



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:04 AM EDT

PDB ID : 6E7V
Title : Heterodimer of the GluN1b-GluN2B NMDA receptor amino-terminal domains bound to allosteric inhibitor 93-88
Authors : Regan, M.C.; Furukawa, H.
Deposited on : 2018-07-27
Resolution : 2.60 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)
Xtrriage (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

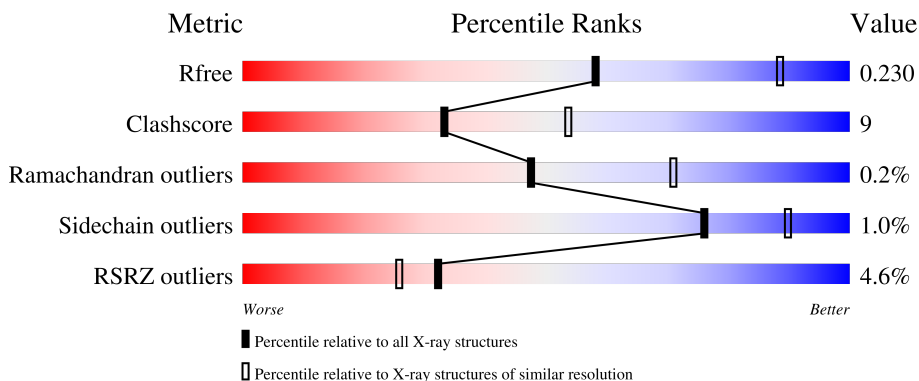
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	385	 0% 76% 17% 7%
1	C	385	 6% 73% 19% 7%
2	B	363	 5% 86% 13%
2	D	363	 6% 83% 15%
3	E	5	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	507	-	-	-	X
4	NAG	C	502	-	-	-	X
6	CL	A	510	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2750	1756	480	504	10	0	0	0
1	C	357	2714	1732	470	501	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
A	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	61	GLN	ASN	engineered mutation	UNP A0A1L8F5J9
C	371	GLN	ASN	engineered mutation	UNP A0A1L8F5J9

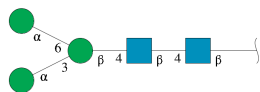
- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	360	2760	1780	436	529	15	0	0	0
2	D	357	2693	1734	429	514	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

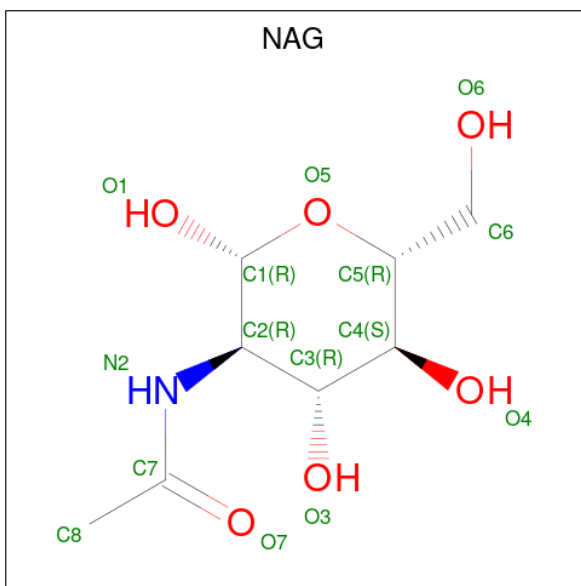
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	C	1	13	7	1	5	0	0
4	C	1	14	8	1	5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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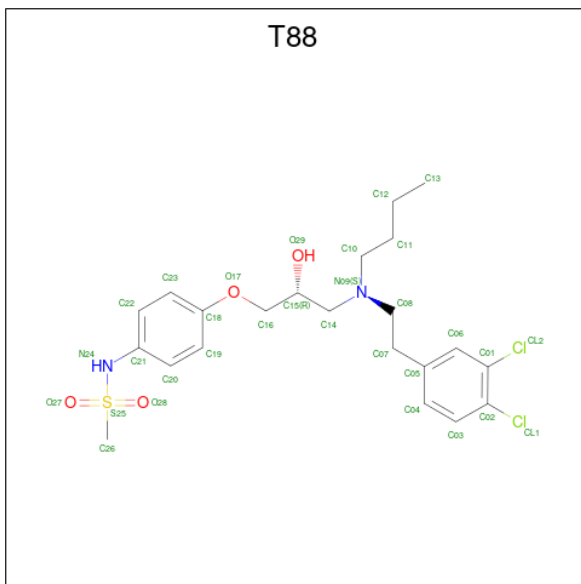
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	B	4	Total Cl 4 4	0	0
6	C	2	Total Cl 2 2	0	0
6	D	3	Total Cl 3 3	0	0

- Molecule 7 is N-{4-[(2R)-3-{butyl[2-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropoxy]phenyl}methanesulfonamide (three-letter code: T88) (formula: C₂₂H₃₀Cl₂N₂O₄S) (labeled as "Ligand of Interest" by depositor).



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

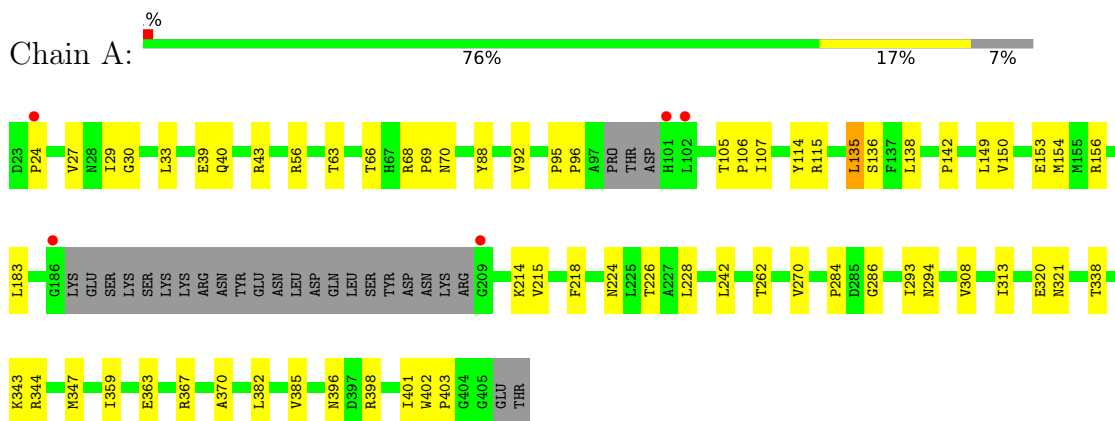
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	99	Total O 99 99	0	0
8	B	54	Total O 54 54	0	0
8	C	56	Total O 56 56	0	0
8	D	34	Total O 34 34	0	0

