



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:28 AM UTC

PDB ID : 4U4G / pdb_00004u4g
Title : Structure of GluA2* in complex with competitive antagonist ZK 200775
Authors : Yelshanskaya, M.V.; Li, M.; Sobolevsky, A.I.
Deposited on : 2014-07-23
Resolution : 4.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

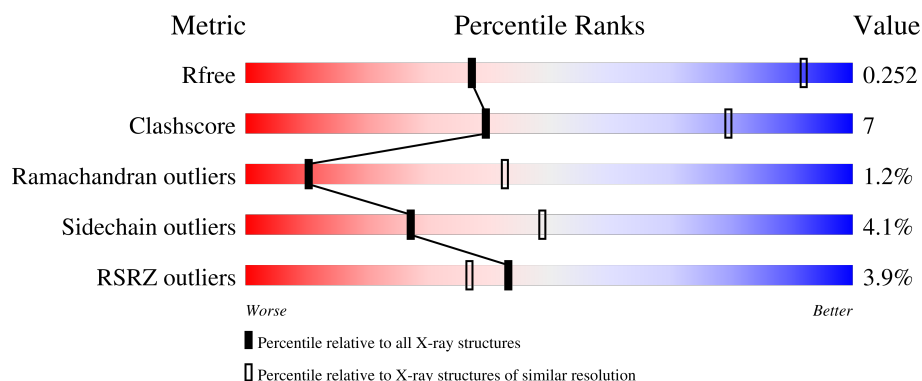
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.49 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	822	4% 75% 18% • 7%
1	B	822	4% 77% 15% • 7%
1	C	822	4% 75% 17% • 7%
1	D	822	4% 74% 18% • 7%
2	E	4	100%

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Mol	Chain	Length	Quality of chain
2	F	4	
2	G	4	
2	H	4	

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
2	NAG	E	1	X	-	-	-
2	BMA	E	3	X	-	-	-
2	NAG	F	1	X	-	-	-
2	NAG	F	2	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23812 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			5889	3781	971	1109	28			
1	B	768	Total	C	N	O	S	0	0	0
			5869	3767	961	1113	28			
1	C	768	Total	C	N	O	S	0	0	0
			5863	3763	963	1109	28			
1	D	768	Total	C	N	O	S	0	0	0
			5883	3776	966	1113	28			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491

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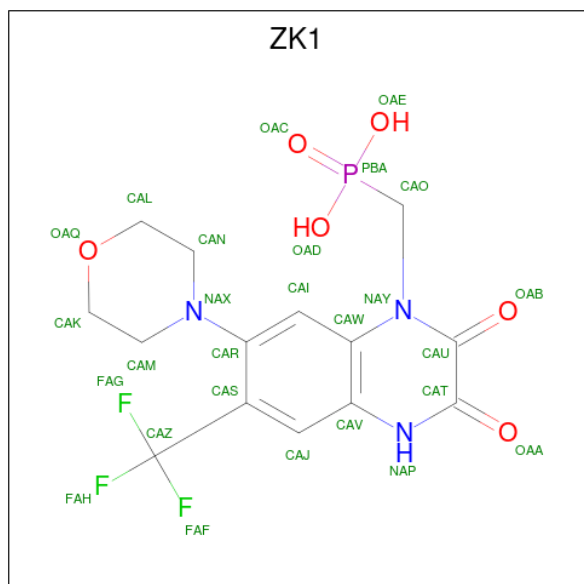
Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-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
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (CCD ID: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			27	14	3	3	6		

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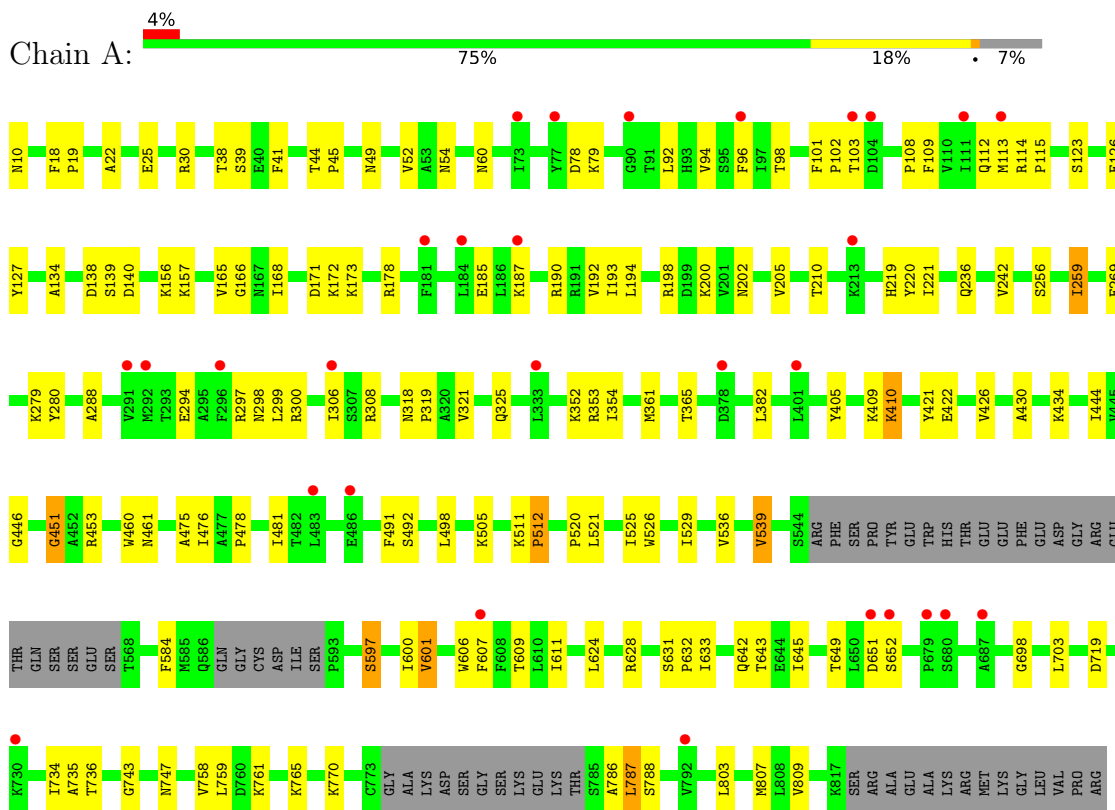
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
3	C	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		
3	D	1	Total	C	F	N	O	P	0	0
			27	14	3	3	6	1		

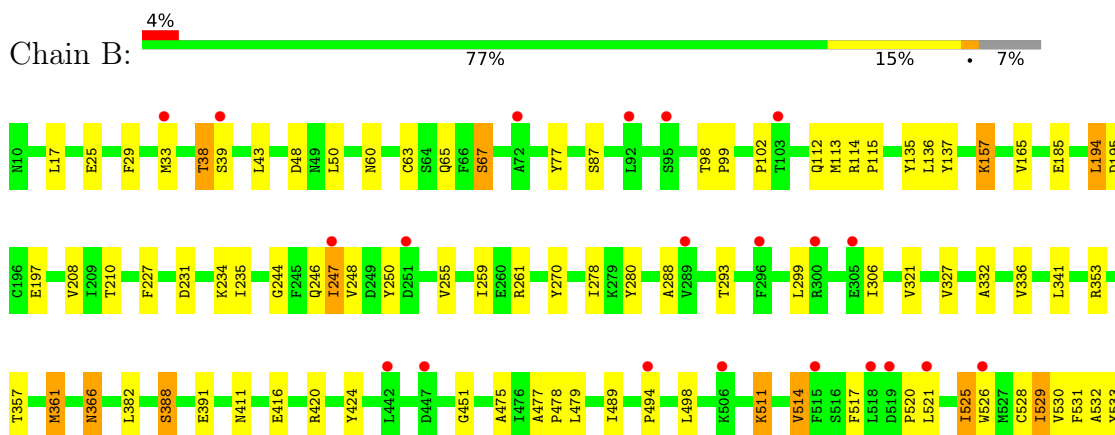
3 Residue-property plots [i](#)

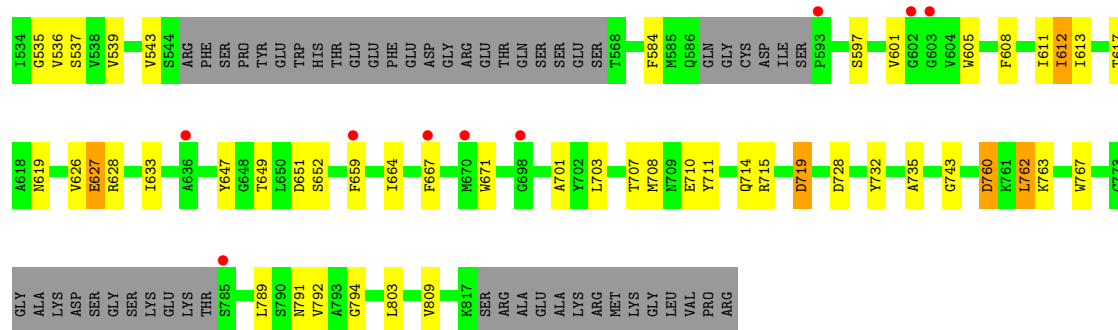
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutamate receptor 2

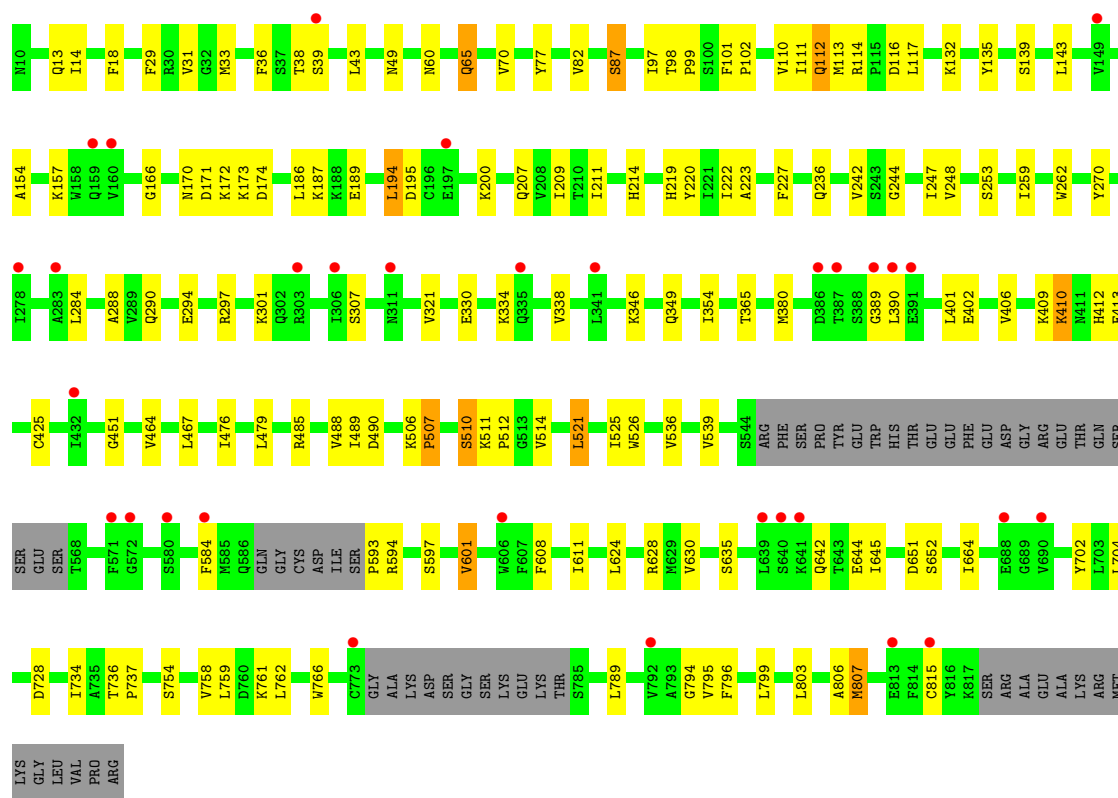
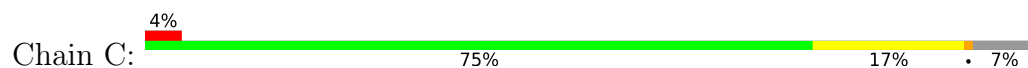


