	A	502	NAG	C1-O5-C5	3.97	117.56	112.19
6	D	503	QEL	C10-N1-C13	2.70	122.08	113.38
6	B	503	QEL	C10-N1-C13	2.57	121.66	113.38
5	C	502	NAG	C1-C2-N2	2.24	114.32	110.49

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	503	QEL	C24-C13-N1-C10

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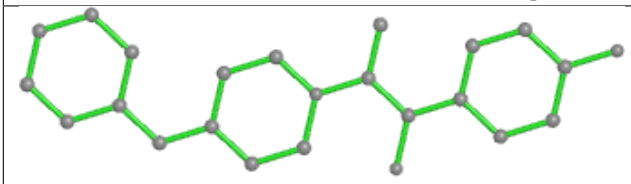
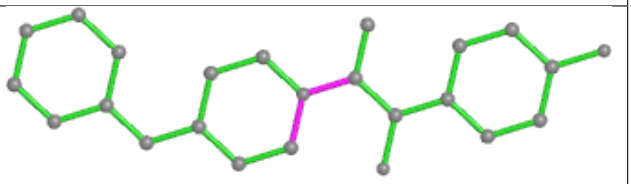
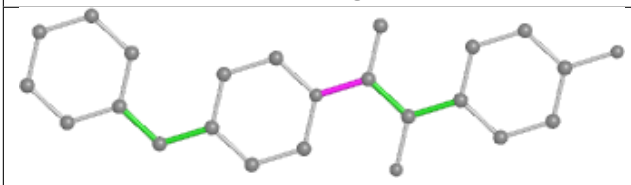
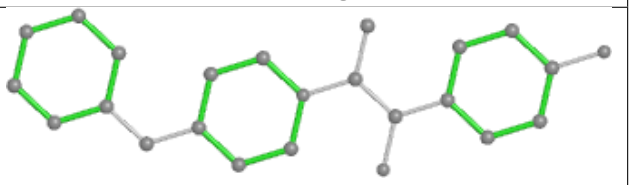
Mol	Chain	Res	Type	Atoms
6	B	503	QEL	C24-C13-N1-C11
6	D	503	QEL	C24-C13-N1-C10
5	A	502	NAG	C4-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	D	502	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
6	D	503	QEL	C24-C13-N1-C11
5	C	502	NAG	C1-C2-N2-C7
5	D	501	NAG	C1-C2-N2-C7
6	B	503	QEL	C14-C13-N1-C11
6	D	503	QEL	C14-C13-N1-C10
6	D	503	QEL	C14-C13-N1-C11

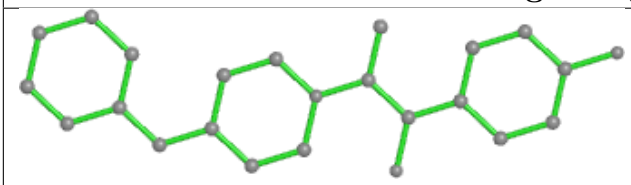
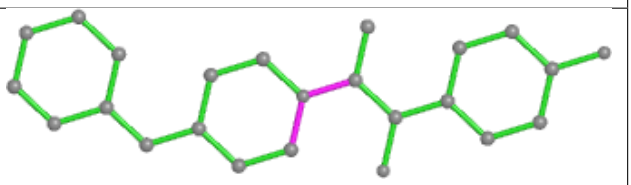
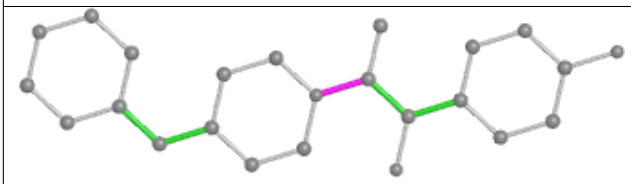
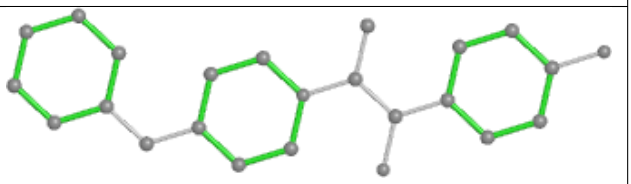
There are no ring outliers.

