



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 5EWM / pdb_00005ewm
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX
WITH EVT-101
Authors : Pandit, J.
Deposited on : 2015-11-20
Resolution : 2.76 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

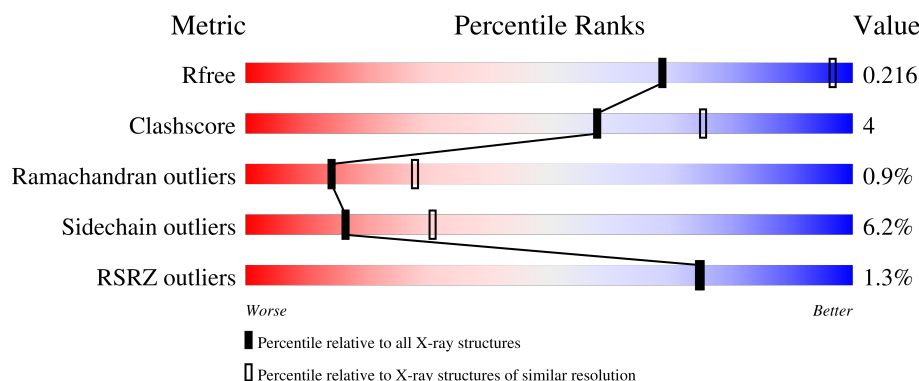
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	% 77% 14% • 8%
1	C	390	% 75% 13% •• 9%
2	B	364	2% 81% 15% •••
2	D	364	% 79% 16% •••

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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 11534 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

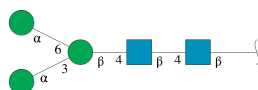
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2781	1793	443	530	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.

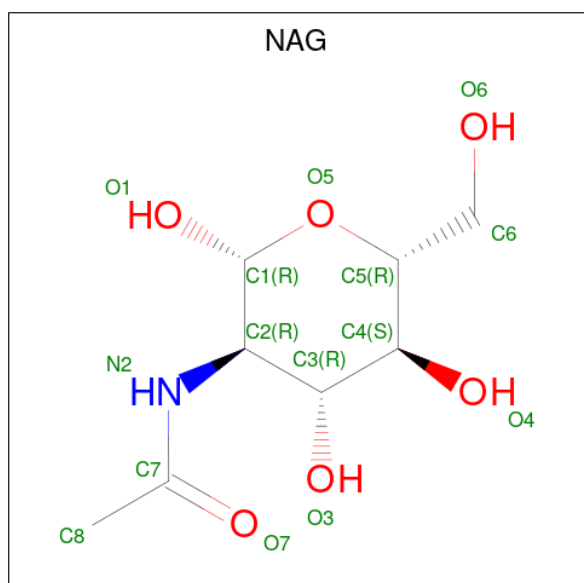


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

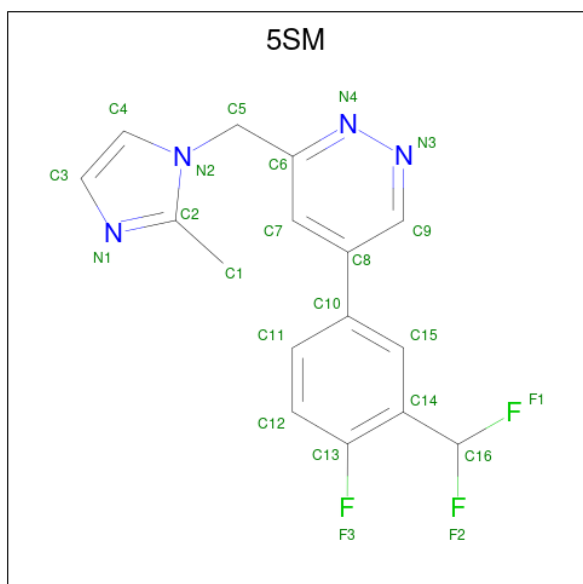
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- 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 5-[3-[bis(fluoranyl)methyl]-4-fluoranyl-phenyl]-3-[(2-methylimidazol-1-yl)methyl]pyridazine (CCD ID: 5SM) (formula: C₁₆H₁₃F₃N₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	F	N	0	0
			23	16	3	4		
6	D	1	Total	C	F	N	0	0
			23	16	3	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	115	Total	O	0	0
			115	115		

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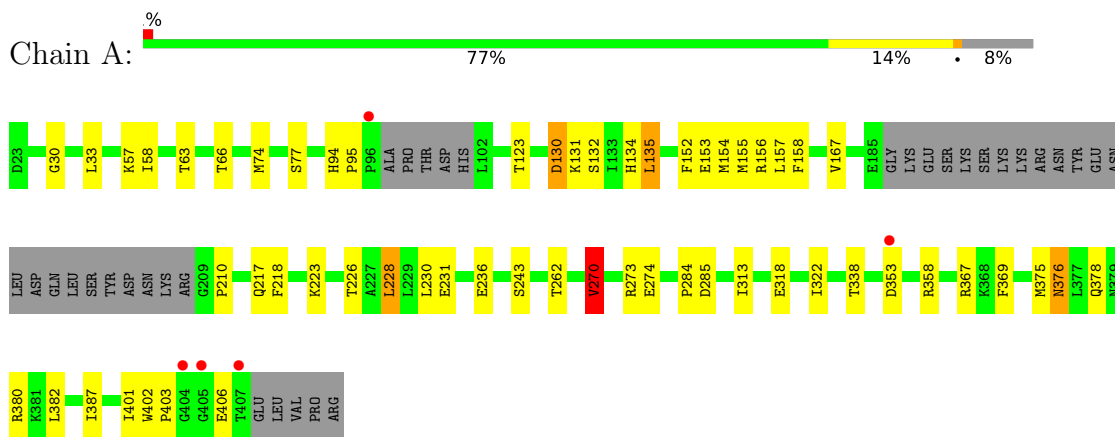
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	86	Total 86	O 86	0	0
7	C	39	Total 39	O 39	0	0
7	D	50	Total 50	O 50	0	0