• Molecule 1: Glutamate receptor 2

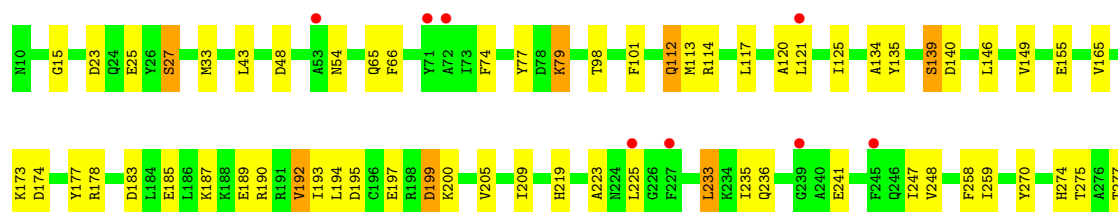
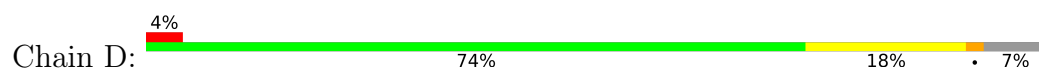


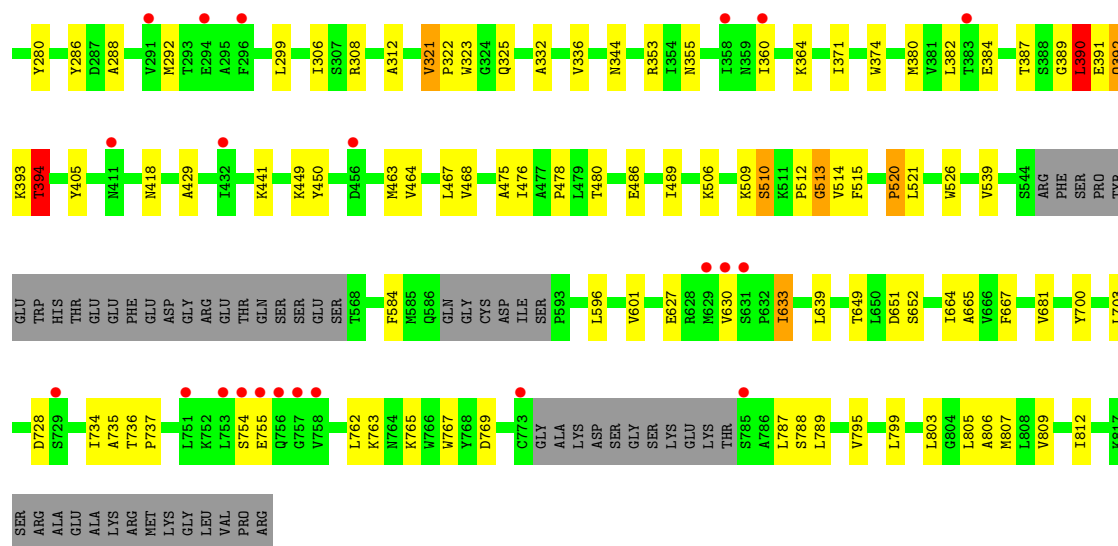


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





- Molecule 2: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  75%  25%



- Molecule 2: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 2: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  75%  25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.00Å 310.36Å 109.50Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	50.00 – 4.49 50.00 – 4.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-4.49) 98.8 (50.00-4.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 4.45Å)	Xtriage
Refinement program	PHENIX PHENIX.REFINE: 1.8_1069	Depositor
R, R_{free}	0.217 , 0.248 0.221 , 0.252	Depositor DCC
R_{free} test set	1797 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	206.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 134.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23812	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: NAG, ZK1, 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	0.30	0/6010	0.72	0/8148
1	B	0.28	0/5990	0.73	3/8128 (0.0%)
1	C	0.28	0/5984	0.72	3/8121 (0.0%)
1	D	0.29	0/6004	0.73	2/8143 (0.0%)
All	All	0.29	0/23988	0.72	8/32540 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	TYR	CA-C-N	6.55	126.58	119.90
1	C	270	TYR	C-N-CA	6.55	126.58	119.90
1	C	807	MET	N-CA-C	-5.92	106.05	113.28
1	D	270	TYR	CA-C-N	5.44	125.75	119.93
1	D	270	TYR	C-N-CA	5.44	125.75	119.93
1	B	185	GLU	N-CA-C	-5.23	106.94	113.38
1	B	270	TYR	CA-C-N	5.03	124.94	119.76
1	B	270	TYR	C-N-CA	5.03	124.94	119.76

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	5889	0	5738	88	0
1	B	5869	0	5680	87	0
1	C	5863	0	5672	86	0
1	D	5883	0	5713	89	0
2	E	50	0	43	0	0
2	F	50	0	43	0	0
2	G	50	0	43	0	0
2	H	50	0	43	1	0
3	A	27	0	13	0	0
3	B	27	0	13	0	0
3	C	27	0	13	0	0
3	D	27	0	13	0	0
All	All	23812	0	23027	315	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 7.