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 then 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 QEL D 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand QEL B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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^{th} 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%)	-0.20	8 (2%)	62	57	34, 52, 82, 101	0
1	C	356/390 (91%)	0.20	26 (7%)	15	10	55, 82, 111, 145	0
2	B	353/364 (96%)	0.17	19 (5%)	25	20	38, 72, 108, 125	0
2	D	355/364 (97%)	0.27	27 (7%)	13	9	55, 80, 121, 144	0
All	All	1421/1508 (94%)	0.11	80 (5%)	24	19	34, 73, 111, 145	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	6.0
2	D	380	LYS	5.7
2	D	193	SER	5.5
1	C	56	ARG	5.1
2	B	381	ASP	4.7
1	C	54	PHE	4.5
2	D	194	PHE	4.4
2	B	32	PRO	4.3
2	D	192	ASN	4.2
1	C	57	LYS	4.1
2	D	353	GLU	3.8
2	B	380	LYS	3.8
2	D	195	VAL	3.6
2	D	285	TRP	3.6
2	B	285	TRP	3.5
2	D	44	THR	3.4
2	D	343	THR	3.4
1	A	405	GLY	3.4
1	C	394	ILE	3.3
2	D	50	ILE	3.3
1	C	327	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	324	THR	3.2
2	D	319	SER	3.1
2	D	344	PHE	3.1
1	A	96	PRO	3.1
2	B	382	LYS	3.0
1	C	353	ASP	3.0
2	B	48	VAL	3.0
2	B	49	ALA	3.0
2	D	257	ILE	2.9
1	C	264	ALA	2.9
2	D	322	TYR	2.9
2	B	257	ILE	2.9
2	D	258	VAL	2.9
2	D	49	ALA	2.9
1	C	406	GLU	2.8
1	C	220	PRO	2.8
1	C	397	ASP	2.8
1	C	241	ILE	2.7
1	C	358	ARG	2.7
2	D	337	ARG	2.6
2	D	229	LEU	2.6
1	C	210	PRO	2.6
2	D	259	PRO	2.6
1	C	405	GLY	2.5
1	C	265	GLY	2.5
1	C	270	VAL	2.5
1	A	242	LEU	2.5
2	B	346	GLY	2.5
2	D	325	HIS	2.5
2	B	258	VAL	2.5
1	C	24	PRO	2.4
2	B	309	SER	2.4
1	A	270	VAL	2.4
1	A	320	GLU	2.4
1	C	331	GLY	2.3
1	A	241	ILE	2.3
1	C	369	PHE	2.3
2	B	232	CYS	2.3
2	B	44	THR	2.2
2	B	194	PHE	2.2
1	A	240	ILE	2.2
2	D	372	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	2.2
1	C	259	LEU	2.2
2	B	283	ASP	2.2
2	B	393	ARG	2.2
2	B	230	LEU	2.2
2	B	267	ASP	2.1
1	C	23	ASP	2.1
1	C	281	ARG	2.1
1	C	322	ILE	2.1
2	B	300	ILE	2.1
1	C	37	LYS	2.1
2	D	333	ASN	2.1
2	D	369	LYS	2.1
2	D	370	GLU	2.1
1	C	89	ALA	2.1
2	D	46	ASP	2.0
1	C	390	GLY	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)