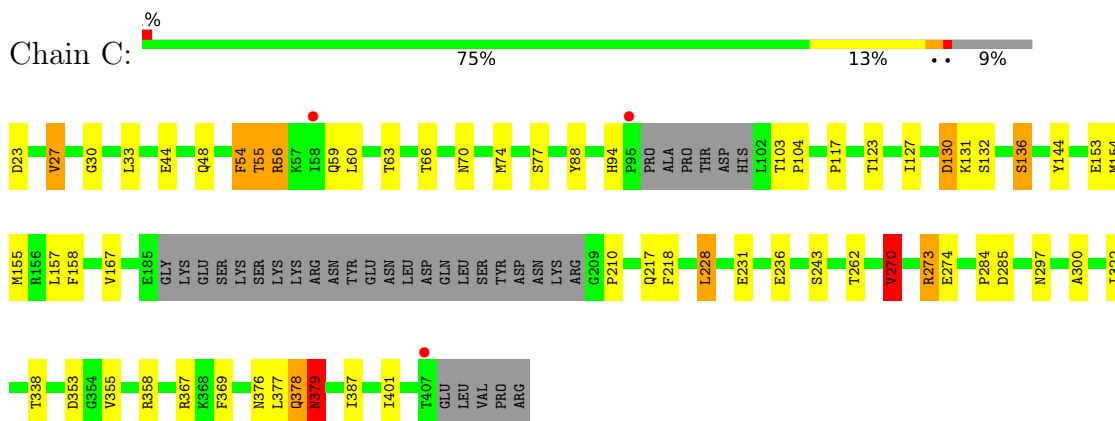
3 Residue-property plots

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.

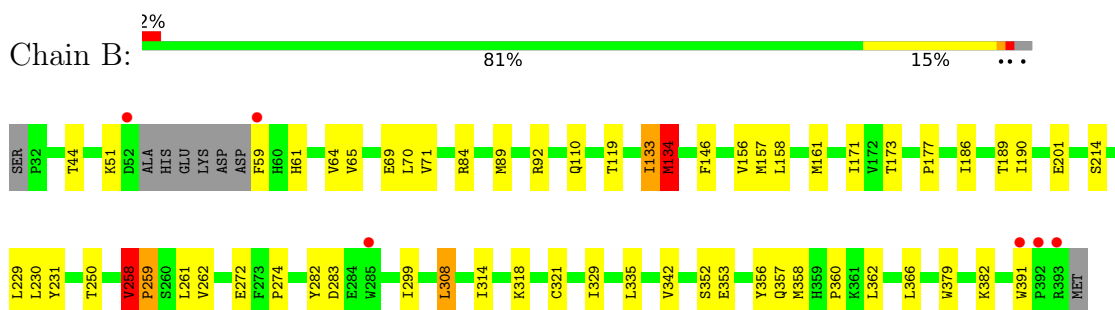
- Molecule 1: NMDA glutamate receptor subunit



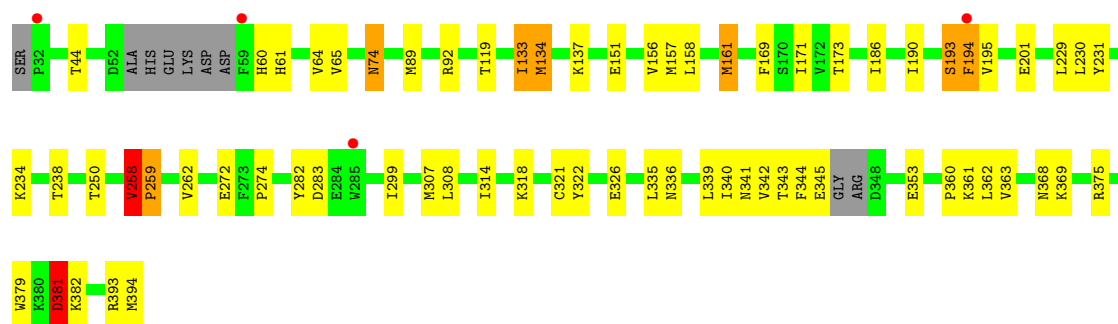
- Molecule 1: NMDA glutamate receptor subunit

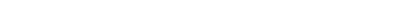


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Chain D:  %



- Chain E:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.40Å 60.61Å 144.50Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	40.41 – 2.76 40.41 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.41-2.76) 98.1 (40.41-2.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.171 , 0.211 0.172 , 0.216	Depositor DCC
R_{free} test set	2608 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.0	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	11534	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: MAN, NAG, 5SM, NA, BMA