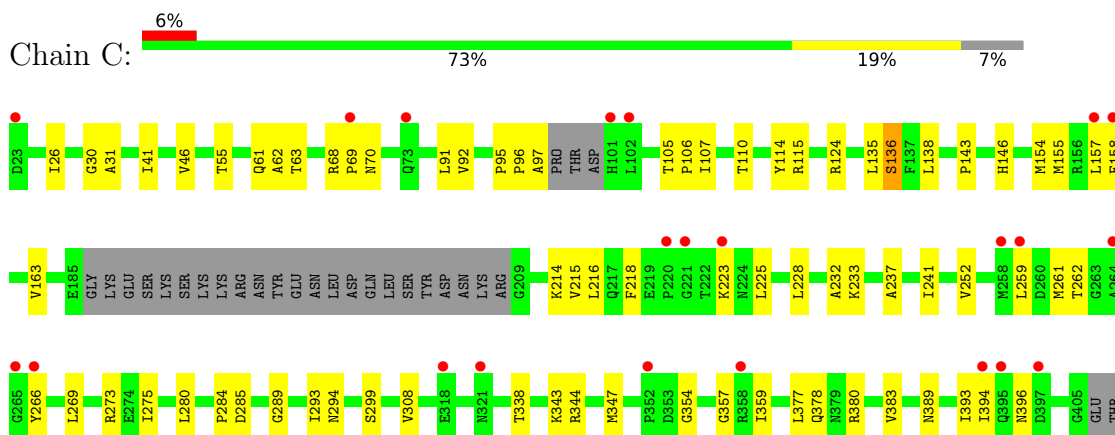
3 Residue-property plots

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.

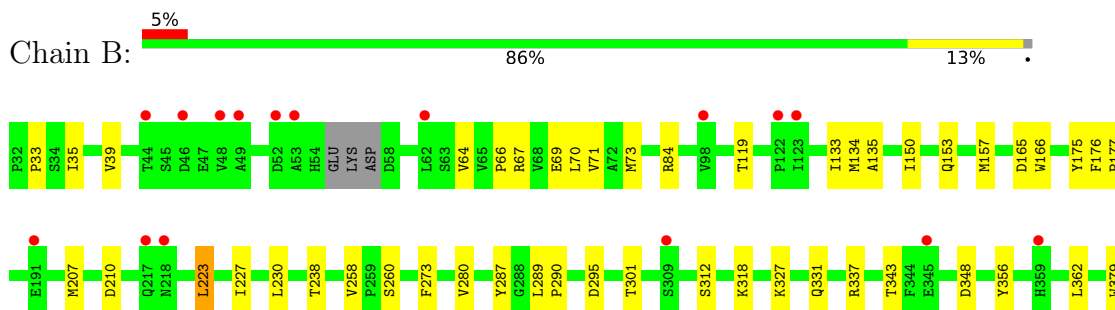
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Glutamate receptor ionotropic, NMDA 1



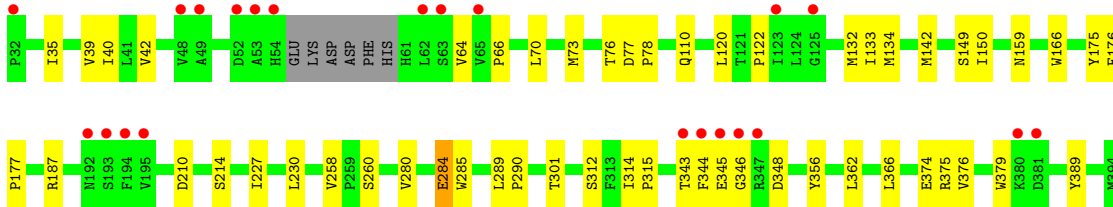
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B





- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D: 6% 83% 15%



- 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: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.13Å 59.61Å 145.53Å 90.00° 116.86° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 34.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	73.6 (25.00-2.60) 73.8 (34.29-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.233 0.195 , 0.230	Depositor DCC
R_{free} test set	2329 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11365	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: T88, MAN, NAG, CL, BMA, 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	0.21	0/2808	0.36	0/3818
1	C	0.20	0/2770	0.36	0/3771
2	B	0.21	0/2824	0.36	0/3853
2	D	0.20	0/2754	0.36	0/3761
All	All	0.21	0/11156	0.36	0/15203

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	389	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2750	0	2714	44	0
1	C	2714	0	2662	63	1
2	B	2760	0	2605	29	1
2	D	2693	0	2527	42	0
3	E	61	0	52	0	0
4	A	28	0	26	1	0
4	B	14	0	13	0	0
4	C	27	0	22	4	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	3	0
6	B	4	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	1	0
7	B	31	0	0	5	0
7	D	31	0	0	9	0
8	A	99	0	0	1	0
8	B	54	0	0	2	0
8	C	56	0	0	4	0
8	D	34	0	0	3	0
All	All	11365	0	10621	186	1

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 9.