All (315) 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:D:510:SER:H	1:D:512:PRO:HD3	1.48	0.79
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.63	0.78
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:A:736:THR:HG21	1:A:743:GLY:HA2	1.72	0.71
1:B:255:VAL:HG13	1:B:341:LEU:HD22	1.73	0.70
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.73	0.70
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.72	0.70
1:A:166:GLY:HA2	1:A:200:LYS:HE2	1.72	0.70
1:B:114:ARG:NH1	1:B:280:TYR:OH	2.25	0.69
1:C:166:GLY:HA2	1:C:200:LYS:HE2	1.75	0.69
1:A:187:LYS:HZ1	1:B:157:LYS:HB3	1.57	0.69
1:A:409:LYS:HD3	1:A:422:GLU:HG3	1.74	0.69
1:C:154:ALA:HB1	1:D:183:ASP:HB3	1.76	0.68
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.77	0.67
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.60	0.66
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.77	0.65
1:D:23:ASP:O	1:D:27:SER:OG	2.14	0.65
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.77	0.65
1:B:525:ILE:HG12	1:C:789:LEU:HD13	1.78	0.65
1:B:601:VAL:HG23	1:C:806:ALA:HB3	1.78	0.64
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.78	0.64
1:B:628:ARG:NH2	1:C:628:ARG:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.32	0.63
1:B:17:LEU:HG	1:B:50:LEU:HD21	1.80	0.63
1:A:220:TYR:HB2	1:A:242:VAL:HG22	1.80	0.62
1:B:528:CYS:HA	1:B:531:PHE:HB2	1.80	0.62
1:B:366:ASN:OD1	1:B:366:ASN:N	2.31	0.62
1:C:758:VAL:HA	1:C:761:LYS:HB3	1.81	0.62
1:A:294:GLU:OE2	1:A:297:ARG:NH1	2.33	0.62
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.81	0.62
1:C:236:GLN:NE2	1:C:365:THR:O	2.31	0.62
1:D:114:ARG:NH1	1:D:280:TYR:OH	2.33	0.62
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.80	0.62
1:D:112:GLN:H	1:D:112:GLN:HE21	1.48	0.62
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.82	0.61
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.82	0.61
1:A:10:ASN:HB3	1:A:300:ARG:HH22	1.66	0.60
1:A:185:GLU:HG3	1:A:190:ARG:HH22	1.66	0.60
1:D:418:ASN:HD21	1:D:441:LYS:HA	1.66	0.60
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.83	0.60
1:B:63:CYS:O	1:B:67:SER:OG	2.19	0.59
1:A:102:PRO:HD3	1:A:114:ARG:HD2	1.85	0.59
1:C:506:LYS:HD2	1:C:507:PRO:HD2	1.85	0.59
1:D:185:GLU:HG3	1:D:190:ARG:HH12	1.66	0.59
1:B:517:PHE:HB2	1:B:791:ASN:HD21	1.69	0.58
1:D:233:LEU:HA	1:D:236:GLN:HB2	1.85	0.58
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.86	0.57
1:C:334:LYS:NZ	1:C:349:GLN:O	2.32	0.57
1:B:613:ILE:O	1:B:617:THR:OG1	2.17	0.57
1:A:78:ASP:OD1	1:A:79:LYS:N	2.32	0.57
1:D:681:VAL:O	1:D:700:TYR:OH	2.20	0.56
1:D:513:GLY:O	1:D:515:PHE:N	2.38	0.56
1:A:236:GLN:NE2	1:A:365:THR:O	2.36	0.56
1:C:101:PHE:HA	1:C:114:ARG:HD3	1.88	0.56
1:A:409:LYS:HG2	1:A:410:LYS:H	1.68	0.56
1:C:464:VAL:HG13	1:C:489:ILE:HD13	1.87	0.55
1:D:633:ILE:HG21	1:D:639:LEU:HG	1.88	0.55
1:C:220:TYR:HB2	1:C:242:VAL:HG22	1.88	0.55
1:D:165:VAL:O	1:D:200:LYS:NZ	2.34	0.55
1:D:450:TYR:HA	1:D:463:MET:HE2	1.88	0.55
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.87	0.55
1:C:490:ASP:HB2	1:C:736:THR:HG23	1.89	0.55
1:B:601:VAL:HG22	1:C:803:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:TYR:HE2	1:C:704:LEU:HD13	1.73	0.54
1:D:728:ASP:N	1:D:728:ASP:OD1	2.39	0.54
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.72	0.54
1:A:758:VAL:HA	1:A:761:LYS:HB3	1.89	0.54
1:B:521:LEU:HD22	1:B:526:TRP:CD2	2.42	0.54
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.88	0.54
1:C:135:TYR:OH	1:C:195:ASP:OD2	2.25	0.54
1:C:451:GLY:O	1:C:485:ARG:NH2	2.38	0.53
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.90	0.53
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.90	0.53
1:D:467:LEU:HD22	1:D:737:PRO:HD3	1.89	0.53
1:B:728:ASP:OD1	1:B:728:ASP:N	2.40	0.53
1:B:261:ARG:O	1:B:261:ARG:NH2	2.42	0.53
1:C:521:LEU:HD22	1:C:526:TRP:CD2	2.44	0.53
1:A:606:TRP:HA	1:A:609:THR:HG22	1.91	0.53
1:A:803:LEU:HD22	1:D:539:VAL:HG11	1.90	0.52
1:D:344:ASN:O	1:D:353:ARG:NH2	2.43	0.52
1:A:113:MET:HE3	1:A:288:ALA:HA	1.91	0.52
1:B:411:ASN:OD1	1:B:411:ASN:N	2.42	0.52
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.44	0.51
1:A:624:LEU:O	1:A:628:ARG:HG2	2.09	0.51
1:D:308:ARG:HG2	1:D:323:TRP:HZ3	1.75	0.51
1:B:521:LEU:HD23	1:B:525:ILE:HB	1.91	0.51
1:A:511:LYS:HG2	1:A:512:PRO:HD2	1.92	0.51
1:B:388:SER:OG	1:B:391:GLU:OE1	2.29	0.51
1:C:186:LEU:HD23	1:C:187:LYS:HG3	1.92	0.51
1:B:115:PRO:HG2	1:B:247:ILE:HD11	1.92	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.46	0.51
1:C:330:GLU:HG2	1:C:334:LYS:HE2	1.93	0.51
1:C:284:LEU:O	1:C:288:ALA:N	2.43	0.50
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.93	0.50
1:D:174:ASP:O	1:D:178:ARG:NH1	2.45	0.50
1:A:633:ILE:HD11	1:A:645:ILE:HD12	1.93	0.50
1:A:809:VAL:HG11	1:D:596:LEU:HD23	1.94	0.50
1:A:601:VAL:HG22	1:B:803:LEU:HD23	1.92	0.50
1:D:332:ALA:O	1:D:336:VAL:HG23	2.11	0.50
1:C:13:GLN:HG2	1:C:70:VAL:HG12	1.93	0.50
1:D:135:TYR:OH	1:D:195:ASP:OD2	2.25	0.50
1:C:409:LYS:HG2	1:C:410:LYS:H	1.77	0.49
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.93	0.49
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:LEU:HD13	1:A:788:SER:H	1.76	0.49
1:A:171:ASP:OD1	1:A:172:LYS:N	2.45	0.49
1:B:477:ALA:O	1:B:479:LEU:N	2.43	0.49
1:B:608:PHE:CG	1:C:799:LEU:HD22	2.47	0.49
1:D:429:ALA:HA	1:D:476:ILE:HD13	1.94	0.49
1:C:476:ILE:HG12	1:C:734:ILE:HD12	1.93	0.49
1:B:255:VAL:HG22	1:B:341:LEU:HA	1.94	0.49
1:C:38:THR:OG1	1:C:39:SER:N	2.45	0.49
1:D:355:ASN:HB3	2:H:1:NAG:H82	1.95	0.49
1:D:33:MET:HE1	1:D:43:LEU:HB2	1.94	0.49
1:A:505:LYS:HB3	1:A:698:GLY:HA2	1.94	0.49
1:B:231:ASP:HB3	1:B:234:LYS:HE2	1.95	0.49
1:C:514:VAL:HG13	1:C:794:GLY:HA3	1.94	0.48
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.47	0.48
1:A:108:PRO:HB2	1:A:109:PHE:HD1	1.78	0.48
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.94	0.48
1:D:788:SER:OG	1:D:789:LEU:N	2.45	0.48
1:C:116:ASP:OD1	1:C:117:LEU:N	2.45	0.48
1:D:199:ASP:OD1	1:D:199:ASP:N	2.46	0.48
1:B:532:ALA:O	1:B:536:VAL:HG23	2.13	0.48
1:C:651:ASP:OD1	1:C:652:SER:N	2.47	0.48
1:A:138:ASP:OD1	1:A:139:SER:N	2.45	0.48
1:A:103:THR:OG1	1:A:352:LYS:NZ	2.47	0.48
1:B:535:GLY:O	1:B:539:VAL:HG23	2.14	0.48
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.96	0.48
1:D:464:VAL:HG13	1:D:489:ILE:HD13	1.96	0.48
1:A:597:SER:O	1:A:600:ILE:HG12	2.14	0.47
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.96	0.47
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.96	0.47
1:A:96:PHE:HE1	1:A:98:THR:HB	1.79	0.47
1:B:760:ASP:HB3	1:C:664:ILE:HD11	1.96	0.47
1:D:205:VAL:O	1:D:209:ILE:HG13	2.14	0.47
1:A:787:LEU:HB2	1:D:520:PRO:O	2.15	0.47
1:C:87:SER:OG	1:D:54:ASN:OD1	2.27	0.47
1:C:642:GLN:OE1	1:C:644:GLU:N	2.47	0.47
1:D:754:SER:OG	1:D:755:GLU:N	2.47	0.47
1:C:157:LYS:HE2	1:D:187:LYS:HG3	1.95	0.47
1:D:288:ALA:O	1:D:292:MET:HG3	2.14	0.47
1:C:412:HIS:CE1	1:C:413:GLU:HG3	2.50	0.47
1:D:25:GLU:OE1	1:D:25:GLU:N	2.46	0.47
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:PHE:HE2	1:D:286:TYR:CZ	2.33	0.47
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.49	0.47
1:B:626:VAL:HB	1:C:628:ARG:NH1	2.30	0.47
1:D:765:LYS:HA	1:D:769:ASP:HB2	1.96	0.47
1:A:115:PRO:HA	1:A:353:ARG:HB2	1.96	0.47
1:C:31:VAL:HG21	1:C:262:TRP:HZ3	1.80	0.47
1:C:754:SER:HB3	1:C:759:LEU:HD12	1.96	0.47
1:B:38:THR:OG1	1:B:39:SER:N	2.48	0.47
1:A:651:ASP:OD1	1:A:652:SER:N	2.48	0.46
1:D:275:THR:OG1	1:D:277:THR:O	2.33	0.46
1:D:382:LEU:H	1:D:382:LEU:HD23	1.80	0.46
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.95	0.46
1:A:405:TYR:CG	1:A:478:PRO:HG3	2.51	0.46
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.80	0.46
1:A:453:ARG:HD2	1:A:460:TRP:CZ2	2.51	0.46
1:A:597:SER:HA	1:B:809:VAL:HB	1.98	0.46
1:C:521:LEU:HD23	1:C:525:ILE:HB	1.97	0.46
1:D:405:TYR:CG	1:D:478:PRO:HG3	2.50	0.46
1:A:430:ALA:O	1:A:434:LYS:N	2.48	0.46
1:B:711:TYR:O	1:B:715:ARG:HG2	2.16	0.46
1:D:146:LEU:HA	1:D:149:VAL:HG22	1.98	0.46
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.80	0.46
1:A:409:LYS:HD3	1:A:422:GLU:CG	2.45	0.46
1:B:135:TYR:OH	1:B:195:ASP:OD2	2.33	0.46
1:C:488:VAL:HG23	1:C:489:ILE:HG23	1.97	0.46
1:C:171:ASP:OD1	1:C:172:LYS:N	2.49	0.45
1:D:219:HIS:ND1	1:D:241:GLU:O	2.47	0.45
1:D:763:LYS:O	1:D:767:TRP:HB2	2.16	0.45
1:B:539:VAL:HG11	1:B:601:VAL:HG21	1.98	0.45
1:C:346:LYS:HD2	1:C:354:ILE:HD11	1.97	0.45
1:C:601:VAL:HG23	1:D:806:ALA:HB3	1.98	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.97	0.45
1:D:48:ASP:OD2	1:D:65:GLN:NE2	2.49	0.45
1:B:539:VAL:HG22	1:C:807:MET:HG2	1.97	0.45
1:D:195:ASP:HA	1:D:223:ALA:HB3	1.98	0.45
1:B:29:PHE:O	1:B:33:MET:HG2	2.16	0.45
1:D:805:LEU:O	1:D:809:VAL:HG23	2.15	0.45
1:A:481:ILE:HG22	1:A:491:PHE:CG	2.52	0.45
1:B:529:ILE:O	1:B:533:TYR:HB2	2.17	0.45
1:C:510:SER:HB3	1:C:511:LYS:HG3	1.99	0.45
1:B:115:PRO:HA	1:B:353:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HH11	1:A:210:THR:HG21	1.82	0.44
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.99	0.44
1:B:539:VAL:O	1:B:543:VAL:HG23	2.17	0.44
1:C:113:MET:HG3	1:C:288:ALA:HB2	1.97	0.44
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.98	0.44
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.82	0.44
1:A:405:TYR:CD2	1:A:478:PRO:HG3	2.52	0.44
1:D:521:LEU:HD22	1:D:526:TRP:CD2	2.52	0.44
1:A:299:LEU:HD13	1:A:306:ILE:HD13	1.99	0.44
1:B:514:VAL:HG11	1:B:794:GLY:HA3	1.98	0.44
1:C:65:GLN:HA	1:C:65:GLN:HE21	1.81	0.44
1:A:114:ARG:NH1	1:A:280:TYR:OH	2.50	0.44
1:B:612:ILE:HD11	1:C:796:PHE:CE1	2.52	0.44
1:A:18:PHE:HA	1:A:19:PRO:HD3	1.87	0.44
1:B:113:MET:O	1:B:353:ARG:NH1	2.49	0.44
1:D:464:VAL:O	1:D:468:VAL:HG23	2.18	0.44
1:A:765:LYS:O	1:A:770:LYS:HB2	2.18	0.44
1:B:511:LYS:HE3	1:B:511:LYS:HB2	1.75	0.44
1:B:651:ASP:OD1	1:B:652:SER:N	2.51	0.44
1:A:294:GLU:O	1:A:298:ASN:ND2	2.36	0.43
1:A:318:ASN:HA	1:A:319:PRO:HA	1.89	0.43
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.99	0.43
1:B:719:ASP:OD1	1:B:719:ASP:N	2.41	0.43
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.76	0.43
1:B:250:TYR:OH	1:B:278:ILE:N	2.37	0.43
1:D:392:GLN:O	1:D:394:THR:N	2.51	0.43
1:B:498:LEU:HD13	1:B:707:THR:HG23	2.00	0.43
1:C:608:PHE:CG	1:D:799:LEU:HD22	2.53	0.43
1:A:108:PRO:HB2	1:A:109:PHE:CD1	2.54	0.43
1:D:173:LYS:HG2	1:D:177:TYR:HE2	1.84	0.43
1:A:539:VAL:HG21	1:B:803:LEU:HB3	2.00	0.43
1:B:619:ASN:HB2	1:C:624:LEU:HD13	2.00	0.43
1:A:38:THR:HG23	1:A:41:PHE:H	1.83	0.43
1:A:198:ARG:HD3	1:A:279:LYS:HE3	2.01	0.43
1:A:492:SER:HB2	1:A:747:ASN:HA	2.00	0.43
1:A:607:PHE:O	1:A:611:ILE:HG12	2.19	0.43
1:B:135:TYR:CE2	1:B:137:TYR:HB3	2.54	0.43
1:B:789:LEU:HD12	1:B:792:VAL:HB	1.99	0.43
1:C:132:LYS:HE2	1:C:189:GLU:HG2	2.00	0.43
1:D:651:ASP:OD1	1:D:652:SER:N	2.51	0.43
1:B:521:LEU:HD22	1:B:526:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:GLU:O	1:B:714:GLN:HG2	2.18	0.43
1:C:101:PHE:HA	1:C:102:PRO:HD3	1.89	0.43
1:C:467:LEU:HD22	1:C:737:PRO:HD3	2.01	0.43
1:A:38:THR:OG1	1:A:39:SER:N	2.50	0.43
1:C:36:PHE:CZ	1:C:290:GLN:HB2	2.54	0.43
1:C:297:ARG:HG2	1:C:301:LYS:HE3	2.00	0.43
1:D:633:ILE:HD13	1:D:639:LEU:HD21	2.00	0.43
1:B:530:VAL:HA	1:B:533:TYR:HB3	2.01	0.43
1:C:593:PRO:HB2	1:C:594:ARG:H	1.64	0.43
1:A:54:ASN:OD1	1:B:87:SER:OG	2.36	0.43
1:A:631:SER:HA	1:A:632:PRO:HD3	1.92	0.43
1:D:134:ALA:HB3	1:D:192:VAL:HG22	2.00	0.43
1:D:325:GLN:H	1:D:325:GLN:CD	2.27	0.43
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.99	0.42
1:B:619:ASN:HD22	1:C:624:LEU:HD13	1.82	0.42
1:D:321:VAL:HA	1:D:322:PRO:HD3	1.85	0.42
1:D:449:LYS:HG2	1:D:450:TYR:H	1.84	0.42
1:C:14:ILE:HD13	1:C:43:LEU:HD23	2.00	0.42
1:D:225:LEU:HD22	1:D:247:ILE:HD13	2.00	0.42
1:A:422:GLU:HA	1:A:426:VAL:HG11	2.01	0.42
1:A:476:ILE:HG12	1:A:734:ILE:HG23	2.01	0.42
1:C:728:ASP:OD1	1:C:728:ASP:N	2.51	0.42
1:A:803:LEU:O	1:A:807:MET:HG2	2.19	0.42
1:D:79:LYS:HE3	1:D:139:SER:HB2	2.00	0.42
1:B:626:VAL:O	1:B:627:GLU:HG2	2.20	0.42
1:C:194:LEU:HG	1:C:222:ILE:HD13	2.01	0.42
1:C:511:LYS:HG2	1:C:512:PRO:HD2	2.01	0.42
1:C:762:LEU:O	1:C:766:TRP:HD1	2.03	0.42
1:D:476:ILE:HG12	1:D:734:ILE:HD12	2.02	0.42
1:B:424:TYR:CE1	1:B:762:LEU:HB3	2.55	0.42
1:A:259:ILE:HA	1:A:259:ILE:HD13	1.82	0.42
1:D:66:PHE:CE2	1:D:312:ALA:HB1	2.54	0.42
1:B:33:MET:HE1	1:B:43:LEU:HB2	2.01	0.42
1:C:29:PHE:O	1:C:33:MET:HG2	2.20	0.42
1:C:209:ILE:HA	1:C:214:HIS:ND1	2.35	0.42
1:D:308:ARG:HG2	1:D:323:TRP:CZ3	2.52	0.42
1:D:360:ILE:HG22	1:D:371:ILE:HG12	2.00	0.42
1:A:44:THR:HA	1:A:45:PRO:HD3	1.82	0.42
1:A:202:ASN:HA	1:A:205:VAL:HB	2.01	0.42
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.91	0.42
1:C:539:VAL:HG13	1:D:807:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ALA:HA	1:D:374:TRP:CE2	2.55	0.42
1:A:521:LEU:HD22	1:A:526:TRP:CD2	2.55	0.41
1:B:332:ALA:O	1:B:336:VAL:HG23	2.20	0.41
1:B:494:PRO:HA	1:B:732:TYR:O	2.20	0.41
1:B:526:TRP:HA	1:B:529:ILE:HG22	2.02	0.41
1:C:601:VAL:HG22	1:D:803:LEU:HD23	2.01	0.41
1:D:389:GLY:O	1:D:391:GLU:N	2.53	0.41
1:A:92:LEU:HB2	1:A:94:VAL:HG23	2.01	0.41
1:A:101:PHE:HA	1:A:114:ARG:HD2	2.01	0.41
1:D:390:LEU:H	1:D:390:LEU:HG	1.58	0.41
1:C:110:VAL:HG12	1:C:112:GLN:HG3	2.02	0.41
1:D:121:LEU:O	1:D:125:ILE:HG13	2.20	0.41
1:D:121:LEU:HD11	1:D:193:ILE:HD13	2.02	0.41
1:A:30:ARG:HH22	1:A:269:GLU:HG3	1.85	0.41
1:A:476:ILE:HG12	1:A:734:ILE:HD12	2.02	0.41
1:A:178:ARG:NH1	1:A:210:THR:HG21	2.36	0.41
1:D:15:GLY:O	1:D:74:PHE:N	2.50	0.41
1:B:98:THR:HA	1:B:99:PRO:HD3	1.83	0.41
1:B:113:MET:HE3	1:B:288:ALA:HA	2.03	0.41
1:C:18:PHE:O	1:C:49:ASN:HA	2.21	0.41
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.55	0.41
1:A:126:GLU:HG3	1:A:156:LYS:HE3	2.02	0.41
1:A:168:ILE:HD13	1:A:173:LYS:HG3	2.02	0.41
1:A:123:SER:O	1:A:127:TYR:N	2.49	0.41
1:A:157:LYS:HA	1:A:157:LYS:HD3	1.87	0.41
1:A:325:GLN:H	1:A:325:GLN:CD	2.29	0.41
1:A:421:TYR:CE1	1:A:444:ILE:HD11	2.55	0.41
1:B:619:ASN:HD22	1:C:624:LEU:HB3	1.86	0.41
1:B:763:LYS:O	1:B:767:TRP:HB2	2.21	0.41
1:C:195:ASP:HA	1:C:223:ALA:HB3	2.02	0.41
1:D:113:MET:HG3	1:D:288:ALA:HB2	2.03	0.41
1:D:364:LYS:HA	1:D:364:LYS:HD3	1.80	0.41
1:A:719:ASP:OD1	1:A:719:ASP:N	2.54	0.41
1:B:25:GLU:OE1	1:B:25:GLU:N	2.52	0.41
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.55	0.41
1:B:246:GLN:HB2	1:B:361:MET:HG3	2.03	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.95	0.41
1:C:98:THR:HA	1:C:99:PRO:HD3	1.84	0.41
1:C:259:ILE:HD13	1:C:259:ILE:HA	1.91	0.41
1:C:425:CYS:HB3	1:C:476:ILE:HG22	2.02	0.40
1:A:18:PHE:O	1:A:49:ASN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HB2	1:B:194:LEU:HD12	2.04	0.40
1:A:803:LEU:HD23	1:D:601:VAL:HG22	2.04	0.40
1:D:380:MET:HE3	1:D:380:MET:HB2	1.99	0.40
1:D:405:TYR:CD1	1:D:478:PRO:HG3	2.56	0.40
1:A:451:GLY:HA2	1:A:461:ASN:O	2.21	0.40
1:D:762:LEU:HD23	1:D:762:LEU:HA	1.97	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	760/822 (92%)	694 (91%)	57 (8%)	9 (1%)	10	43
1	B	760/822 (92%)	701 (92%)	52 (7%)	7 (1%)	14	49
1	C	760/822 (92%)	683 (90%)	70 (9%)	7 (1%)	14	49
1	D	760/822 (92%)	689 (91%)	58 (8%)	13 (2%)	7	35
All	All	3040/3288 (92%)	2767 (91%)	237 (8%)	36 (1%)	10	43