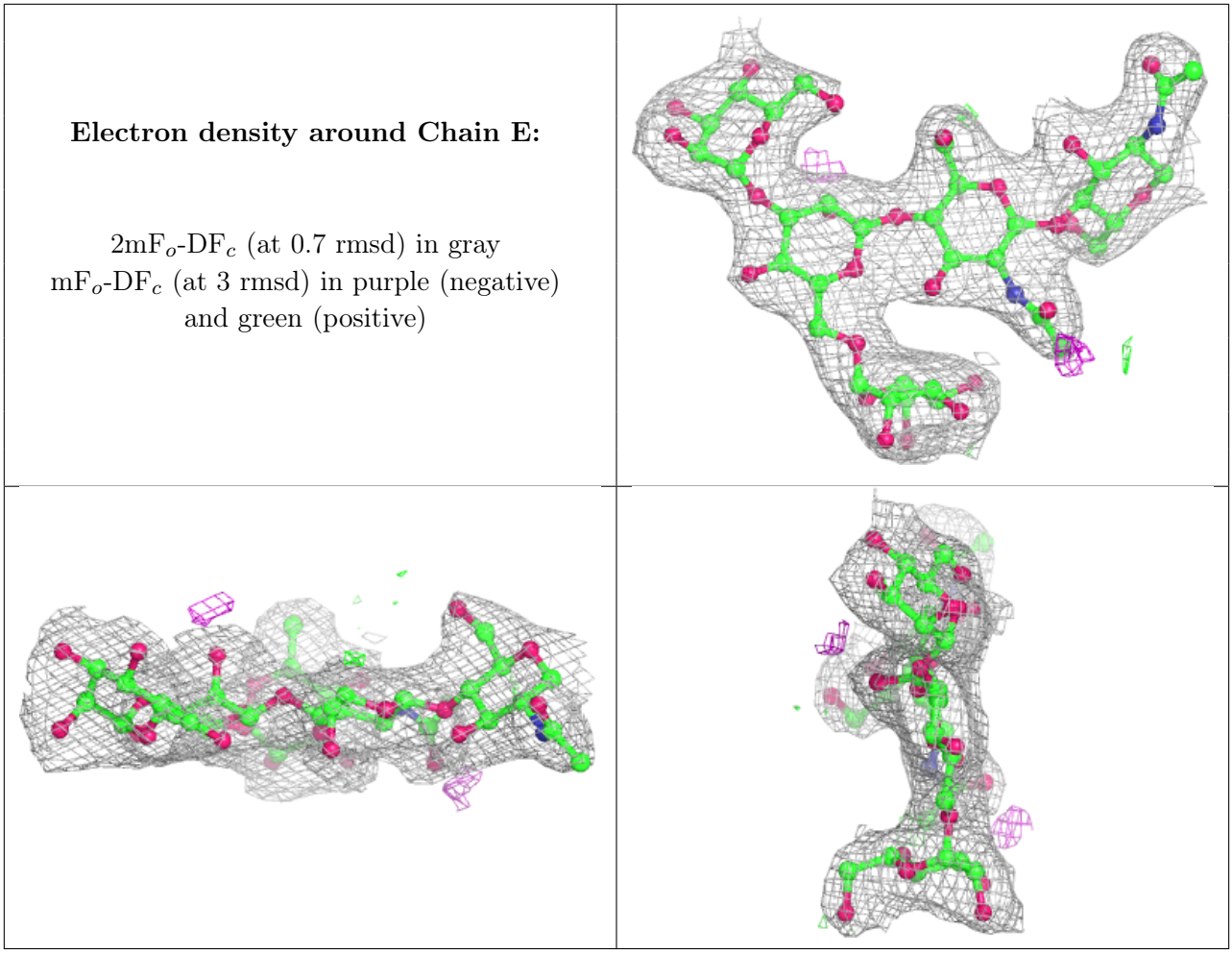
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.91	0.22	80,81,85,85	0
3	MAN	E	5	11/12	0.95	0.12	55,62,68,70	0
3	BMA	E	3	11/12	0.97	0.19	62,69,77,78	0
3	NAG	E	1	14/15	0.97	0.17	50,57,64,70	0
3	NAG	E	2	14/15	0.97	0.18	62,63,71,73	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.