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	0/2809	1.32	13/3819 (0.3%)
1	C	0.81	0/2792	1.32	8/3794 (0.2%)
2	B	0.88	1/2846 (0.0%)	1.32	7/3874 (0.2%)
2	D	0.85	1/2841 (0.0%)	1.36	17/3864 (0.4%)
All	All	0.88	2/11288 (0.0%)	1.33	45/15351 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	134	MET	SD-CE	-6.71	1.62	1.79
2	D	161	MET	SD-CE	-5.79	1.65	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	VAL	N-CA-CB	-9.61	101.27	112.32
1	C	130	ASP	CA-C-N	9.56	134.33	120.38
1	C	130	ASP	C-N-CA	9.56	134.33	120.38
2	D	341	ASN	CA-CB-CG	9.26	121.86	112.60
1	A	130	ASP	CA-C-N	8.27	132.46	120.38
1	A	130	ASP	C-N-CA	8.27	132.46	120.38
2	D	344	PHE	CA-CB-CG	8.14	121.94	113.80
2	D	61	HIS	N-CA-C	-8.12	104.25	114.56
1	A	270	VAL	N-CA-CB	-7.21	101.61	112.35
2	D	341	ASN	CB-CG-ND2	-7.21	105.59	116.40
2	B	189	THR	CA-C-N	7.05	130.47	120.53
2	B	189	THR	C-N-CA	7.05	130.47	120.53
2	D	381	ASP	CA-C-N	6.72	134.38	121.54
2	D	381	ASP	C-N-CA	6.72	134.38	121.54
2	D	341	ASN	OD1-CG-ND2	6.68	129.28	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PRO	N-CA-C	6.58	118.73	110.70
2	B	61	HIS	CA-C-N	6.56	135.41	123.27
2	B	61	HIS	C-N-CA	6.56	135.41	123.27
2	B	258	VAL	N-CA-CB	-6.01	102.79	111.21
1	C	131	LYS	CA-C-N	5.93	128.71	120.29
1	C	131	LYS	C-N-CA	5.93	128.71	120.29
1	A	134	HIS	CA-C-N	5.84	128.70	120.28
1	A	134	HIS	C-N-CA	5.84	128.70	120.28
2	D	195	VAL	N-CA-C	-5.72	106.19	113.22
2	D	258	VAL	N-CA-CB	-5.71	103.21	111.21
2	D	74	ASN	OD1-CG-ND2	5.63	128.24	122.60
1	A	131	LYS	CA-C-N	5.61	128.26	120.29
1	A	131	LYS	C-N-CA	5.61	128.26	120.29
2	D	60	HIS	CA-C-N	5.49	130.48	122.08
2	D	60	HIS	C-N-CA	5.49	130.48	122.08
1	C	231	GLU	CA-C-N	5.47	127.61	120.28
1	C	231	GLU	C-N-CA	5.47	127.61	120.28
1	A	231	GLU	CA-C-N	5.41	127.53	120.28
1	A	231	GLU	C-N-CA	5.41	127.53	120.28
1	C	54	PHE	CA-CB-CG	5.40	119.20	113.80
2	D	61	HIS	CA-C-N	5.33	130.44	120.95
2	D	61	HIS	C-N-CA	5.33	130.44	120.95
2	B	259	PRO	CA-C-N	5.25	128.69	120.82
2	B	259	PRO	C-N-CA	5.25	128.69	120.82
2	D	259	PRO	CA-C-N	5.19	128.61	120.82
2	D	259	PRO	C-N-CA	5.19	128.61	120.82
1	A	135	LEU	N-CA-C	5.19	117.68	111.71
2	D	393	ARG	N-CA-C	5.17	117.12	108.23
1	A	376	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	318	GLU	N-CA-C	-5.04	106.64	112.89