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASP
1	A	410	LYS
1	A	512	PRO
1	A	597	SER
1	D	514	VAL
1	A	786	ALA
1	B	157	LYS
1	B	520	PRO
1	B	584	PHE

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Mol	Chain	Res	Type
1	B	597	SER
1	C	389	GLY
1	C	584	PHE
1	D	140	ASP
1	D	390	LEU
1	D	393	LYS
1	D	394	THR
1	A	520	PRO
1	A	584	PHE
1	C	410	LYS
1	C	630	VAL
1	D	510	SER
1	D	584	PHE
1	C	390	LEU
1	D	384	GLU
1	D	665	ALA
1	B	478	PRO
1	C	507	PRO
1	C	597	SER
1	D	392	GLN
1	D	506	LYS
1	D	513	GLY
1	A	451	GLY
1	B	451	GLY
1	A	446	GLY
1	D	520	PRO
1	B	743	GLY

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	615/702 (88%)	597 (97%)	18 (3%)	37	58
1	B	611/702 (87%)	578 (95%)	33 (5%)	20	42
1	C	609/702 (87%)	587 (96%)	22 (4%)	31	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	614/702 (88%)	587 (96%)	27 (4%)	25	47
All	All	2449/2808 (87%)	2349 (96%)	100 (4%)	27	49

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	60	ASN
1	A	112	GLN
1	A	165	VAL
1	A	219	HIS
1	A	256	SER
1	A	259	ILE
1	A	308	ARG
1	A	321	VAL
1	A	354	ILE
1	A	361	MET
1	A	382	LEU
1	A	498	LEU
1	A	529	ILE
1	A	539	VAL
1	A	601	VAL
1	A	643	THR
1	A	787	LEU
1	B	38	THR
1	B	60	ASN
1	B	67	SER
1	B	112	GLN
1	B	165	VAL
1	B	194	LEU
1	B	197	GLU
1	B	208	VAL
1	B	210	THR
1	B	235	ILE
1	B	247	ILE
1	B	248	VAL
1	B	259	ILE
1	B	293	THR
1	B	321	VAL
1	B	327	VAL
1	B	357	THR
1	B	361	MET

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Mol	Chain	Res	Type
1	B	366	ASN
1	B	382	LEU
1	B	388	SER
1	B	511	LYS
1	B	514	VAL
1	B	525	ILE
1	B	529	ILE
1	B	537	SER
1	B	612	ILE
1	B	627	GLU
1	B	633	ILE
1	B	708	MET
1	B	719	ASP
1	B	760	ASP
1	B	762	LEU
1	C	60	ASN
1	C	65	GLN
1	C	82	VAL
1	C	87	SER
1	C	112	GLN
1	C	139	SER
1	C	143	LEU
1	C	194	LEU
1	C	211	ILE
1	C	219	HIS
1	C	247	ILE
1	C	248	VAL
1	C	253	SER
1	C	307	SER
1	C	321	VAL
1	C	380	MET
1	C	402	GLU
1	C	510	SER
1	C	521	LEU
1	C	601	VAL
1	C	635	SER
1	C	815	CYS
1	D	27	SER
1	D	79	LYS
1	D	112	GLN
1	D	139	SER
1	D	155	GLU

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Mol	Chain	Res	Type
1	D	189	GLU
1	D	192	VAL
1	D	194	LEU
1	D	197	GLU
1	D	199	ASP
1	D	233	LEU
1	D	235	ILE
1	D	248	VAL
1	D	259	ILE
1	D	274	HIS
1	D	321	VAL
1	D	387	THR
1	D	390	LEU
1	D	394	THR
1	D	480	THR
1	D	486	GLU
1	D	509	LYS
1	D	627	GLU
1	D	630	VAL
1	D	633	ILE
1	D	736	THR
1	D	787	LEU