Electron density around Chain E:

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



6.4 Ligands

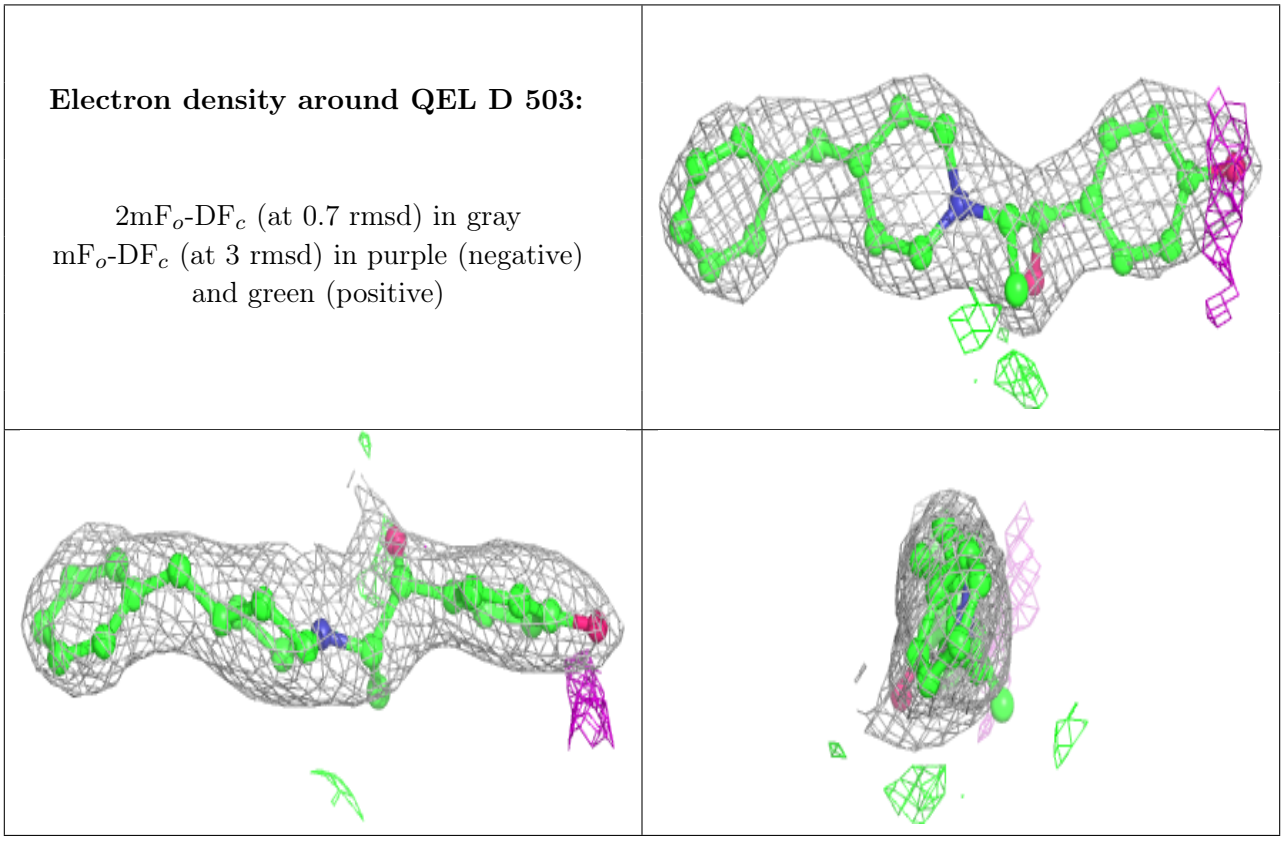
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NAG	D	502	14/15	0.64	0.47	164,170,173,174	0
5	NAG	D	501	14/15	0.71	0.48	154,160,163,164	0
5	NAG	B	502	14/15	0.72	0.36	142,147,153,153	0
4	NA	C	501	1/1	0.80	0.62	100,100,100,100	0
5	NAG	B	501	14/15	0.84	0.42	140,145,148,149	0
5	NAG	C	502	14/15	0.86	0.31	88,94,97,100	0
4	NA	A	501	1/1	0.91	0.17	65,65,65,65	0
6	QEL	D	503	24/24	0.93	0.18	64,69,73,77	0
5	NAG	A	502	14/15	0.96	0.18	58,69,76,77	0
6	QEL	B	503	24/24	0.98	0.14	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.