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	23	0
1	C	2737	0	2705	28	0
2	B	2781	0	2685	25	0
2	D	2778	0	2691	25	0
3	E	61	0	52	0	0
4	A	3	0	0	0	0
4	B	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	1	0
5	D	28	0	26	0	0
6	B	23	0	0	1	0
6	D	23	0	0	0	0
7	A	115	0	0	1	0
7	B	86	0	0	0	0
7	C	39	0	0	1	0
7	D	50	0	0	0	0
All	All	11534	0	10928	99	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 (99) 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:HD21	1:A:401:ILE:H	1.36	0.73
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.60	0.65
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.81	0.62
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.82	0.62
2:B:157:MET:HE2	2:B:229:LEU:HD22	1.83	0.61
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.84	0.60
2:B:230:LEU:O	2:B:259:PRO:HD3	2.02	0.60
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.84	0.58
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.84	0.58
2:B:110:GLN:HA	2:B:134:MET:HE3	1.84	0.58
2:D:157:MET:HE2	2:D:229:LEU:HD22	1.84	0.58
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.85	0.58
2:D:134:MET:HE2	2:D:137:LYS:HG2	1.86	0.58
2:D:230:LEU:O	2:D:259:PRO:HD3	2.03	0.58
1:C:70:ASN:HD21	2:D:322:TYR:HA	1.69	0.57
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG23	1:C:60:LEU:HD23	1.87	0.56
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.86	0.56
1:C:262:THR:HB	1:C:284:PRO:HB3	1.87	0.56
1:C:358:ARG:HD2	1:C:369:PHE:CD2	2.42	0.55
2:D:89:MET:HE1	2:D:119:THR:HG21	1.90	0.54
2:B:89:MET:HE1	2:B:119:THR:HG21	1.90	0.53
1:C:130:ASP:OD1	1:C:132:SER:HB3	2.08	0.53
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.90	0.53
2:B:258:VAL:HG13	2:B:262:VAL:HB	1.92	0.52
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.93	0.51
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.92	0.51
2:B:158:LEU:HA	2:B:161:MET:HE3	1.93	0.51
1:A:130:ASP:OD1	1:A:132:SER:HB3	2.10	0.51
2:D:368:ASN:HA	2:D:394:MET:HE2	1.91	0.51
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.92	0.51
2:B:133:ILE:HD11	2:B:261:LEU:HD22	1.92	0.50
1:A:262:THR:HB	1:A:284:PRO:HB3	1.93	0.49
1:C:379:ASN:HB2	7:C:615:HOH:O	2.12	0.49
2:D:158:LEU:HA	2:D:161:MET:HE3	1.93	0.49
1:C:74:MET:HE3	1:C:77:SER:HB3	1.93	0.49
1:C:117:PRO:HA	1:C:136:SER:HB3	1.94	0.49
1:A:57:LYS:HB2	7:A:695:HOH:O	2.13	0.48
2:B:329:ILE:HD12	2:D:314:ILE:HD11	1.95	0.48
1:A:74:MET:HE3	1:A:77:SER:HB3	1.94	0.48
1:A:33:LEU:O	1:A:66:THR:HA	2.14	0.48
1:C:55:THR:HG23	1:C:59:GLN:HB2	1.96	0.48
2:B:146:PHE:HA	2:B:357:GLN:HG3	1.95	0.47
2:D:307:MET:HE2	2:D:314:ILE:HA	1.95	0.47
1:C:27:VAL:HG12	1:C:88:TYR:CE1	2.49	0.47
1:C:94:HIS:CE1	1:C:123:THR:HG23	2.50	0.47
1:C:33:LEU:O	1:C:66:THR:HA	2.15	0.47
1:A:402:TRP:CD1	1:A:406:GLU:HA	2.47	0.46
1:C:155:MET:HE2	1:C:210:PRO:HB2	1.98	0.46
2:B:89:MET:CE	2:B:321:CYS:SG	3.04	0.46
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.80	0.46
1:A:30:GLY:HA2	1:A:63:THR:O	2.16	0.46
2:B:352:SER:HA	2:B:358:MET:HE2	1.98	0.46
2:D:250:THR:HB	2:D:274:PRO:HB3	1.97	0.46
1:A:155:MET:HE2	1:A:210:PRO:HB2	1.97	0.45
2:D:89:MET:CE	2:D:321:CYS:SG	3.05	0.45
2:B:299:ILE:HA	2:B:342:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:THR:HB	2:B:274:PRO:HB3	1.99	0.44
1:C:157:LEU:HD23	1:C:158:PHE:CE1	2.53	0.44
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.99	0.44
1:C:167:VAL:O	1:C:217:GLN:HA	2.17	0.44
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.99	0.44
2:B:133:ILE:HG22	2:B:356:TYR:CE1	2.53	0.43
2:B:282:TYR:HE1	2:B:360:PRO:HB3	1.84	0.43
1:A:157:LEU:HD23	1:A:158:PHE:CE1	2.53	0.43
1:A:322:ILE:HG23	1:A:338:THR:HG21	2.01	0.43
1:A:376:ASN:HD22	1:A:378:GLN:HE21	1.67	0.43
1:C:297:ASN:HB3	1:C:300:ALA:HB3	2.00	0.43
1:A:167:VAL:O	1:A:217:GLN:HA	2.18	0.43
1:A:375:MET:HB3	1:A:382:LEU:HD22	2.00	0.43
1:C:376:ASN:HD21	1:C:401:ILE:H	1.66	0.43
2:B:177:PRO:HG2	6:B:503:5SM:C1	2.48	0.42
1:C:30:GLY:HA2	1:C:63:THR:O	2.19	0.42
1:C:322:ILE:HG23	1:C:338:THR:HG21	2.01	0.42
1:A:154:MET:HE2	1:A:154:MET:HB2	1.81	0.42
1:A:167:VAL:HG12	1:A:243:SER:HB3	2.02	0.42
1:C:378:GLN:HG2	1:C:401:ILE:HD12	2.01	0.42
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.55	0.42
2:D:282:TYR:HE1	2:D:360:PRO:CB	2.33	0.42
1:A:152:PHE:CE2	1:A:156:ARG:HD2	2.55	0.41
2:B:51:LYS:HE3	2:B:70:LEU:HD22	2.02	0.41
1:C:154:MET:HE2	1:C:154:MET:HB2	1.82	0.41
2:D:308:LEU:HB2	2:D:314:ILE:HG23	2.01	0.41
2:D:363:VAL:HG11	2:D:375:ARG:HG2	2.00	0.41
2:B:156:VAL:HG22	2:B:379:TRP:CD2	2.55	0.41
1:C:378:GLN:CG	1:C:401:ILE:HD12	2.50	0.41
1:C:355:VAL:HG11	5:C:502:NAG:H82	2.01	0.41
1:A:58:ILE:HD13	1:A:313:ILE:HG22	2.02	0.41
1:C:167:VAL:HG12	1:C:243:SER:HB3	2.02	0.40
2:D:156:VAL:HG22	2:D:379:TRP:CD2	2.55	0.40
2:B:308:LEU:HB2	2:B:314:ILE:HG23	2.02	0.40
1:A:94:HIS:CE1	1:A:123:THR:HG23	2.57	0.40
1:A:358:ARG:HD3	1:A:369:PHE:CD2	2.56	0.40
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.37	0.40
2:D:234:LYS:O	2:D:238:THR:HG23	2.22	0.40
2:B:366:LEU:HD13	2:B:391:TRP:HZ2	1.86	0.40
1:C:103:THR:HB	1:C:104:PRO:CD	2.52	0.40
2:D:134:MET:CE	2:D:137:LYS:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:ASN:HA	2:D:339:LEU:HD12	2.04	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%)	343 (98%)	7 (2%)	1 (0%)	36	56
1	C	350/390 (90%)	338 (97%)	8 (2%)	4 (1%)	11	22
2	B	352/364 (97%)	334 (95%)	17 (5%)	1 (0%)	36	56
2	D	349/364 (96%)	334 (96%)	9 (3%)	6 (2%)	7	14
All	All	1402/1508 (93%)	1349 (96%)	41 (3%)	12 (1%)	14	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	382	LYS
2	B	283	ASP
1	C	54	PHE
1	C	56	ARG
2	D	194	PHE
2	D	283	ASP
1	C	379	ASN
2	D	381	ASP
2	D	193	SER
1	C	55	THR
2	D	133	ILE
1	A	403	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	292/336 (87%)	278 (95%)	14 (5%)	23	44
1	C	289/336 (86%)	270 (93%)	19 (7%)	15	29
2	B	301/326 (92%)	283 (94%)	18 (6%)	17	32
2	D	305/326 (94%)	282 (92%)	23 (8%)	12	24
All	All	1187/1324 (90%)	1113 (94%)	74 (6%)	16	31