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	24	GLN
1	A	337	GLN
1	A	412	HIS
1	B	619	ASN
1	B	726	ASN
1	C	13	GLN
1	C	24	GLN
1	C	65	GLN
1	C	392	GLN
1	C	412	HIS
1	D	83	ASN
1	D	202	ASN
1	D	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.56	0	17,19,21	0.85	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.67	0
2	BMA	E	3	2	11,11,12	0.60	0	15,15,17	0.72	0
2	BMA	E	4	2	11,11,12	0.62	0	15,15,17	0.76	0
2	NAG	F	1	2,1	14,14,15	0.55	0	17,19,21	0.71	0
2	NAG	F	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	BMA	F	3	2	11,11,12	0.60	0	15,15,17	0.75	0
2	BMA	F	4	2	11,11,12	0.59	0	15,15,17	0.77	0
2	NAG	G	1	2,1	14,14,15	0.58	0	17,19,21	0.73	0
2	NAG	G	2	2	14,14,15	0.51	0	17,19,21	0.64	0
2	BMA	G	3	2	11,11,12	0.59	0	15,15,17	0.75	0
2	BMA	G	4	2	11,11,12	0.65	0	15,15,17	0.73	0
2	NAG	H	1	2,1	14,14,15	0.69	0	17,19,21	1.57	2 (11%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	0.67	0
2	BMA	H	3	2	11,11,12	0.56	0	15,15,17	0.72	0
2	BMA	H	4	2	11,11,12	0.65	0	15,15,17	0.74	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
2	NAG	E	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	BMA	E	4	2	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	BMA	F	4	2	-	1/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	BMA	G	4	2	-	1/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	BMA	H	4	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C2-N2-C7	-4.66	116.65	122.90
2	F	2	NAG	C1-O5-C5	2.63	115.71	112.19
2	H	1	NAG	C1-O5-C5	2.23	115.17	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1
2	E	3	BMA	C1
2	F	1	NAG	C1
2	F	2	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O7-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	H	4	BMA	O5-C5-C6-O6
2	G	4	BMA	O5-C5-C6-O6
2	F	4	BMA	O5-C5-C6-O6
2	E	4	BMA	O5-C5-C6-O6

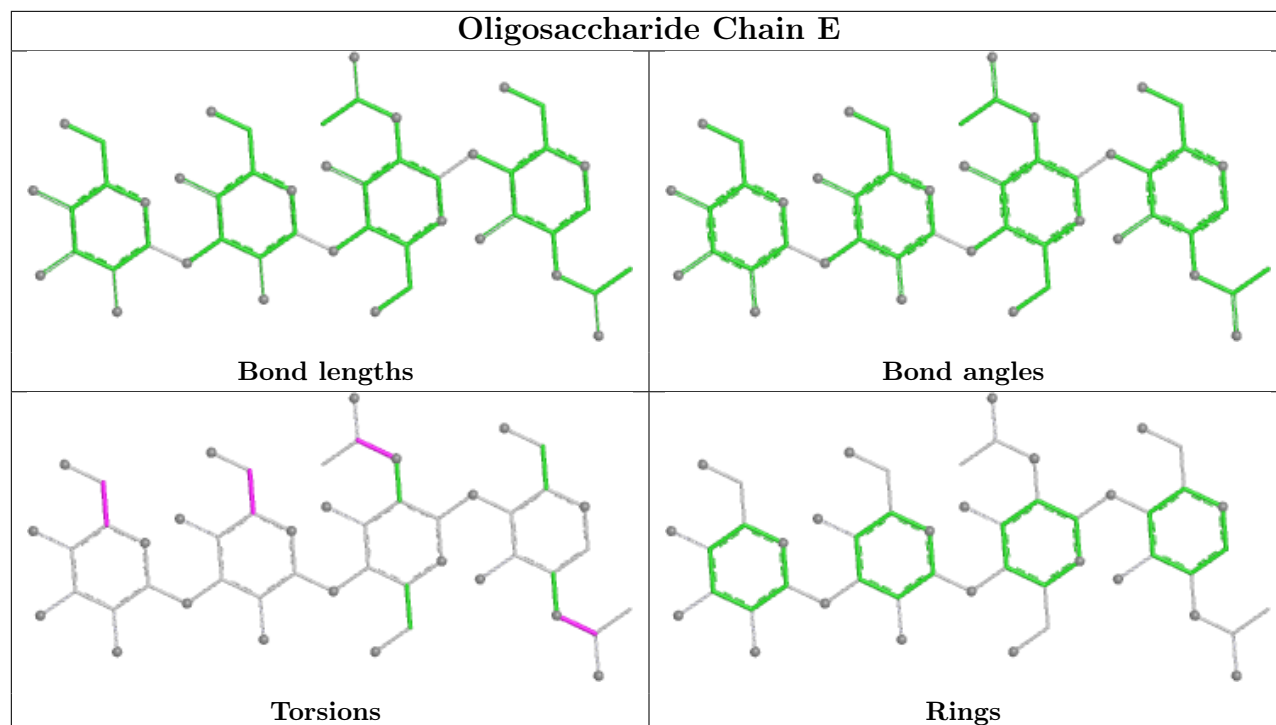
There are no ring outliers.

1 monomer is involved in 1 short contact:

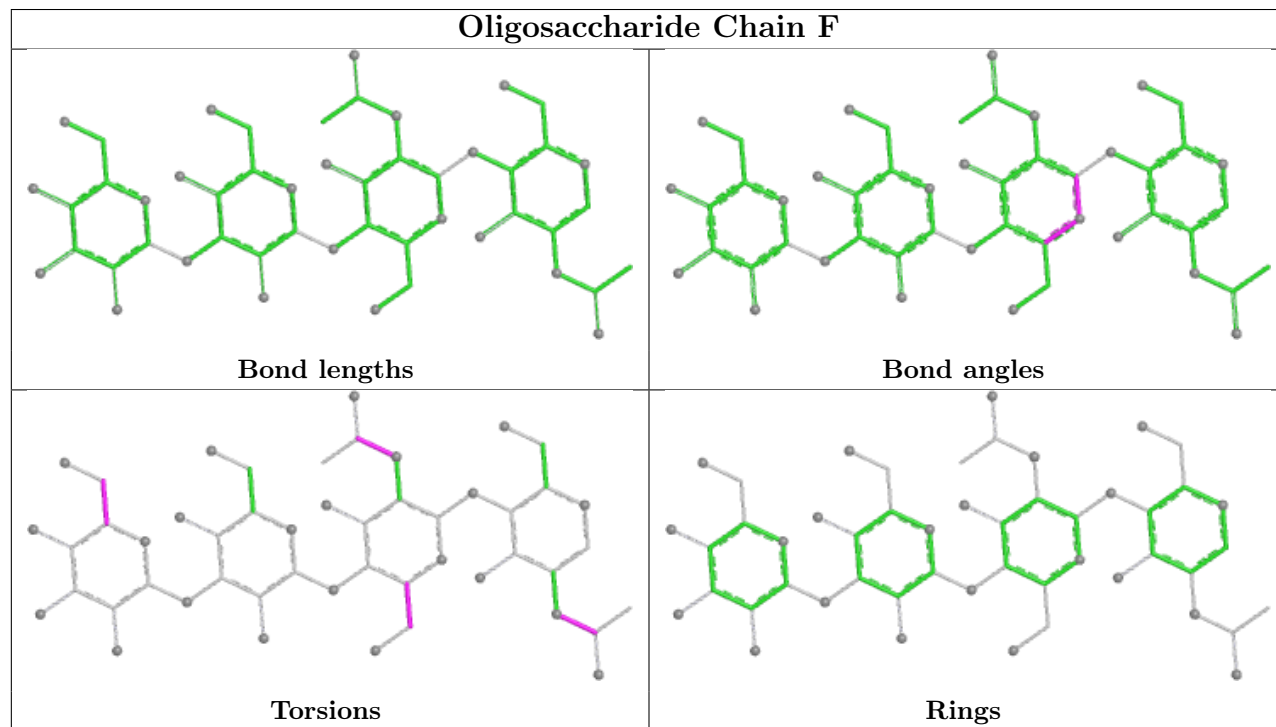
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

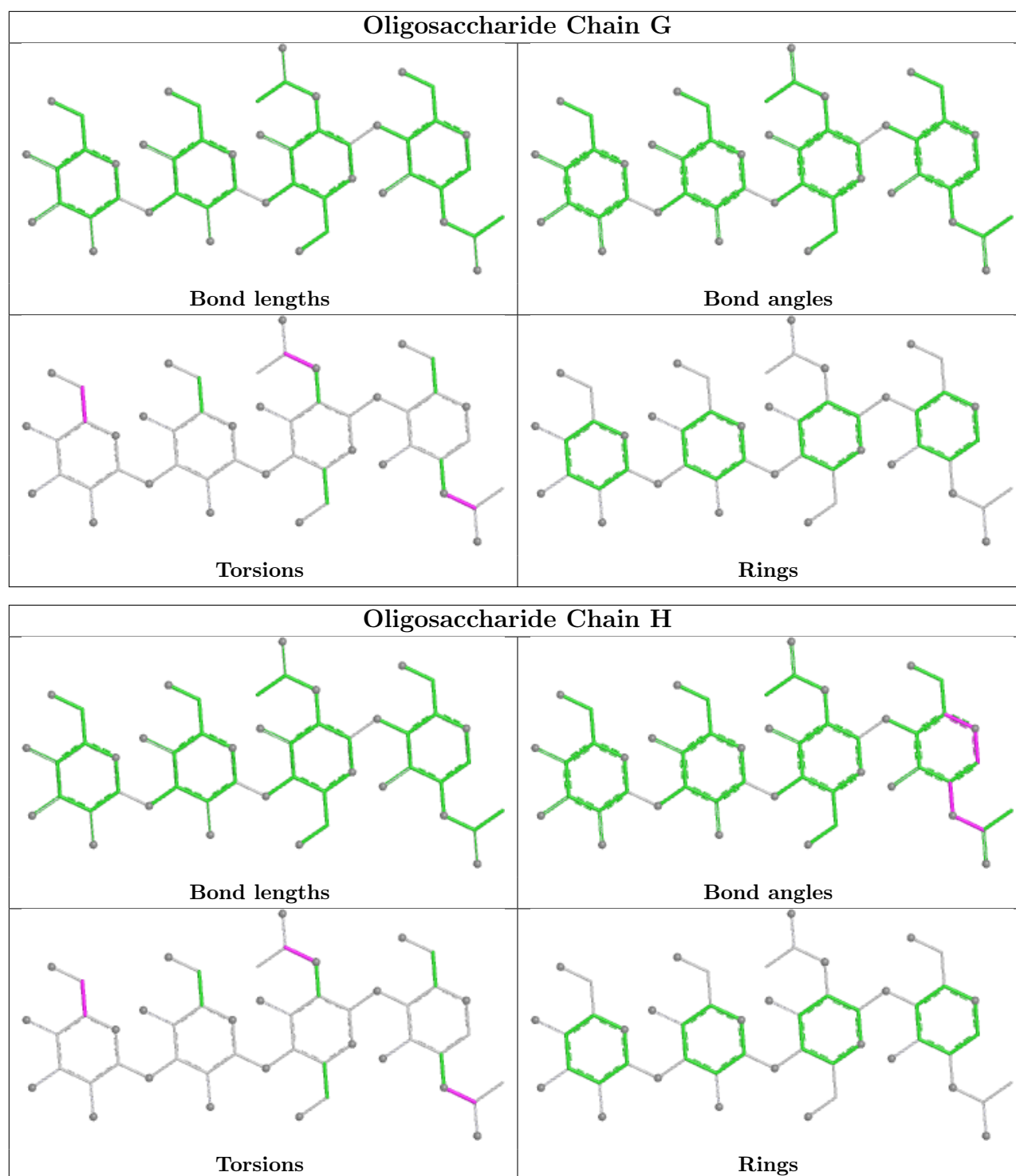
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F