All (186) 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:C:232:ALA:O	8:C:601:HOH:O	1.73	1.03
4:C:501:NAG:C8	4:C:501:NAG:N2	2.25	1.00
4:C:501:NAG:C8	4:C:501:NAG:O7	2.15	0.95
1:C:233:LYS:O	8:C:602:HOH:O	1.87	0.92
1:C:157:LEU:HD23	1:C:158:PHE:CE2	2.08	0.89
1:A:135:LEU:HD23	7:B:502:T88:C16	2.04	0.88
2:B:312:SER:O	8:B:601:HOH:O	1.97	0.83
2:D:343:THR:HG22	2:D:348:ASP:HA	1.60	0.83
4:C:501:NAG:N2	4:C:501:NAG:O7	2.18	0.76
1:A:29:ILE:HD11	1:A:313:ILE:CD1	2.15	0.76
1:A:40:GLN:OE1	1:A:43:ARG:NH1	2.20	0.75
1:A:29:ILE:HD11	1:A:313:ILE:HD11	1.68	0.74
1:A:218:PHE:HB3	1:A:228:LEU:HD13	1.70	0.74
2:B:175:TYR:HB2	7:B:502:T88:C26	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:HG21	1:C:359:ILE:HG21	1.73	0.70
1:C:261:MET:HA	1:C:266:TYR:CE2	2.27	0.70
1:C:259:LEU:HB2	1:C:261:MET:HE2	1.74	0.69
2:B:343:THR:HG22	2:B:348:ASP:HA	1.76	0.68
1:C:155:MET:HE3	1:C:163:VAL:HG21	1.77	0.67
1:A:153:GLU:OE2	1:A:156:ARG:NH1	2.27	0.67
2:D:120:LEU:C	2:D:142:MET:CE	2.63	0.67
2:D:133:ILE:HG23	6:D:503:CL:CL	2.31	0.67
1:C:262:THR:HB	1:C:284:PRO:HB3	1.77	0.67
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.75	0.67
1:C:273:ARG:HD3	8:C:636:HOH:O	1.94	0.66
1:A:218:PHE:HB3	1:A:228:LEU:CD1	2.25	0.66
1:C:110:THR:HA	7:D:502:T88:CL2	2.33	0.66
1:A:135:LEU:CD2	7:B:502:T88:C16	2.73	0.65
1:A:396:ASN:O	6:A:510:CL:CL	2.52	0.65
1:A:398:ARG:O	6:A:510:CL:CL	2.52	0.64
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.78	0.64
1:C:228:LEU:C	1:C:228:LEU:HD23	2.18	0.63
1:A:359:ILE:HD13	1:A:367:ARG:CZ	2.29	0.63
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.34	0.63
1:C:157:LEU:HD23	1:C:158:PHE:CD2	2.33	0.63
1:C:68:ARG:HB3	1:C:69:PRO:HD2	1.79	0.62
2:B:119:THR:O	2:B:318:LYS:HE3	1.99	0.62
1:C:218:PHE:HB3	1:C:228:LEU:CD1	2.31	0.61
2:D:35:ILE:HG23	2:D:64:VAL:HG11	1.82	0.61
7:B:502:T88:C10	7:B:502:T88:C04	2.79	0.61
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.83	0.60
2:B:165:ASP:OD1	8:B:602:HOH:O	2.15	0.60
1:C:26:ILE:HG21	1:C:61:GLN:OE1	2.03	0.59
2:D:133:ILE:HD12	2:D:150:ILE:HG12	1.85	0.58
1:C:354:GLY:HA3	1:C:359:ILE:HD11	1.85	0.58
1:C:154:MET:HG2	1:C:393:ILE:CD1	2.34	0.58
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.85	0.58
7:B:502:T88:C11	7:B:502:T88:O29	2.52	0.58
2:D:110:GLN:HA	2:D:134:MET:SD	2.43	0.58
2:D:133:ILE:HG13	2:D:133:ILE:O	2.03	0.58
1:A:242:LEU:HB3	1:A:270:VAL:HG12	1.85	0.57
2:B:35:ILE:HG23	2:B:64:VAL:HG21	1.86	0.57
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.85	0.57
2:D:35:ILE:HG23	2:D:64:VAL:CG1	2.35	0.56
2:D:175:TYR:HB2	7:D:502:T88:C26	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:GLY:O	1:C:359:ILE:HD12	2.07	0.55
1:C:293:ILE:O	1:C:294:ASN:HB2	2.07	0.54
1:C:218:PHE:HB3	1:C:228:LEU:HD13	1.87	0.54
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.89	0.54
1:A:293:ILE:O	1:A:294:ASN:HB2	2.08	0.53
1:C:228:LEU:HD23	1:C:228:LEU:O	2.07	0.53
2:D:187:ARG:NH1	8:D:605:HOH:O	2.35	0.53
1:A:114:TYR:O	1:A:115:ARG:HB2	2.08	0.53
1:C:394:ILE:HD11	4:C:502:NAG:H61	1.90	0.53
1:A:344:ARG:NE	2:B:210:ASP:OD1	2.38	0.53
1:C:30:GLY:HA2	1:C:63:THR:O	2.08	0.52
1:C:105:THR:HB	1:C:106:PRO:HD3	1.92	0.52
1:C:261:MET:HG2	1:C:266:TYR:CZ	2.45	0.52
1:C:354:GLY:HA3	1:C:359:ILE:CD1	2.40	0.52
2:D:312:SER:O	8:D:601:HOH:O	2.18	0.51
2:B:327:LYS:O	2:B:331:GLN:HG3	2.10	0.51
1:C:154:MET:HG2	1:C:393:ILE:HD11	1.92	0.51
1:A:150:VAL:O	1:A:154:MET:HG3	2.09	0.51
1:C:285:ASP:HA	1:C:377:LEU:HD23	1.92	0.51
2:D:120:LEU:C	2:D:142:MET:HE2	2.30	0.51
1:A:385:VAL:O	6:A:510:CL:CL	2.66	0.51
2:D:149:SER:HB3	2:D:356:TYR:CE1	2.46	0.51
1:A:105:THR:HB	1:A:106:PRO:HD3	1.93	0.51
1:A:343:LYS:O	1:A:347:MET:HG2	2.10	0.51
1:C:389:ASN:OD1	1:C:389:ASN:C	2.48	0.50
2:D:366:LEU:HB3	2:D:376:VAL:HG21	1.93	0.50
1:C:261:MET:HG2	1:C:266:TYR:OH	2.11	0.50
2:D:176:PHE:CD1	2:D:177:PRO:HD2	2.46	0.50
1:A:338:THR:O	1:A:338:THR:HG22	2.12	0.50
1:C:155:MET:HE3	1:C:163:VAL:CG2	2.40	0.50
2:D:374:GLU:O	2:D:376:VAL:HG23	2.12	0.49
1:C:41:ILE:HD12	1:C:299:SER:OG	2.11	0.49
2:B:39:VAL:HB	2:B:70:LEU:HD23	1.94	0.49
1:C:124:ARG:O	1:C:143:PRO:HA	2.12	0.49
1:C:157:LEU:CD2	1:C:158:PHE:CE2	2.89	0.49
1:C:275:ILE:HD13	1:C:289:GLY:HA3	1.94	0.49
2:D:35:ILE:CG2	2:D:64:VAL:HG11	2.41	0.49
2:D:284:GLU:HG3	2:D:284:GLU:O	2.12	0.49
1:C:343:LYS:O	1:C:347:MET:HG2	2.12	0.49
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.49	0.48
1:A:149:LEU:HD23	1:A:183:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD23	7:D:502:T88:C16	2.43	0.48
1:A:138:LEU:HD12	1:A:138:LEU:N	2.29	0.48
7:D:502:T88:C04	7:D:502:T88:C11	2.91	0.48
2:D:78:PRO:HB3	7:D:502:T88:CL2	2.51	0.48
1:C:138:LEU:HD12	1:C:138:LEU:N	2.29	0.47
2:D:133:ILE:CD1	2:D:150:ILE:HG12	2.44	0.47
1:A:105:THR:N	1:A:106:PRO:CD	2.77	0.47
2:B:35:ILE:HG23	2:B:64:VAL:CG2	2.44	0.47
7:D:502:T88:C12	7:D:502:T88:O29	2.63	0.47
2:D:285:TRP:CE3	2:D:375:ARG:HD2	2.49	0.47
1:C:105:THR:N	1:C:106:PRO:CD	2.77	0.47
1:C:136:SER:HB3	8:C:627:HOH:O	2.14	0.47
1:C:259:LEU:CB	1:C:261:MET:HE2	2.43	0.47
1:C:95:PRO:HA	1:C:96:PRO:HD3	1.74	0.47
1:C:135:LEU:C	1:C:135:LEU:HD12	2.34	0.47
1:C:214:LYS:HE2	1:C:216:LEU:HD23	1.97	0.47
2:B:71:VAL:HG13	2:B:84:ARG:NH2	2.30	0.47
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.95	0.47
2:D:344:PHE:O	2:D:344:PHE:CG	2.67	0.46
1:A:24:PRO:HB3	1:A:56:ARG:O	2.14	0.46
1:C:92:VAL:CG2	1:C:107:ILE:HD13	2.45	0.46
2:D:122:PRO:HD3	2:D:142:MET:HE1	1.97	0.46
1:A:228:LEU:C	1:A:228:LEU:HD23	2.36	0.46
1:A:363:GLU:H	1:A:363:GLU:CD	2.19	0.46
2:D:260:SER:HA	2:D:280:VAL:O	2.15	0.46
2:B:67:ARG:HG2	2:B:67:ARG:O	2.16	0.46
2:B:318:LYS:N	2:B:318:LYS:HD3	2.30	0.46
1:C:396:ASN:OD1	1:C:396:ASN:C	2.53	0.46
2:D:77:ASP:HB2	2:D:78:PRO:HD2	1.97	0.46
2:D:230:LEU:HB3	2:D:258:VAL:HG12	1.97	0.46
1:A:321:ASN:HD22	4:A:507:NAG:C7	2.29	0.45
2:B:66:PRO:HD3	2:B:301:THR:HG21	1.99	0.45
7:D:502:T88:C26	7:D:502:T88:C22	2.95	0.45
2:B:260:SER:HA	2:B:280:VAL:O	2.16	0.45
2:D:133:ILE:HD12	2:D:150:ILE:CG1	2.45	0.45
1:A:402:TRP:HB3	1:A:403:PRO:HD2	1.99	0.45
2:D:39:VAL:HB	2:D:70:LEU:HD23	1.98	0.44
1:A:286:GLY:HA2	1:A:401:ILE:O	2.17	0.44
1:C:214:LYS:HE2	1:C:216:LEU:CD2	2.47	0.44
1:C:214:LYS:HG3	1:C:215:VAL:N	2.32	0.44
2:D:344:PHE:O	2:D:345:GLU:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:TYR:OH	2:B:295:ASP:OD2	2.28	0.44
1:C:225:LEU:HD13	1:C:252:VAL:HG22	1.97	0.44
1:A:224:ASN:OD1	1:A:226:THR:OG1	2.30	0.44
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.47	0.44
1:A:30:GLY:HA2	1:A:63:THR:O	2.18	0.44
2:D:40:ILE:HG21	2:D:73:MET:CE	2.48	0.44
2:B:289:LEU:N	2:B:290:PRO:CD	2.81	0.43
1:C:338:THR:HG22	1:C:338:THR:O	2.17	0.43
7:D:502:T88:C04	7:D:502:T88:C10	2.96	0.43
1:A:142:PRO:HG3	1:A:370:ALA:CB	2.48	0.43
2:B:135:ALA:HB2	2:B:150:ILE:HD11	1.99	0.43
2:B:33:PRO:O	2:B:64:VAL:HG23	2.19	0.43
7:D:502:T88:C12	7:D:502:T88:C15	2.97	0.43
1:C:70:ASN:OD1	1:C:70:ASN:C	2.57	0.43
1:C:223:LYS:HA	1:C:223:LYS:HD3	1.80	0.43
1:A:214:LYS:HG3	1:A:215:VAL:N	2.34	0.42
1:C:31:ALA:HA	1:C:91:LEU:O	2.18	0.42
2:D:66:PRO:HD3	2:D:301:THR:HG21	2.01	0.42
1:C:55:THR:HG22	1:C:55:THR:O	2.19	0.42
1:C:344:ARG:NE	2:D:210:ASP:OD1	2.47	0.42
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.88	0.42
1:A:33:LEU:O	1:A:66:THR:HA	2.20	0.42
2:B:133:ILE:HG22	2:B:356:TYR:CE1	2.54	0.42
1:C:46:VAL:HG21	1:C:62:ALA:HB2	2.02	0.42
1:A:92:VAL:CG2	1:A:107:ILE:HG21	2.50	0.41
1:C:114:TYR:O	1:C:115:ARG:HB2	2.19	0.41
1:C:228:LEU:C	1:C:228:LEU:CD2	2.88	0.41
1:A:95:PRO:HA	1:A:96:PRO:HD3	1.75	0.41
2:D:214:SER:HA	8:D:613:HOH:O	2.19	0.41
2:D:289:LEU:N	2:D:290:PRO:CD	2.83	0.41
2:B:223:LEU:HD12	2:B:223:LEU:HA	1.85	0.41
2:D:132:MET:O	2:D:133:ILE:C	2.59	0.41
1:A:70:ASN:C	1:A:70:ASN:OD1	2.59	0.41
1:A:320:GLU:O	1:A:321:ASN:HB2	2.21	0.41
1:A:262:THR:HB	1:A:284:PRO:HB3	2.03	0.41
1:C:241:ILE:HA	1:C:269:LEU:O	2.20	0.41
2:D:35:ILE:HG13	2:D:35:ILE:O	2.20	0.41
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.03	0.41
1:C:92:VAL:HG21	1:C:107:ILE:HD13	2.02	0.41
1:C:96:PRO:O	1:C:97:ALA:HB3	2.20	0.41
2:D:149:SER:HB3	2:D:356:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLN:OE1	1:C:383:VAL:HG21	2.21	0.41
2:D:314:ILE:HB	2:D:315:PRO:HD2	2.02	0.41
2:B:289:LEU:N	2:B:290:PRO:HD2	2.35	0.40
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.82	0.40
2:B:153:GLN:O	2:B:157:MET:HG3	2.22	0.40
2:B:238:THR:HG22	2:B:273:PHE:CE1	2.56	0.40
1:A:39:GLU:OE2	8:A:601:HOH:O	2.21	0.40
1:A:308:VAL:HG21	1:A:359:ILE:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:TYR:O	1:C:380:ARG:NH1[4_758]	2.19	0.01