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	153	GLU
1	A	223	LYS
1	A	226	THR
1	A	228	LEU
1	A	230	LEU
1	A	236	GLU
1	A	270	VAL
1	A	273	ARG
1	A	285	ASP
1	A	353	ASP
1	A	367	ARG
1	A	380	ARG
1	A	387	ILE
2	B	44	THR
2	B	59	PHE
2	B	64	VAL
2	B	65	VAL
2	B	69	GLU
2	B	92	ARG
2	B	133	ILE
2	B	134	MET
2	B	190	ILE
2	B	201	GLU

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Mol	Chain	Res	Type
2	B	214	SER
2	B	258	VAL
2	B	272	GLU
2	B	308	LEU
2	B	318	LYS
2	B	335	LEU
2	B	353	GLU
2	B	382	LYS
1	C	23	ASP
1	C	27	VAL
1	C	44	GLU
1	C	48	GLN
1	C	56	ARG
1	C	127	ILE
1	C	136	SER
1	C	153	GLU
1	C	228	LEU
1	C	236	GLU
1	C	270	VAL
1	C	273	ARG
1	C	285	ASP
1	C	353	ASP
1	C	367	ARG
1	C	377	LEU
1	C	378	GLN
1	C	379	ASN
1	C	387	ILE
2	D	44	THR
2	D	64	VAL
2	D	65	VAL
2	D	74	ASN
2	D	92	ARG
2	D	133	ILE
2	D	134	MET
2	D	151	GLU
2	D	193	SER
2	D	194	PHE
2	D	201	GLU
2	D	258	VAL
2	D	272	GLU
2	D	318	LYS
2	D	326	GLU

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Mol	Chain	Res	Type
2	D	335	LEU
2	D	340	ILE
2	D	343	THR
2	D	345	GLU
2	D	353	GLU
2	D	361	LYS
2	D	369	LYS
2	D	381	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	73	GLN
1	A	376	ASN
1	A	384	GLN
2	B	311	HIS
1	C	53	HIS
1	C	61	GLN
1	C	73	GLN
1	C	147	GLN
1	C	376	ASN
1	C	384	GLN
2	D	110	GLN
2	D	311	HIS
2	D	323	ASN
2	D	357	GLN

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	0.39	0	17,19,21	0.57	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
3	BMA	E	3	3	11,11,12	0.26	0	15,15,17	0.87	1 (6%)
3	MAN	E	4	3	11,11,12	0.34	0	15,15,17	0.69	0
3	MAN	E	5	3	11,11,12	0.32	0	15,15,17	0.76	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(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	2.60	115.67	112.19
3	E	2	NAG	C1-C2-N2	-2.59	106.35	110.43

There are no chirality outliers.

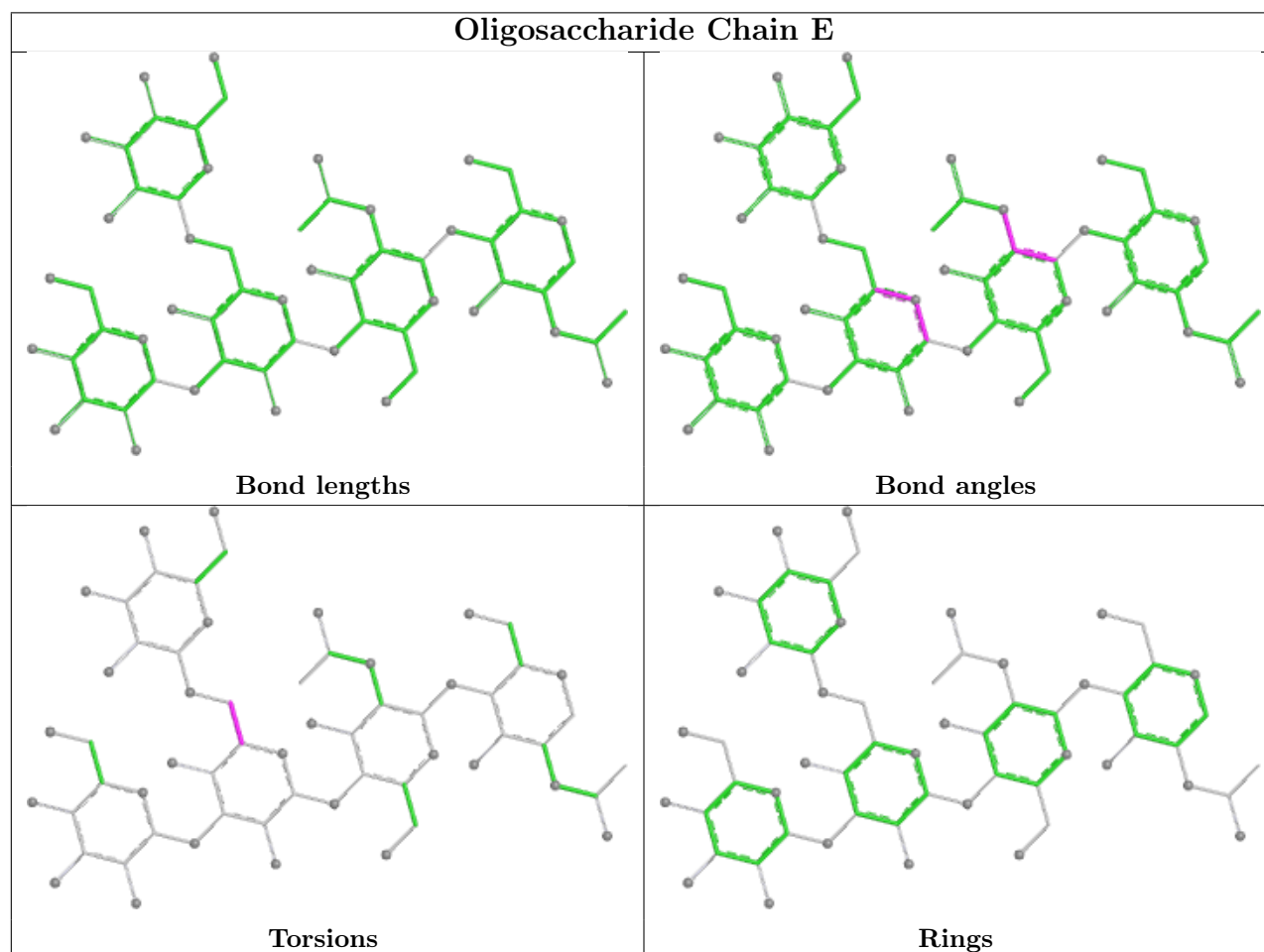
All (1) torsion outliers are listed below:

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 13 ligands modelled in this entry, 5 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	D	501	2	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	D	502	2	14,14,15	0.34	0	17,19,21	0.70	0
5	NAG	A	502	1	14,14,15	0.32	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	502	2	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
6	5SM	D	503	-	24,25,25	0.26	0	30,35,35	0.64	0
5	NAG	C	502	1	14,14,15	0.42	0	17,19,21	0.74	0
6	5SM	B	503	-	24,25,25	0.30	0	30,35,35	0.95	1 (3%)
5	NAG	B	501	2	14,14,15	0.31	0	17,19,21	0.88	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	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	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	B	502	2	-	0/6/23/26	0/1/1/1
6	5SM	D	503	-	-	2/12/12/12	0/3/3/3
5	NAG	C	502	1	-	0/6/23/26	0/1/1/1
6	5SM	B	503	-	-	1/12/12/12	0/3/3/3
5	NAG	B	501	2	-	1/6/23/26	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(°)
6	B	503	5SM	F1-C16-C14	-3.45	106.97	110.64
5	A	502	NAG	C1-O5-C5	3.37	116.70	112.19
5	B	502	NAG	O5-C1-C2	2.93	115.83	111.29
5	B	501	NAG	O5-C1-C2	2.19	114.67	111.29
5	B	502	NAG	C1-O5-C5	2.07	114.97	112.19
5	B	501	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
6	B	503	5SM	C13-C14-C16-F1
6	D	503	5SM	C13-C14-C16-F1

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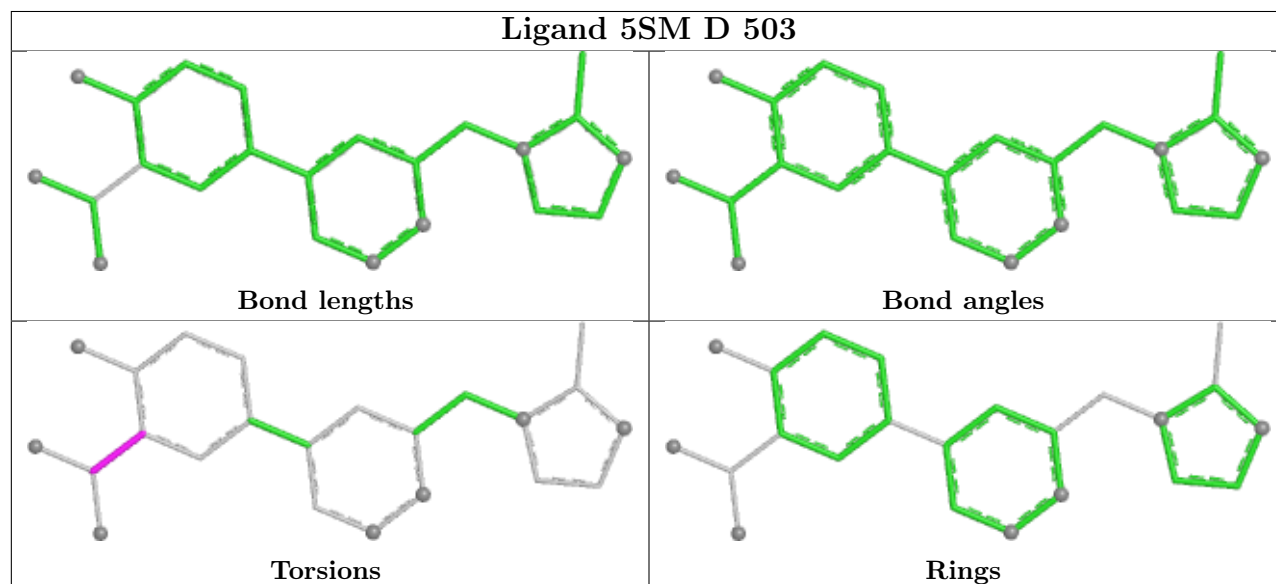
Mol	Chain	Res	Type	Atoms
6	D	503	5SM	C13-C14-C16-F2
5	D	502	NAG	C4-C5-C6-O6