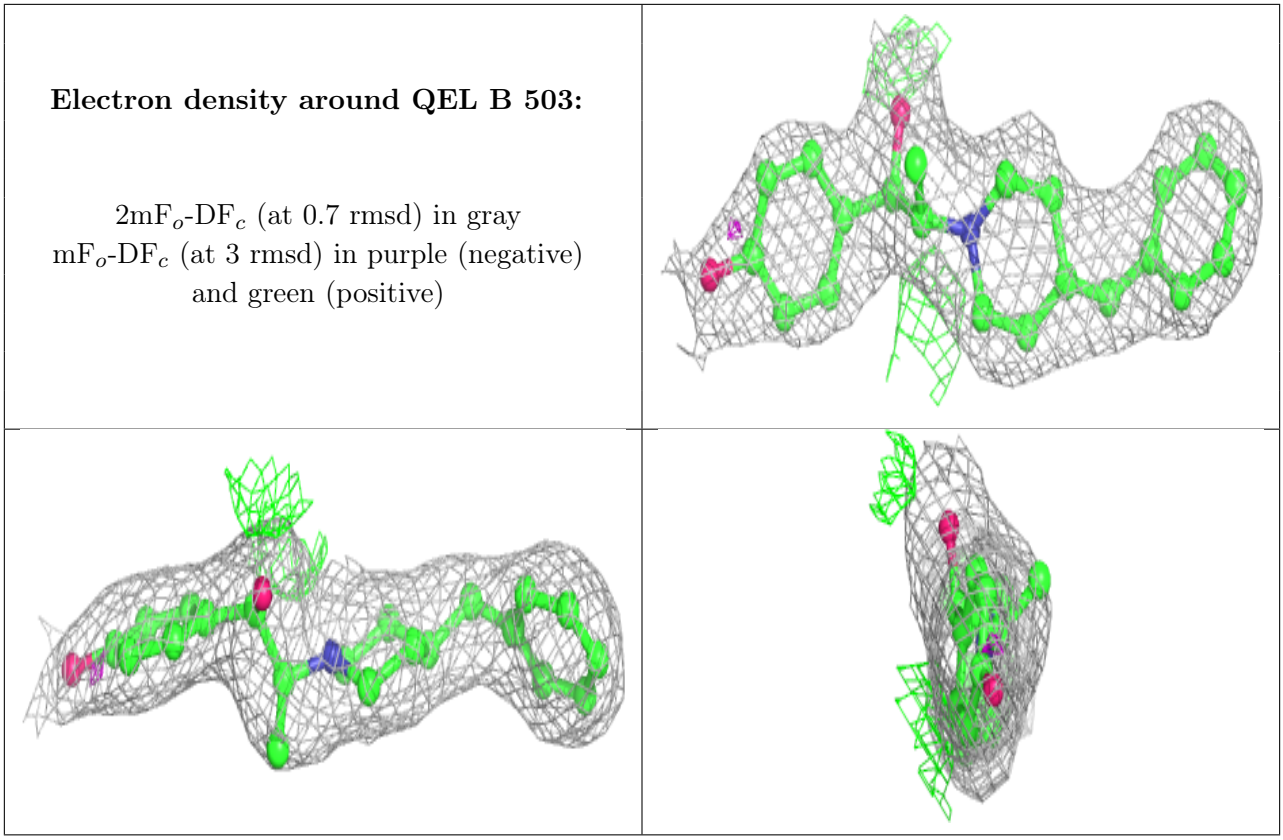
Electron density around QEL D 503:

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



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.