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	352/385 (91%)	338 (96%)	14 (4%)	0	100	100
1	C	351/385 (91%)	336 (96%)	14 (4%)	1 (0%)	41	64
2	B	356/363 (98%)	343 (96%)	13 (4%)	0	100	100
2	D	353/363 (97%)	336 (95%)	15 (4%)	2 (1%)	25	47
All	All	1412/1496 (94%)	1353 (96%)	56 (4%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	284	GLU
2	D	346	GLY

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Mol	Chain	Res	Type
1	C	237	ALA

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	287/331 (87%)	285 (99%)	2 (1%)	84	94
1	C	282/331 (85%)	280 (99%)	2 (1%)	84	94
2	B	289/326 (89%)	283 (98%)	6 (2%)	53	77
2	D	278/326 (85%)	277 (100%)	1 (0%)	91	97
All	All	1136/1314 (86%)	1125 (99%)	11 (1%)	76	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	136	SER
2	B	69	GLU
2	B	73	MET
2	B	134	MET
2	B	207	MET
2	B	223	LEU
2	B	337	ARG
1	C	136	SER
1	C	146	HIS
2	D	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	219	GLN
1	C	48	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	0.32	0	17,19,21	0.59	0
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.78	0
3	BMA	E	3	3	11,11,12	0.23	0	15,15,17	0.59	0
3	MAN	E	4	3	11,11,12	0.26	0	15,15,17	0.68	0
3	MAN	E	5	3	11,11,12	0.25	0	15,15,17	0.60	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	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