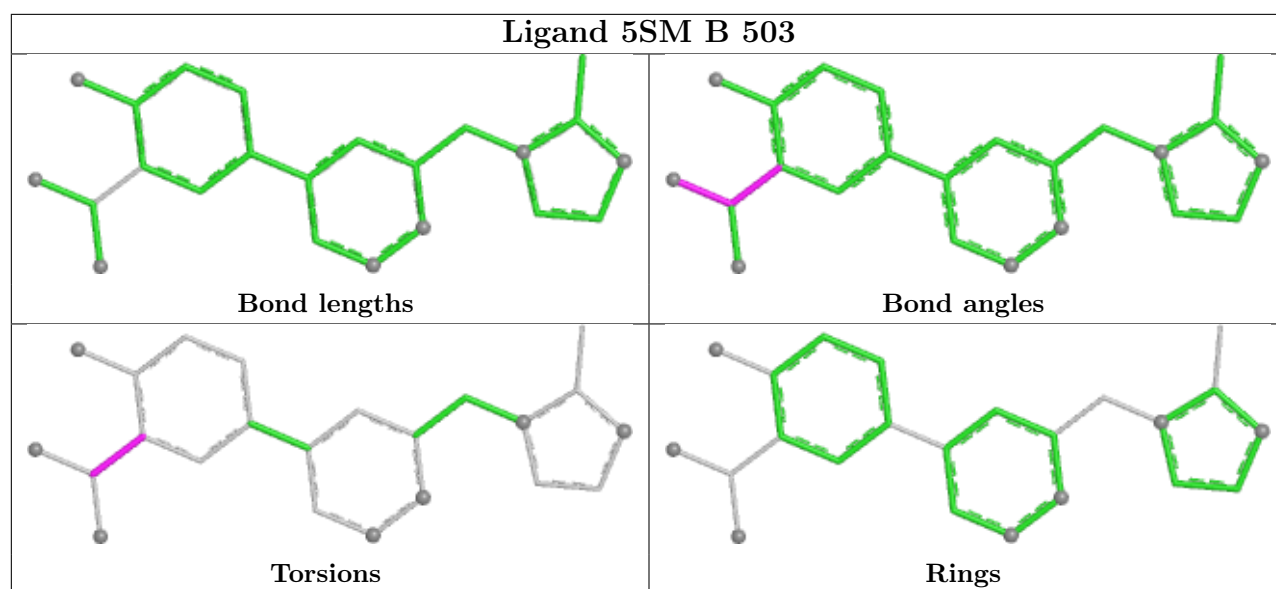
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	NAG	1	0
6	B	503	5SM	1	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%)	-0.50	5 (1%) 73 73	36, 53, 85, 109	0
1	C	356/390 (91%)	0.01	3 (0%) 82 82	61, 87, 116, 145	0
2	B	356/364 (97%)	-0.18	6 (1%) 69 67	44, 73, 109, 142	0
2	D	355/364 (97%)	-0.07	4 (1%) 78 77	55, 80, 120, 139	0
All	All	1424/1508 (94%)	-0.19	18 (1%) 75 75	36, 76, 113, 145	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	392	PRO	4.5
2	B	52	ASP	3.4
2	D	32	PRO	3.2
2	B	393	ARG	3.1
2	D	194	PHE	3.0
2	B	391	TRP	2.9
2	B	59	PHE	2.9
1	A	353	ASP	2.8
1	A	96	PRO	2.8
1	C	407	THR	2.7
2	D	285	TRP	2.6
1	C	95	PRO	2.6
1	A	405	GLY	2.6
2	B	285	TRP	2.6
2	D	59	PHE	2.5
1	A	407	THR	2.2
1	A	404	GLY	2.1
1	C	58	ILE	2.0

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

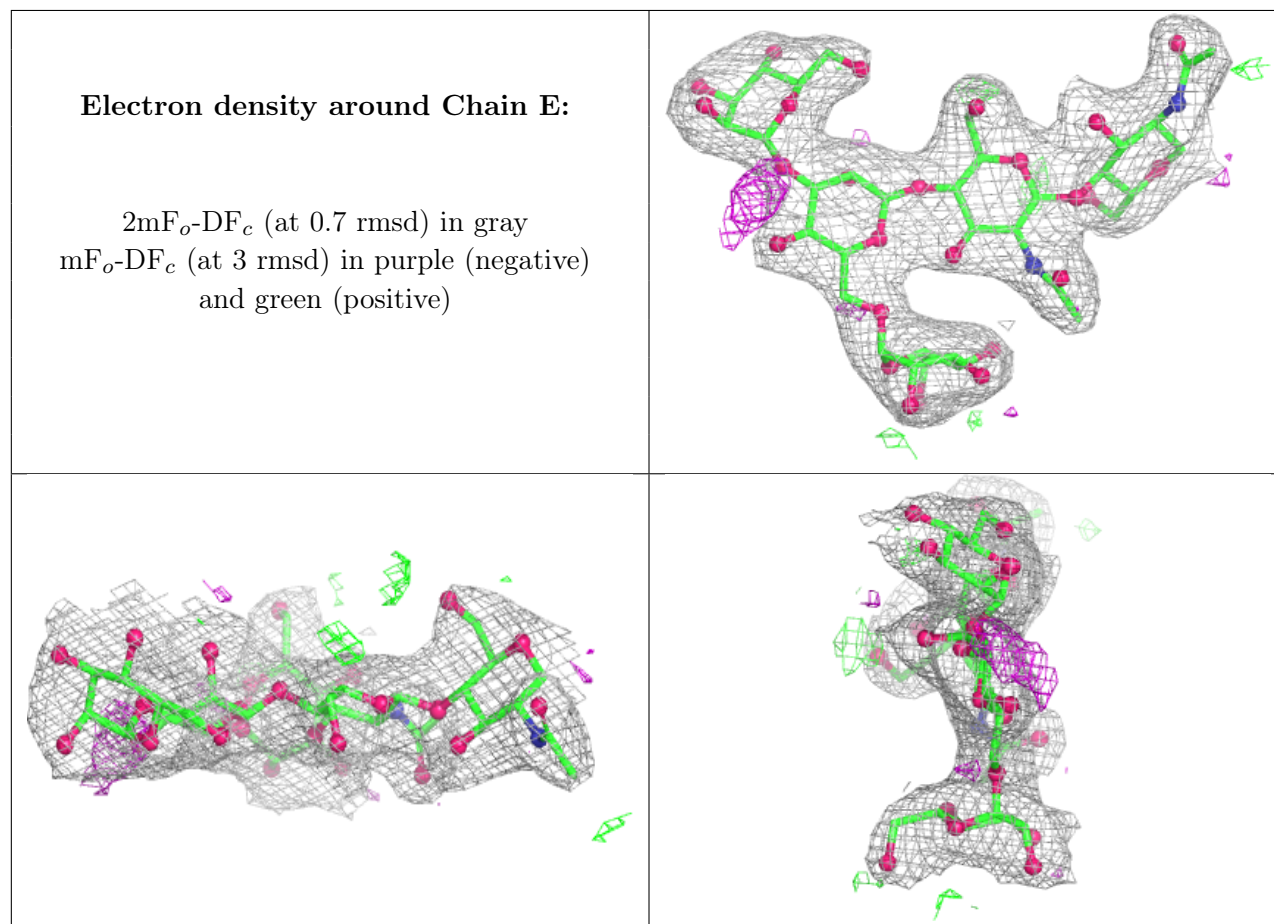
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.85	0.10	88,89,93,96	0
3	BMA	E	3	11/12	0.93	0.08	62,69,75,83	0
3	NAG	E	2	14/15	0.94	0.07	61,65,68,69	0
3	NAG	E	1	14/15	0.95	0.08	45,59,64,68	0
3	MAN	E	5	11/12	0.96	0.07	55,61,69,71	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