5.6 Ligand geometry [i](#)

4 ligands 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	ZK1	B	901	-	29,29,29	3.77	13 (44%)	45,45,45	1.84	7 (15%)
3	ZK1	A	901	-	29,29,29	3.79	13 (44%)	45,45,45	1.83	9 (20%)
3	ZK1	C	901	-	29,29,29	3.74	13 (44%)	45,45,45	1.81	7 (15%)
3	ZK1	D	901	-	29,29,29	3.70	11 (37%)	45,45,45	1.84	8 (17%)

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	ZK1	B	901	-	-	4/13/23/23	0/3/3/3
3	ZK1	A	901	-	-	4/13/23/23	0/3/3/3
3	ZK1	C	901	-	-	4/13/23/23	0/3/3/3
3	ZK1	D	901	-	-	5/13/23/23	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ZK1	OAA-CAT	9.45	1.41	1.23
3	A	901	ZK1	OAA-CAT	9.41	1.41	1.23
3	D	901	ZK1	OAA-CAT	9.37	1.41	1.23
3	B	901	ZK1	OAA-CAT	9.37	1.41	1.23
3	B	901	ZK1	OAB-CAU	8.80	1.41	1.23
3	A	901	ZK1	OAB-CAU	8.80	1.41	1.23
3	C	901	ZK1	OAB-CAU	8.77	1.40	1.23
3	D	901	ZK1	CAU-CAT	-8.76	1.41	1.53
3	D	901	ZK1	OAB-CAU	8.73	1.40	1.23
3	B	901	ZK1	CAU-CAT	-8.72	1.41	1.53
3	A	901	ZK1	CAU-CAT	-8.60	1.41	1.53
3	C	901	ZK1	CAU-CAT	-8.57	1.41	1.53
3	D	901	ZK1	CAN-NAX	-6.76	1.35	1.46
3	A	901	ZK1	CAN-NAX	-6.75	1.35	1.46
3	B	901	ZK1	CAN-NAX	-6.74	1.35	1.46
3	C	901	ZK1	CAM-NAX	-6.70	1.35	1.46
3	A	901	ZK1	CAM-NAX	-6.65	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ZK1	CAN-NAX	-6.65	1.35	1.46
3	D	901	ZK1	CAM-NAX	-6.58	1.35	1.46
3	B	901	ZK1	CAM-NAX	-6.55	1.35	1.46
3	B	901	ZK1	CAI-CAW	4.73	1.47	1.39
3	D	901	ZK1	CAI-CAW	4.67	1.47	1.39
3	C	901	ZK1	CAI-CAW	4.60	1.47	1.39
3	A	901	ZK1	CAI-CAW	4.59	1.47	1.39
3	A	901	ZK1	PBA-OAC	3.76	1.57	1.50
3	A	901	ZK1	CAR-CAS	3.22	1.44	1.40
3	B	901	ZK1	CAR-CAS	3.21	1.44	1.40
3	C	901	ZK1	CAR-CAS	3.14	1.44	1.40
3	B	901	ZK1	CAJ-CAV	3.06	1.44	1.39
3	A	901	ZK1	CAJ-CAV	3.01	1.44	1.39
3	D	901	ZK1	CAR-CAS	2.99	1.43	1.40
3	D	901	ZK1	CAJ-CAV	2.97	1.44	1.39
3	C	901	ZK1	CAJ-CAV	2.90	1.44	1.39
3	B	901	ZK1	CAR-NAX	2.81	1.47	1.41
3	C	901	ZK1	CAR-NAX	2.78	1.47	1.41
3	A	901	ZK1	CAR-NAX	2.74	1.47	1.41
3	D	901	ZK1	CAR-NAX	2.69	1.47	1.41
3	B	901	ZK1	PBA-CAO	2.36	1.86	1.81
3	B	901	ZK1	PBA-OAC	2.34	1.54	1.50
3	A	901	ZK1	PBA-CAO	2.32	1.86	1.81
3	A	901	ZK1	PBA-OAE	-2.29	1.49	1.55
3	B	901	ZK1	PBA-OAE	-2.28	1.49	1.55
3	C	901	ZK1	PBA-OAE	-2.27	1.49	1.55
3	D	901	ZK1	PBA-CAO	2.25	1.86	1.81
3	C	901	ZK1	PBA-OAC	2.25	1.54	1.50
3	C	901	ZK1	PBA-CAO	2.19	1.86	1.81
3	A	901	ZK1	CAJ-CAS	2.11	1.42	1.39
3	D	901	ZK1	CAJ-CAS	2.08	1.42	1.39
3	B	901	ZK1	CAJ-CAS	2.05	1.42	1.39
3	C	901	ZK1	CAJ-CAS	2.03	1.42	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ZK1	CAN-NAX-CAM	7.75	129.01	111.57
3	B	901	ZK1	CAN-NAX-CAM	7.67	128.83	111.57
3	C	901	ZK1	CAN-NAX-CAM	7.44	128.30	111.57
3	A	901	ZK1	CAN-NAX-CAM	7.30	128.00	111.57
3	A	901	ZK1	CAI-CAR-NAX	-3.69	117.22	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ZK1	CAI-CAR-NAX	-3.52	117.46	122.59
3	B	901	ZK1	CAO-NAY-CAW	3.52	124.40	120.12
3	A	901	ZK1	CAV-NAP-CAT	-3.42	120.03	124.82
3	C	901	ZK1	CAV-NAP-CAT	-3.31	120.19	124.82
3	C	901	ZK1	CAO-NAY-CAW	3.23	124.05	120.12
3	D	901	ZK1	CAV-NAP-CAT	-3.21	120.32	124.82
3	D	901	ZK1	CAI-CAR-NAX	-3.20	117.92	122.59
3	B	901	ZK1	CAV-NAP-CAT	-3.20	120.34	124.82
3	D	901	ZK1	CAO-NAY-CAW	3.19	124.00	120.12
3	A	901	ZK1	CAO-NAY-CAW	3.18	123.99	120.12
3	B	901	ZK1	CAI-CAR-NAX	-3.15	118.00	122.59
3	D	901	ZK1	CAT-CAU-NAY	3.08	120.75	117.41
3	B	901	ZK1	CAT-CAU-NAY	3.02	120.69	117.41
3	C	901	ZK1	CAT-CAU-NAY	2.99	120.66	117.41
3	A	901	ZK1	CAT-CAU-NAY	2.90	120.56	117.41
3	A	901	ZK1	CAS-CAR-NAX	2.70	123.01	119.92
3	C	901	ZK1	CAS-CAR-NAX	2.50	122.79	119.92
3	D	901	ZK1	CAW-NAY-CAU	-2.15	120.20	122.84
3	A	901	ZK1	FAG-CAZ-CAS	-2.14	108.86	112.65
3	A	901	ZK1	CAU-CAT-NAP	2.13	119.63	117.46
3	A	901	ZK1	CAW-NAY-CAU	-2.11	120.25	122.84
3	D	901	ZK1	CAL-CAN-NAX	2.10	113.91	109.93
3	B	901	ZK1	CAK-CAM-NAX	2.09	113.89	109.93
3	C	901	ZK1	CAW-NAY-CAU	-2.09	120.27	122.84
3	B	901	ZK1	CAW-NAY-CAU	-2.08	120.28	122.84
3	D	901	ZK1	CAS-CAR-NAX	2.03	122.25	119.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ZK1	NAY-CAO-PBA-OAD
3	D	901	ZK1	NAY-CAO-PBA-OAC
3	D	901	ZK1	NAY-CAO-PBA-OAD
3	D	901	ZK1	CAI-CAR-NAX-CAN
3	A	901	ZK1	NAY-CAO-PBA-OAE
3	B	901	ZK1	NAY-CAO-PBA-OAD
3	B	901	ZK1	NAY-CAO-PBA-OAE
3	C	901	ZK1	NAY-CAO-PBA-OAD
3	C	901	ZK1	NAY-CAO-PBA-OAE
3	D	901	ZK1	NAY-CAO-PBA-OAE
3	A	901	ZK1	CAI-CAR-NAX-CAN