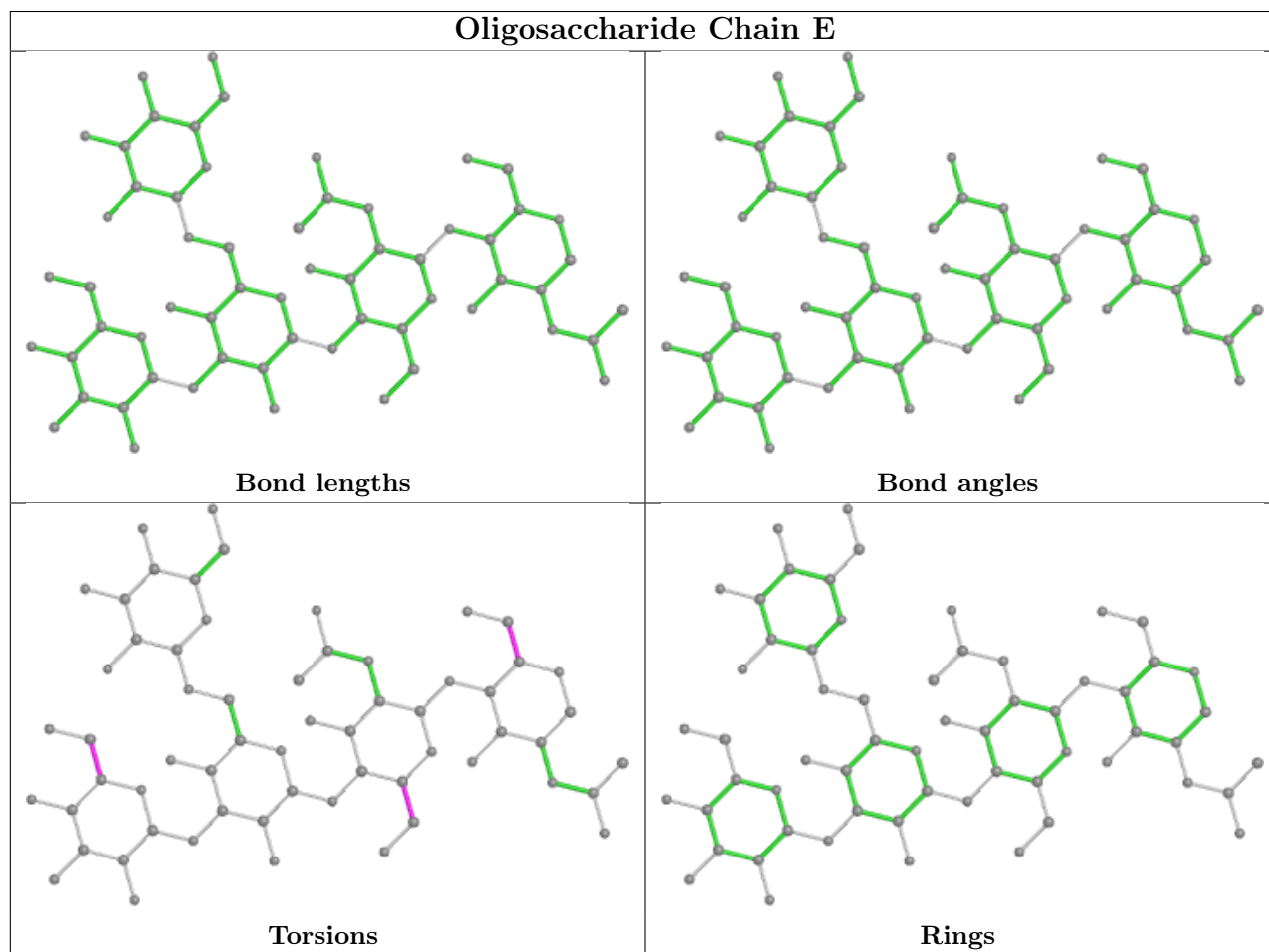
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-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 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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
7	T88	B	502	-	32,32,32	1.44	4 (12%)	43,43,43	2.17	3 (6%)
7	T88	D	502	-	32,32,32	1.44	4 (12%)	43,43,43	2.13	4 (9%)
4	NAG	C	502	1	14,14,15	0.26	0	17,19,21	1.03	1 (5%)
4	NAG	A	507	1	14,14,15	0.28	0	17,19,21	0.73	0
4	NAG	B	501	2	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	C	501	1	11,11,15	0.34	0	12,15,21	0.64	0
4	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.64	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
7	T88	B	502	-	-	9/23/23/23	0/2/2/2
7	T88	D	502	-	-	9/23/23/23	0/2/2/2
4	NAG	C	502	1	-	2/6/23/26	0/1/1/1
4	NAG	A	507	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	2	-	2/6/23/26	0/1/1/1
4	NAG	C	501	1	-	0/2/19/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	502	T88	S25-N24	5.78	1.71	1.63
7	B	502	T88	S25-N24	5.70	1.70	1.63
7	B	502	T88	C26-S25	2.83	1.82	1.75
7	D	502	T88	C26-S25	2.80	1.82	1.75
7	D	502	T88	C02-CL1	2.20	1.78	1.73
7	B	502	T88	C02-CL1	2.20	1.78	1.73
7	D	502	T88	C01-CL2	2.16	1.78	1.73
7	B	502	T88	C01-CL2	2.14	1.78	1.73

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	T88	O28-S25-O27	-12.18	101.33	118.85
7	B	502	T88	O28-S25-O27	-12.13	101.41	118.85
7	B	502	T88	C26-S25-N24	3.35	110.45	106.63
7	D	502	T88	C26-S25-N24	3.32	110.42	106.63
4	C	502	NAG	C1-O5-C5	3.18	116.49	112.19
7	B	502	T88	C16-O17-C18	-2.65	112.29	117.93
7	D	502	T88	O27-S25-N24	2.09	111.37	107.10
7	D	502	T88	C16-O17-C18	-2.04	113.59	117.93

There are no chirality outliers.

All (26) torsion outliers are listed below:

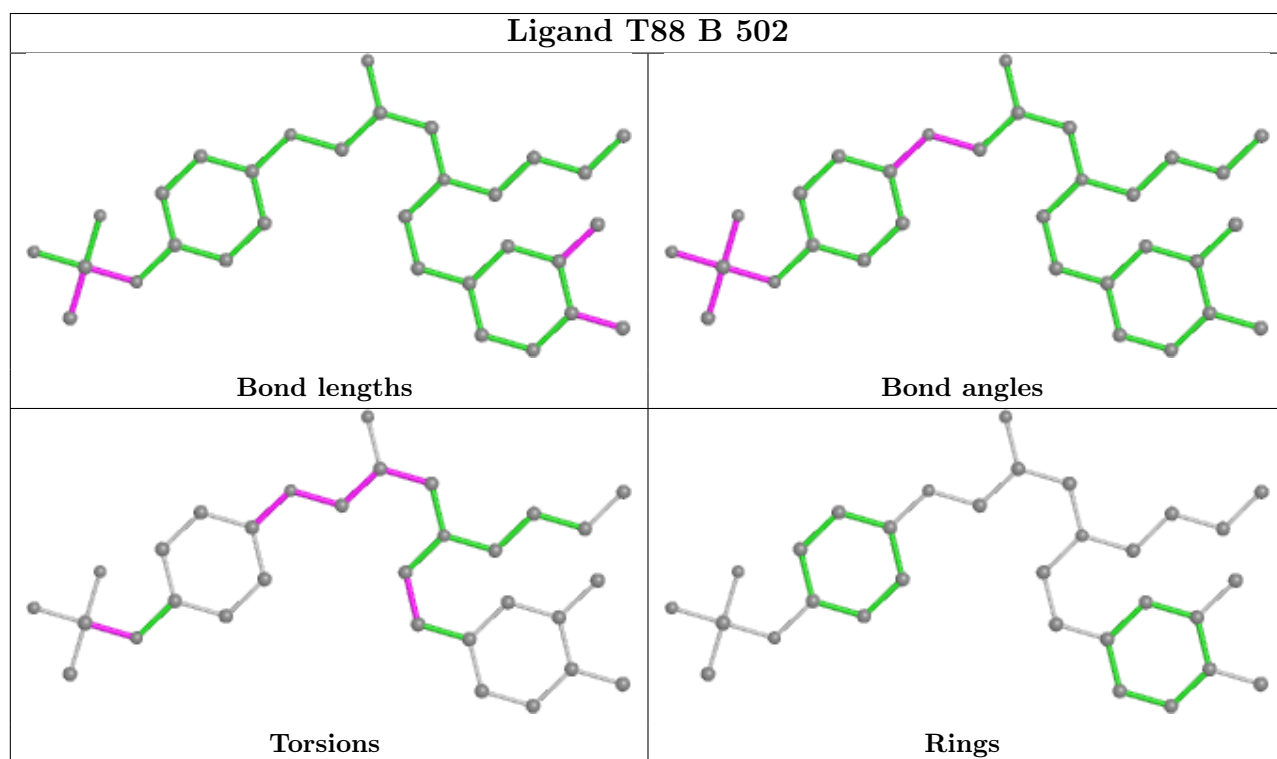
Mol	Chain	Res	Type	Atoms
7	B	502	T88	N09-C14-C15-C16
7	B	502	T88	O29-C15-C16-O17
7	D	502	T88	C21-N24-S25-C26
7	D	502	T88	C21-N24-S25-O28
4	C	502	NAG	O5-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	C	502	NAG	C4-C5-C6-O6
4	A	507	NAG	C4-C5-C6-O6
4	B	501	NAG	C4-C5-C6-O6
7	B	502	T88	C19-C18-O17-C16
4	A	507	NAG	O5-C5-C6-O6
7	B	502	T88	C14-C15-C16-O17
7	B	502	T88	C23-C18-O17-C16
7	D	502	T88	N09-C10-C11-C12
7	B	502	T88	C21-N24-S25-O27
7	D	502	T88	C11-C10-N09-C14
7	B	502	T88	C05-C07-C08-N09
4	A	501	NAG	C4-C5-C6-O6
7	B	502	T88	C15-C16-O17-C18
7	D	502	T88	C11-C10-N09-C08
7	D	502	T88	C19-C18-O17-C16
7	B	502	T88	N09-C14-C15-O29
4	A	501	NAG	O5-C5-C6-O6
7	D	502	T88	C05-C07-C08-N09
7	D	502	T88	N09-C14-C15-O29
7	D	502	T88	N09-C14-C15-C16

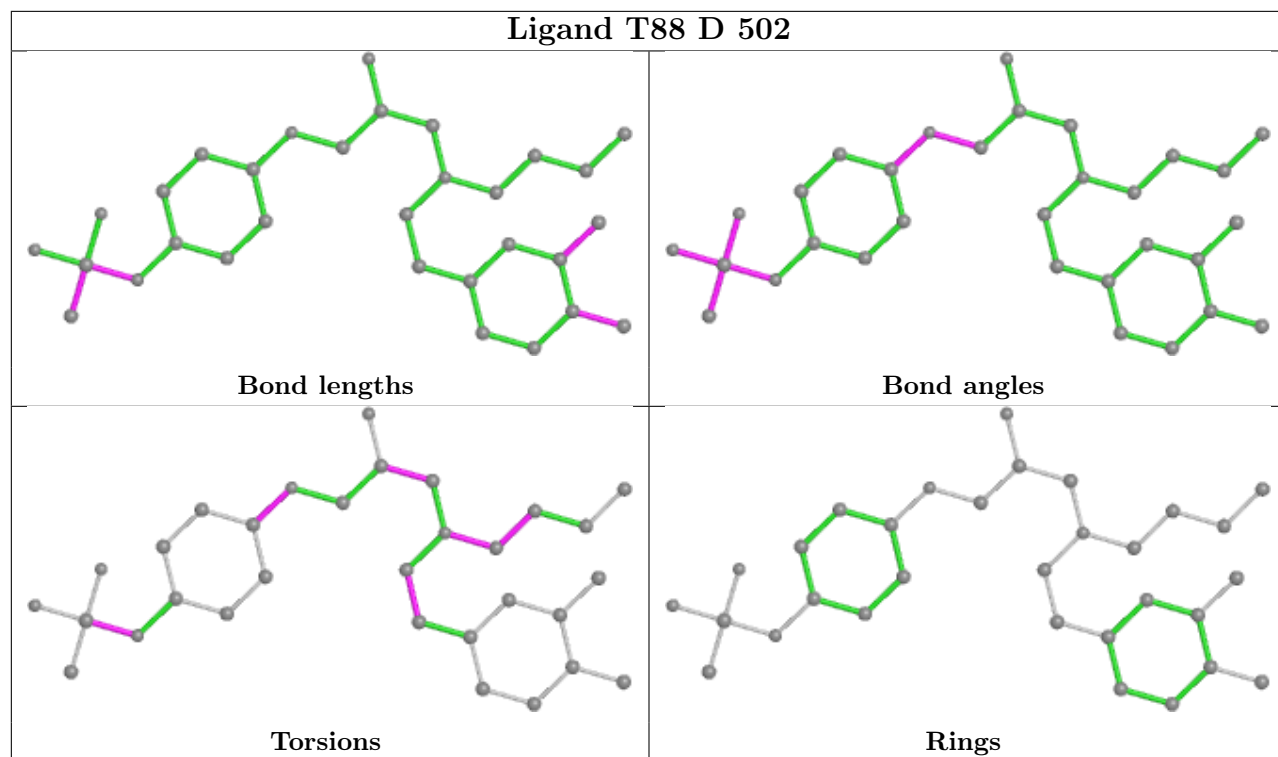
There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	T88	5	0
7	D	502	T88	9	0
4	C	502	NAG	1	0
4	A	507	NAG	1	0
4	C	501	NAG	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	358/385 (92%)	-0.32	5 (1%) 75 71	23, 40, 73, 102	0
1	C	357/385 (92%)	0.02	22 (6%) 20 15	31, 55, 92, 115	0
2	B	360/363 (99%)	0.10	17 (4%) 31 25	27, 54, 95, 113	0
2	D	357/363 (98%)	0.15	22 (6%) 20 15	33, 55, 97, 127	0
All	All	1432/1496 (95%)	-0.01	66 (4%) 32 26	23, 51, 92, 127	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	194	PHE	6.1
2	B	48	VAL	5.6
1	C	102	LEU	5.3
2	B	49	ALA	5.2
2	B	44	THR	4.9
2	D	345	GLU	4.7
2	B	52	ASP	4.6
1	A	102	LEU	4.5
1	C	101	HIS	4.2
2	D	48	VAL	4.2
2	D	343	THR	4.0
1	C	264	ALA	4.0
2	D	192	ASN	4.0
2	D	195	VAL	3.7
2	D	62	LEU	3.7
1	C	321	ASN	3.6
2	D	344	PHE	3.5
1	C	223	LYS	3.4
2	B	394	MET	3.4
2	D	49	ALA	3.3
2	D	65	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	395	GLN	3.2
1	C	265	GLY	3.2
2	D	54	HIS	3.1
1	C	358	ARG	3.1
2	D	347	ARG	3.0
1	C	397	ASP	2.9
2	D	346	GLY	2.9
2	D	193	SER	2.9
2	B	62	LEU	2.9
1	C	258	MET	2.8
2	D	52	ASP	2.8
2	B	191	GLU	2.7
2	B	53	ALA	2.7
2	D	53	ALA	2.7
1	A	101	HIS	2.7
2	B	122	PRO	2.7
1	C	259	LEU	2.6
1	A	186	GLY	2.6
2	B	345	GLU	2.5
2	D	32	PRO	2.5
1	A	209	GLY	2.5
2	D	381	ASP	2.5
2	B	218	ASN	2.4
1	C	266	TYR	2.4
2	B	98	VAL	2.4
1	C	157	LEU	2.4
2	D	123	ILE	2.4
2	B	359	HIS	2.4
1	C	73	GLN	2.3
1	C	221	GLY	2.3
1	C	158	PHE	2.3
2	B	123	ILE	2.3
2	B	46	ASP	2.3
1	C	23	ASP	2.2
1	C	394	ILE	2.2
1	C	220	PRO	2.2
2	D	380	LYS	2.1
1	C	318	GLU	2.1
2	B	217	GLN	2.1
2	B	309	SER	2.1
1	C	352	PRO	2.1
2	D	63	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	69	PRO	2.0
2	D	125	GLY	2.0
1	A	24	PRO	2.0