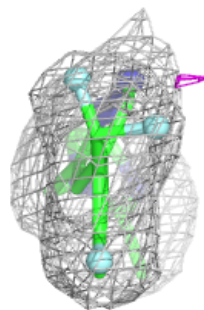
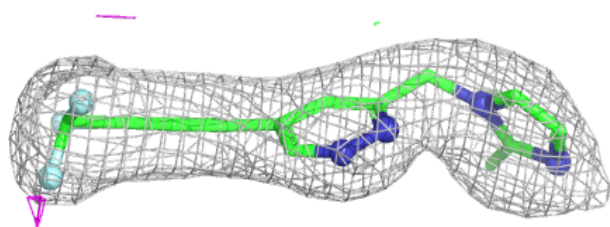
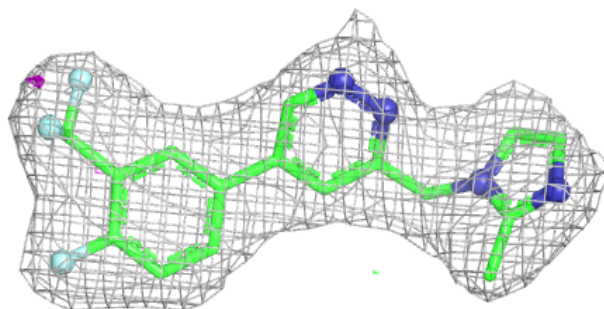
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	D	501	14/15	0.28	0.14	150,154,158,160	0
5	NAG	B	502	14/15	0.46	0.15	128,136,142,145	0
5	NAG	D	502	14/15	0.50	0.14	152,158,161,163	0
5	NAG	B	501	14/15	0.59	0.14	140,143,145,147	0
5	NAG	C	502	14/15	0.82	0.13	98,105,107,111	0
4	NA	C	501	1/1	0.84	0.23	80,80,80,80	0
4	NA	A	501	1/1	0.85	0.27	67,67,67,67	0
4	NA	A	509	1/1	0.90	0.09	62,62,62,62	0
4	NA	A	508	1/1	0.93	0.07	45,45,45,45	0
5	NAG	A	502	14/15	0.94	0.07	56,69,75,79	0
6	5SM	B	503	23/23	0.97	0.07	42,48,57,60	0
4	NA	B	504	1/1	0.98	0.05	57,57,57,57	0
6	5SM	D	503	23/23	0.98	0.07	66,71,72,73	0

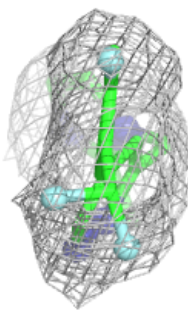
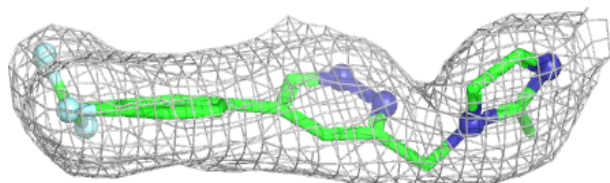
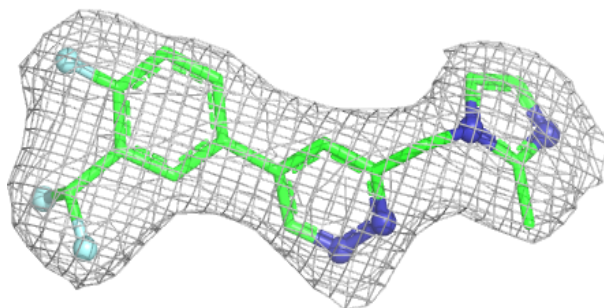
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5SM 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 5SM D 503:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.