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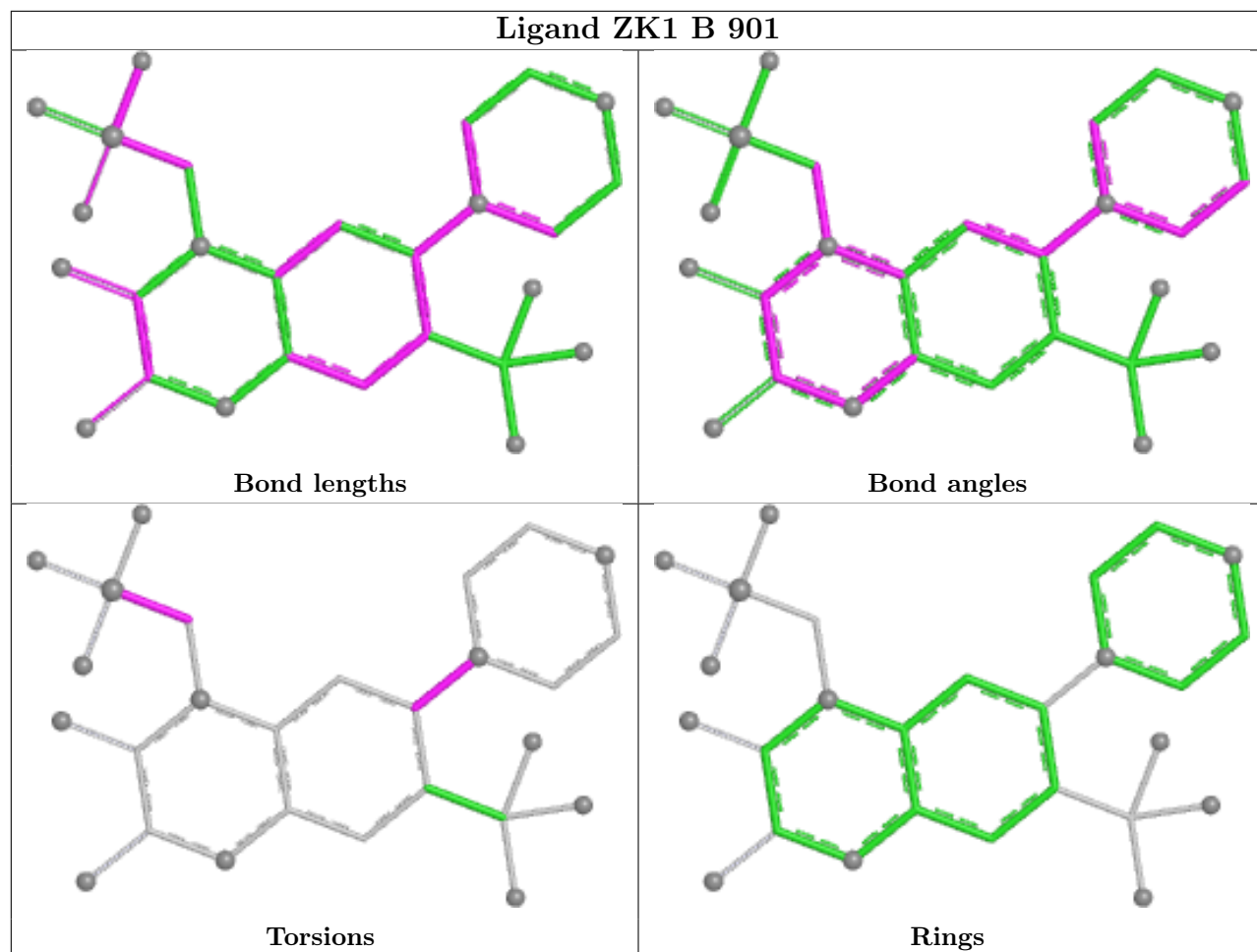
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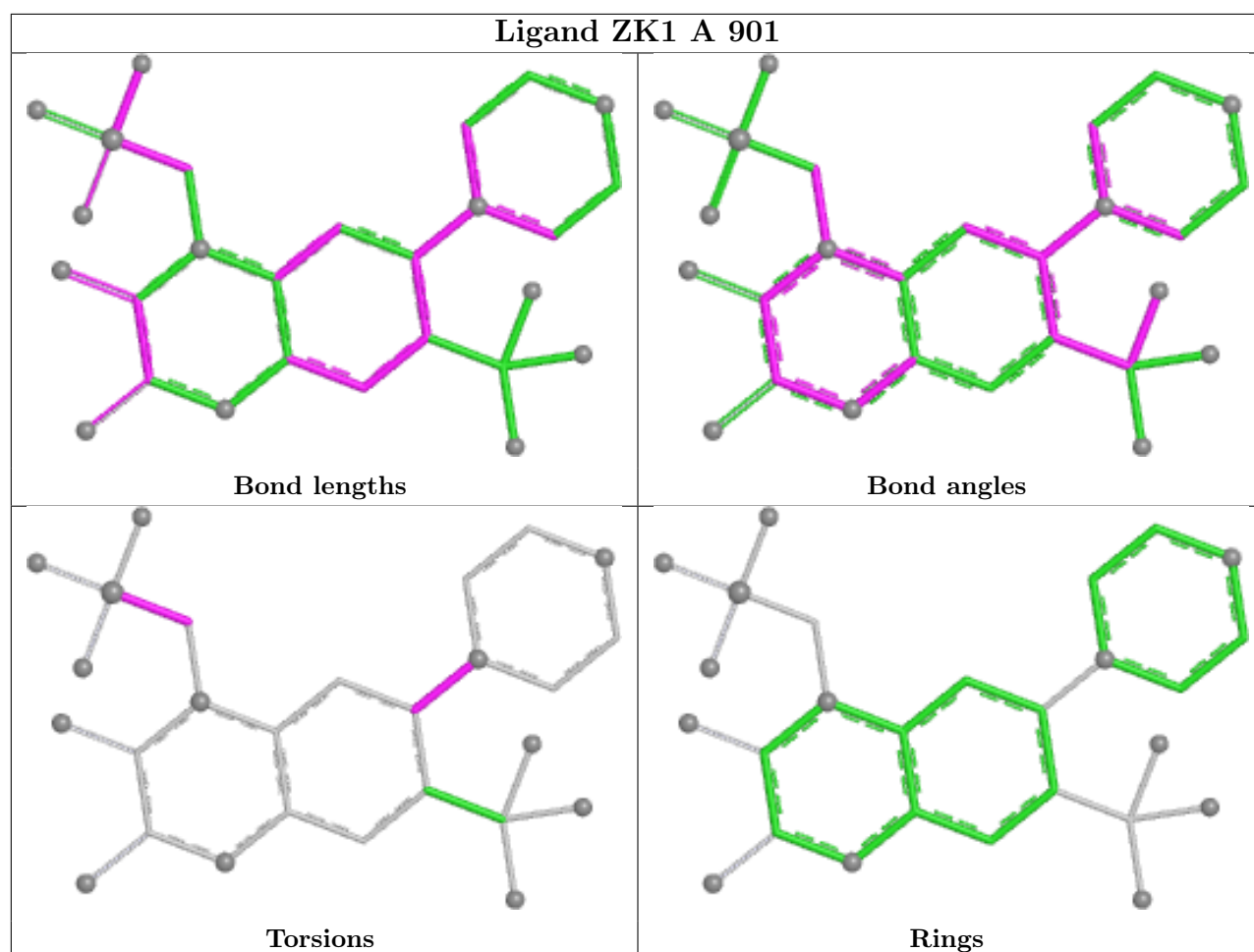
Mol	Chain	Res	Type	Atoms
3	B	901	ZK1	CAI-CAR-NAX-CAN
3	C	901	ZK1	CAI-CAR-NAX-CAN
3	A	901	ZK1	NAY-CAO-PBA-OAC
3	B	901	ZK1	NAY-CAO-PBA-OAC
3	C	901	ZK1	NAY-CAO-PBA-OAC
3	D	901	ZK1	CAS-CAR-NAX-CAN

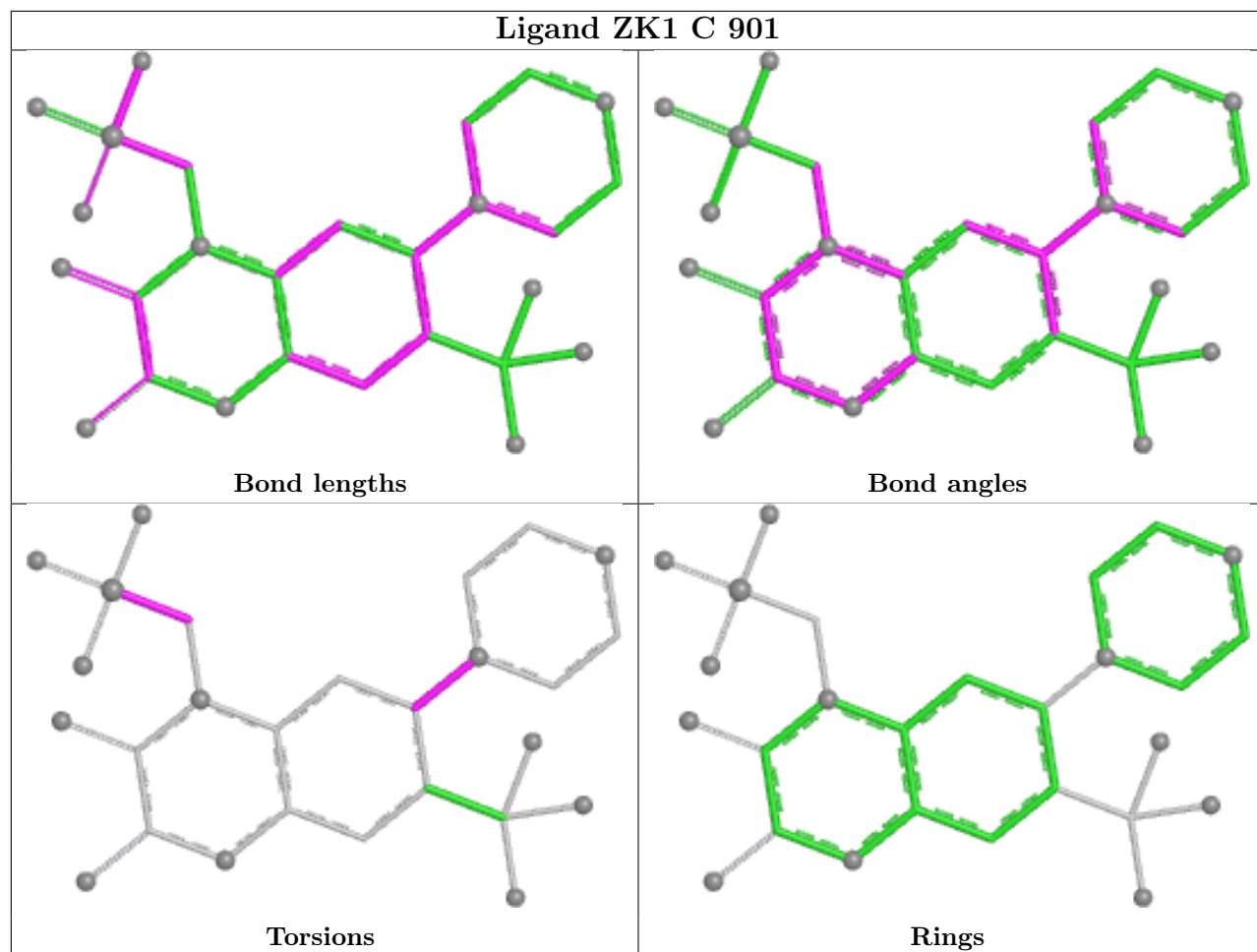
There are no ring outliers.