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

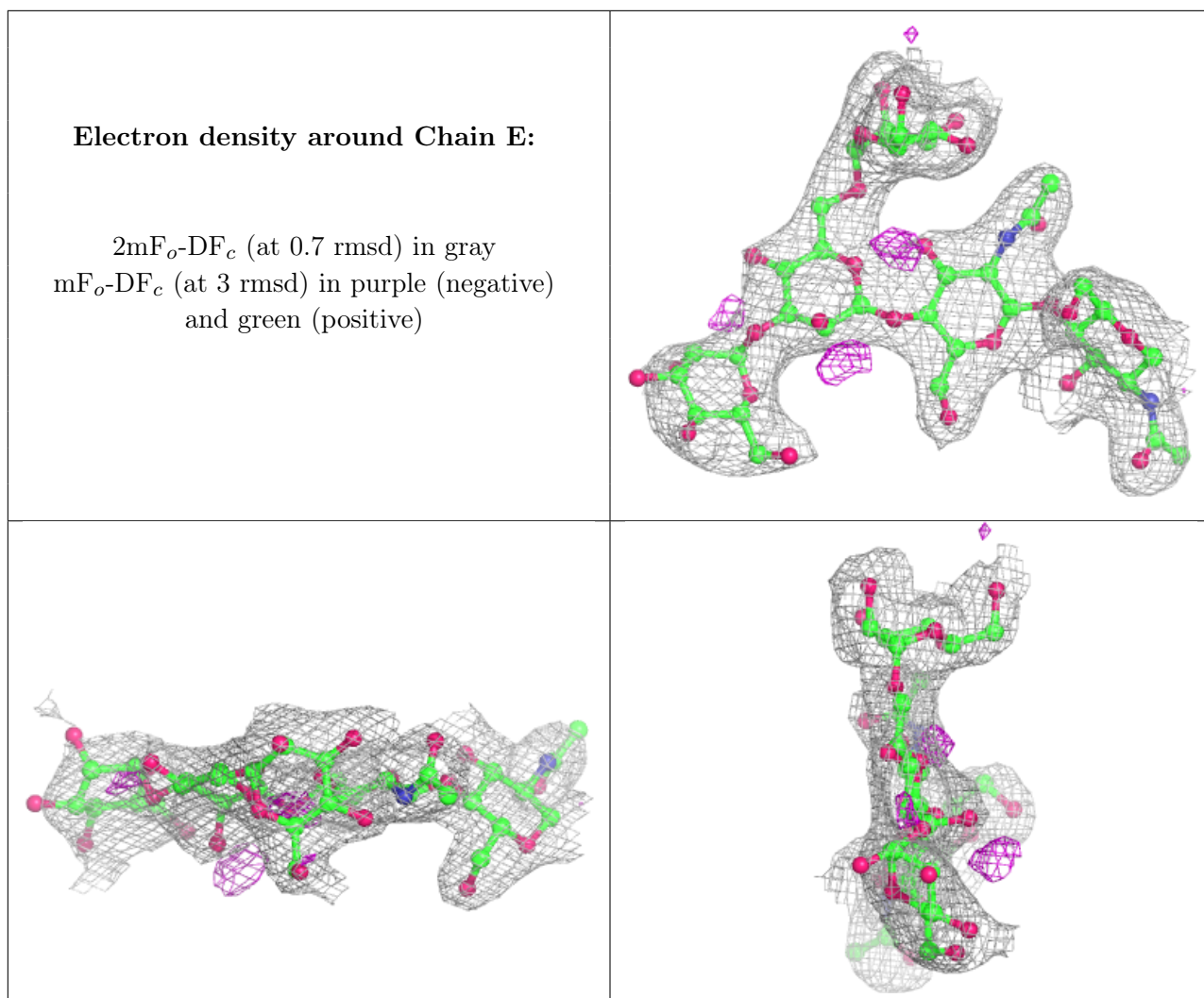
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	MAN	E	4	11/12	0.81	0.24	104,107,110,113	0
3	NAG	E	1	14/15	0.93	0.17	49,54,58,61	0
3	BMA	E	3	11/12	0.94	0.21	70,76,86,97	0
3	NAG	E	2	14/15	0.94	0.17	61,69,74,80	0
3	MAN	E	5	11/12	0.94	0.14	58,65,70,70	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 [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.

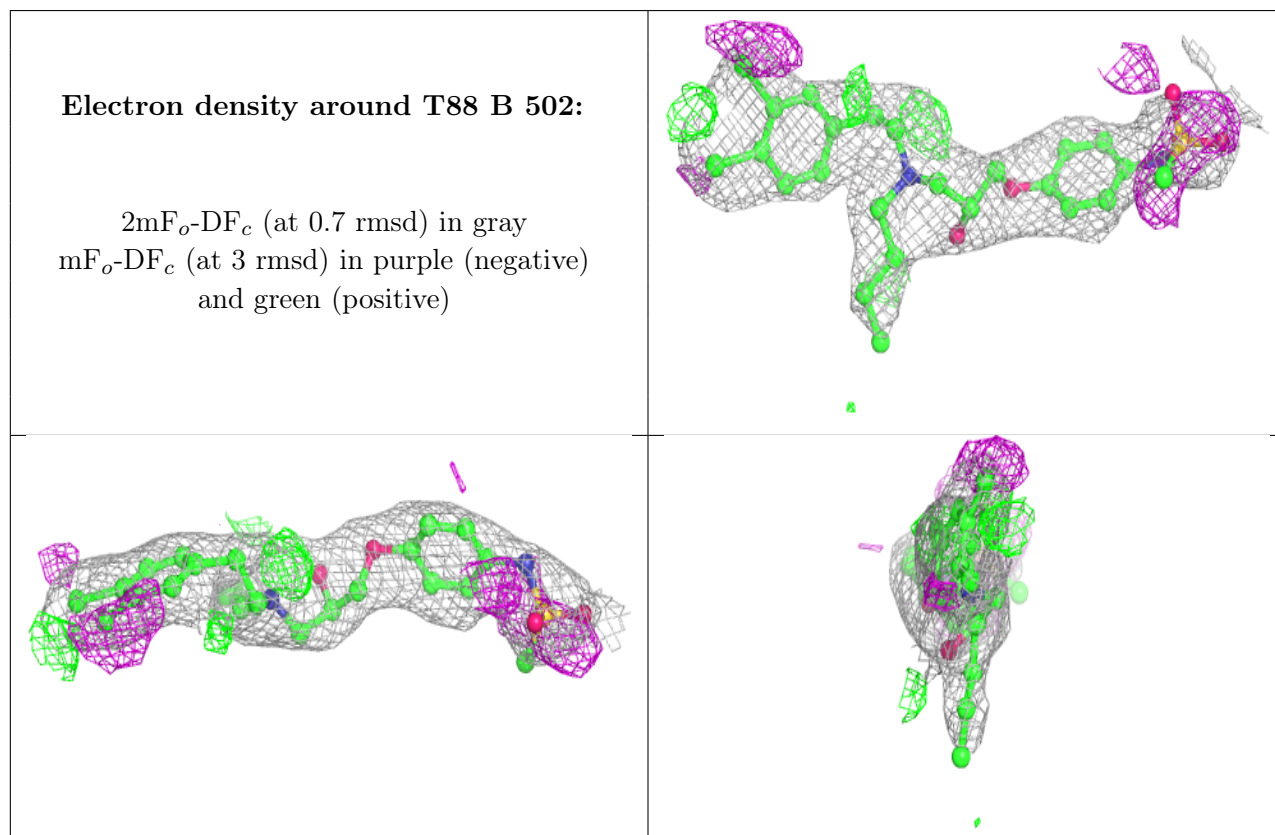
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	507	14/15	0.68	0.53	109,120,123,124	0
4	NAG	B	501	14/15	0.68	0.36	91,99,112,120	0
4	NAG	C	502	14/15	0.74	0.49	92,114,123,129	0
4	NAG	C	501	13/15	0.89	0.14	42,55,60,61	0
7	T88	B	502	31/31	0.90	0.22	37,56,82,103	0
7	T88	D	502	31/31	0.90	0.22	47,63,95,99	0
6	CL	A	510	1/1	0.91	0.12	56,56,56,56	0
6	CL	B	504	1/1	0.92	0.18	73,73,73,73	0
4	NAG	A	501	14/15	0.93	0.18	44,52,60,76	0

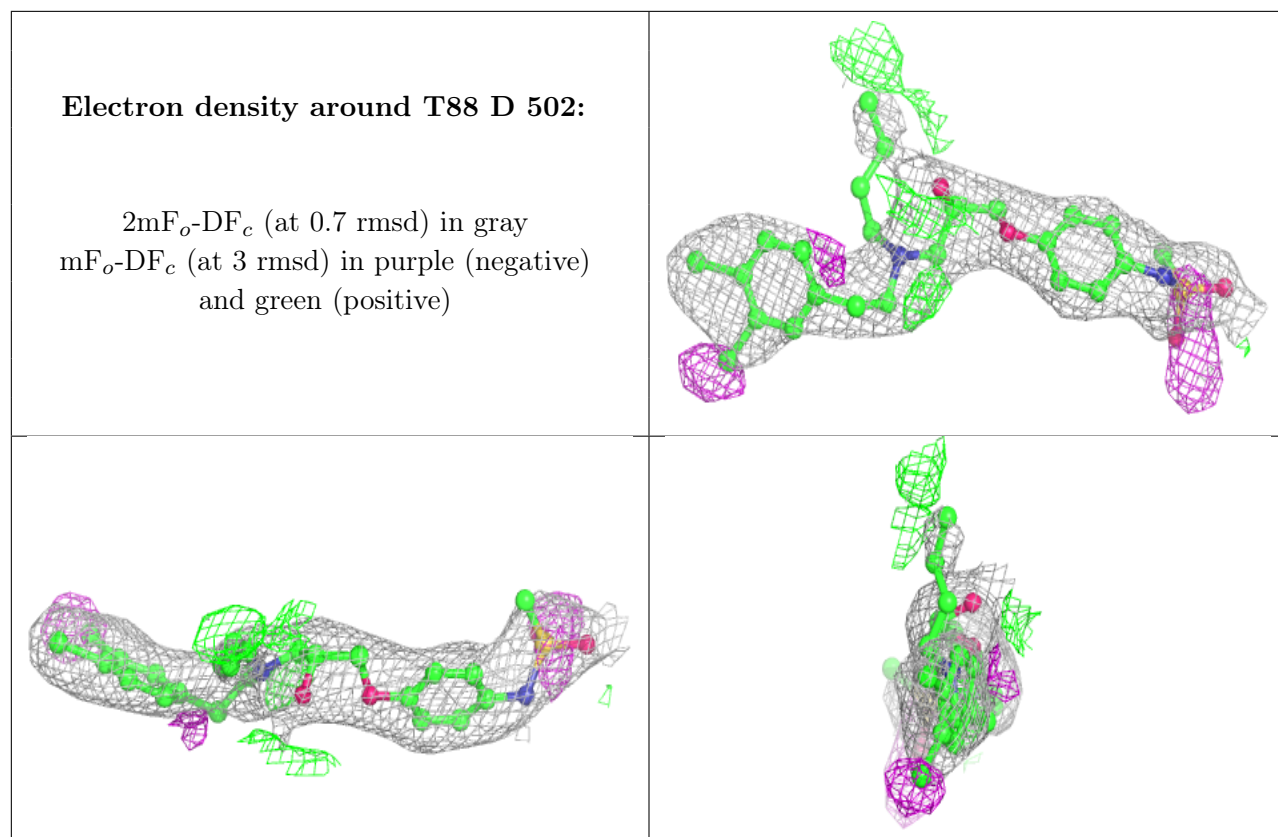
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	D	505	1/1	0.93	0.15	79,79,79,79	0
6	CL	B	503	1/1	0.94	0.20	72,72,72,72	0
6	CL	B	505	1/1	0.95	0.07	67,67,67,67	0
6	CL	D	504	1/1	0.96	0.22	83,83,83,83	0
6	CL	A	509	1/1	0.96	0.17	71,71,71,71	0
5	NA	C	503	1/1	0.97	0.07	37,37,37,37	0
6	CL	D	503	1/1	0.97	0.23	70,70,70,70	0
6	CL	C	505	1/1	0.98	0.07	61,61,61,61	0
5	NA	A	508	1/1	0.98	0.17	30,30,30,30	0
6	CL	C	504	1/1	0.98	0.26	68,68,68,68	0
6	CL	B	506	1/1	0.99	0.22	72,72,72,72	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.