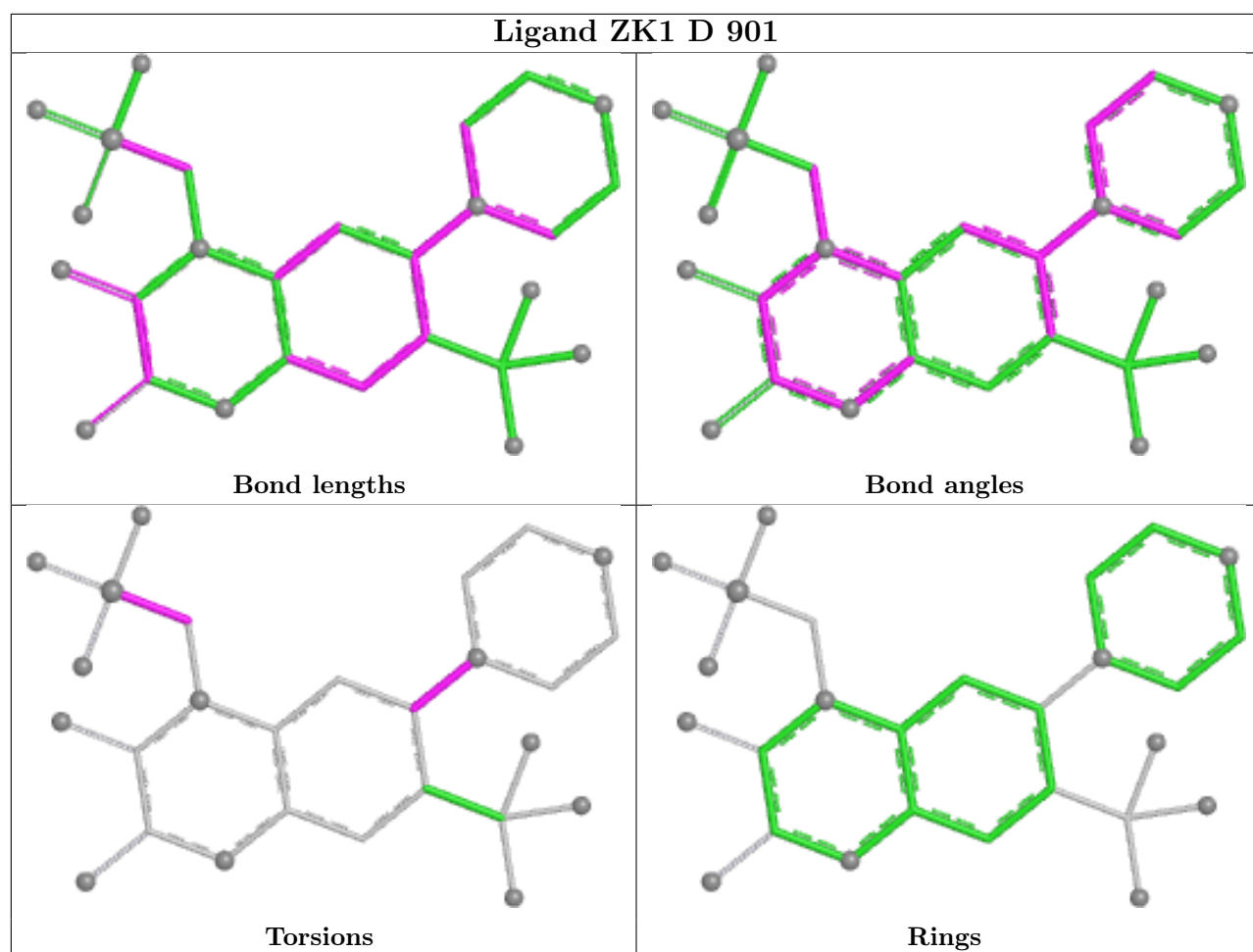
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	768/822 (93%)	-0.04	29 (3%)	44	37	58, 155, 265, 497	0
1	B	768/822 (93%)	0.02	30 (3%)	43	37	41, 167, 300, 506	0
1	C	768/822 (93%)	0.07	32 (4%)	40	35	45, 148, 265, 547	0
1	D	768/822 (93%)	0.05	30 (3%)	43	37	27, 135, 288, 515	0
All	All	3072/3288 (93%)	0.03	121 (3%)	43	37	27, 151, 276, 547	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	VAL	5.7
1	B	518	LEU	5.6
1	D	629	MET	5.4
1	C	571	PHE	5.3
1	D	756	GLN	5.2
1	A	291	VAL	5.1
1	B	659	PHE	4.9
1	B	526	TRP	4.7
1	B	636	ALA	4.6
1	D	757	GLY	4.6
1	A	187	LYS	4.5
1	C	432	ILE	4.4
1	D	758	VAL	4.4
1	D	245	PHE	4.3
1	D	729	SER	4.3
1	C	306	ILE	4.3
1	D	72	ALA	4.2
1	A	181	PHE	4.1
1	A	292	MET	4.0
1	A	296	PHE	3.9
1	A	679	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	631	SER	3.9
1	B	72	ALA	3.8
1	D	53	ALA	3.8
1	A	306	ILE	3.8
1	D	225	LEU	3.8
1	A	792	VAL	3.7
1	D	227	PHE	3.7
1	A	401	LEU	3.7
1	B	39	SER	3.7
1	C	792	VAL	3.6
1	D	358	ILE	3.6
1	B	494	PRO	3.5
1	D	239	GLY	3.5
1	D	71	TYR	3.5
1	A	103	THR	3.4
1	D	360	ILE	3.4
1	D	291	VAL	3.3
1	B	667	PHE	3.3
1	C	197	GLU	3.3
1	B	785	SER	3.2
1	C	149	VAL	3.2
1	C	813	GLU	3.2
1	A	652	SER	3.1
1	B	33	MET	3.1
1	A	77	TYR	3.1
1	B	521	LEU	3.1
1	A	73	ILE	3.1
1	C	387	THR	3.1
1	C	815	CYS	3.1
1	D	755	GLU	3.1
1	B	698	GLY	3.0
1	C	160	VAL	3.0
1	D	753	LEU	3.0
1	C	391	GLU	3.0
1	A	213	LYS	2.9
1	C	640	SER	2.9
1	D	121	LEU	2.9
1	A	687	ALA	2.8
1	C	386	ASP	2.8
1	A	378	ASP	2.8
1	B	670	MET	2.8
1	A	111	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	278	ILE	2.8
1	C	341	LEU	2.8
1	C	390	LEU	2.8
1	C	159	GLN	2.8
1	C	688	GLU	2.7
1	B	519	ASP	2.6
1	A	90	GLY	2.6
1	B	602	GLY	2.6
1	A	607	PHE	2.5
1	D	456	ASP	2.5
1	B	300	ARG	2.5
1	B	92	LEU	2.5
1	D	754	SER	2.5
1	C	584	PHE	2.5
1	C	639	LEU	2.4
1	D	432	ILE	2.4
1	A	113	MET	2.4
1	D	411	ASN	2.4
1	C	303	ARG	2.4
1	C	572	GLY	2.4
1	C	283	ALA	2.3
1	D	751	LEU	2.3
1	C	311	ASN	2.3
1	B	103	THR	2.3
1	B	442	LEU	2.3
1	A	184	LEU	2.3
1	A	96	PHE	2.3
1	C	773	CYS	2.2
1	B	251	ASP	2.2
1	B	447	ASP	2.2
1	A	730	LYS	2.2
1	B	603	GLY	2.2
1	B	247	ILE	2.2
1	A	486	GLU	2.2
1	B	515	PHE	2.2
1	D	773	CYS	2.2
1	C	606	TRP	2.2
1	B	296	PHE	2.1
1	B	95	SER	2.1
1	D	785	SER	2.1
1	D	294	GLU	2.1
1	A	483	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	39	SER	2.1
1	A	651	ASP	2.1
1	A	333	LEU	2.1
1	B	506	LYS	2.1
1	D	296	PHE	2.1
1	B	593	PRO	2.1
1	C	389	GLY	2.1
1	A	680	SER	2.1
1	B	305	GLU	2.1
1	C	641	LYS	2.0
1	A	104	ASP	2.0
1	C	335	GLN	2.0
1	C	690	VAL	2.0
1	D	383	THR	2.0
1	C	580	SER	2.0
1	B	289	VAL	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.

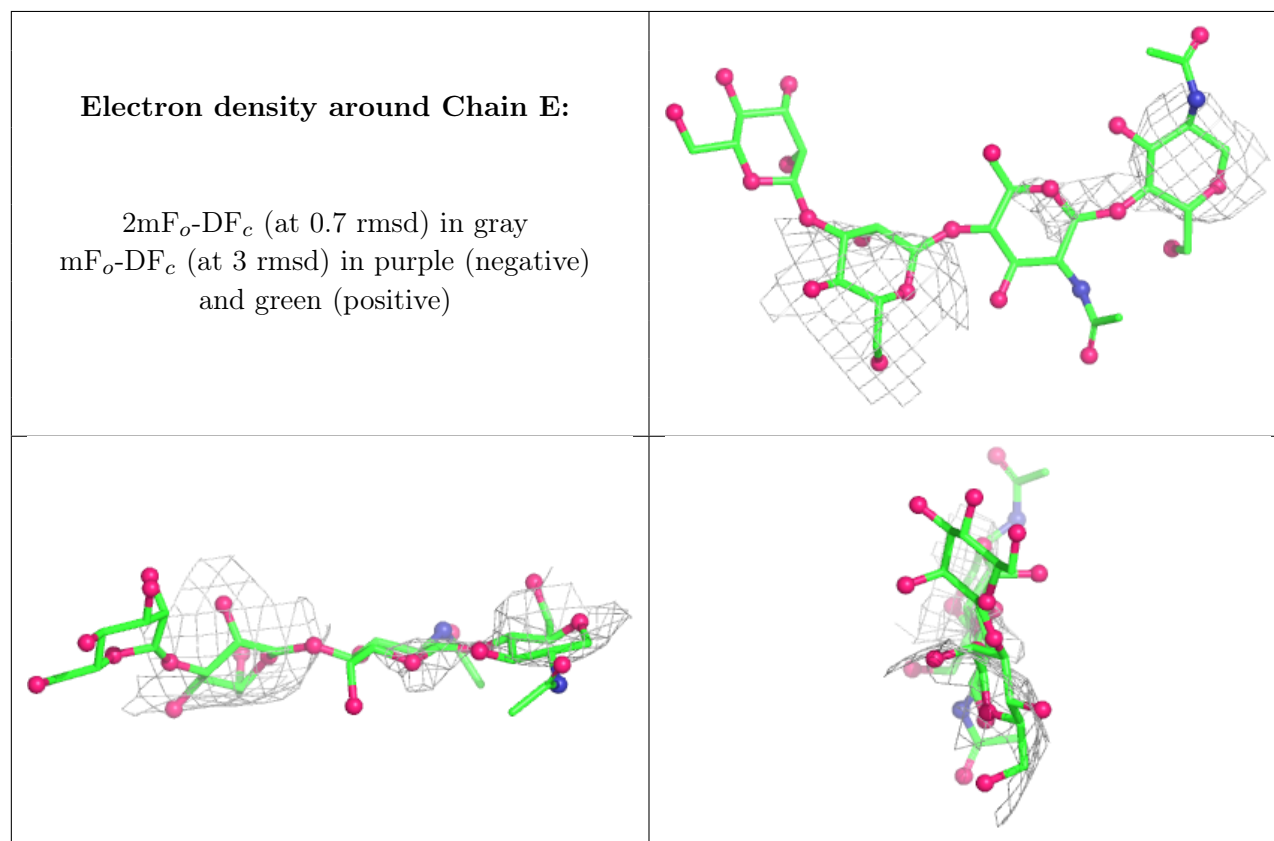
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	G	3	11/12	-0.30	0.14	254,254,254,254	0
2	BMA	F	3	11/12	0.04	0.14	232,232,232,232	0
2	BMA	E	3	11/12	0.13	0.14	280,280,280,280	0
2	BMA	E	4	11/12	0.27	0.08	269,269,269,269	0
2	BMA	H	3	11/12	0.27	0.09	233,233,233,233	0
2	NAG	F	2	14/15	0.54	0.09	180,180,180,180	0
2	NAG	H	1	14/15	0.55	0.09	336,336,336,336	0
2	BMA	G	4	11/12	0.66	0.09	287,287,287,287	0
2	BMA	H	4	11/12	0.67	0.07	264,264,264,264	0
2	BMA	F	4	11/12	0.72	0.08	231,231,231,231	0
2	NAG	E	2	14/15	0.74	0.10	269,269,269,269	0
2	NAG	G	2	14/15	0.75	0.09	225,225,225,225	0

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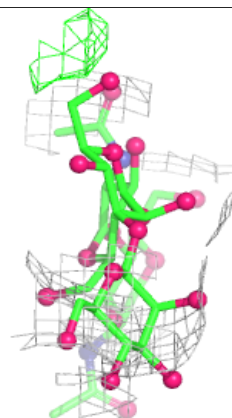
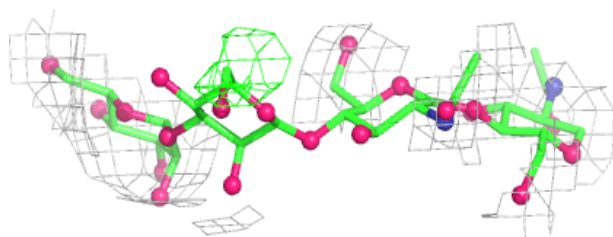
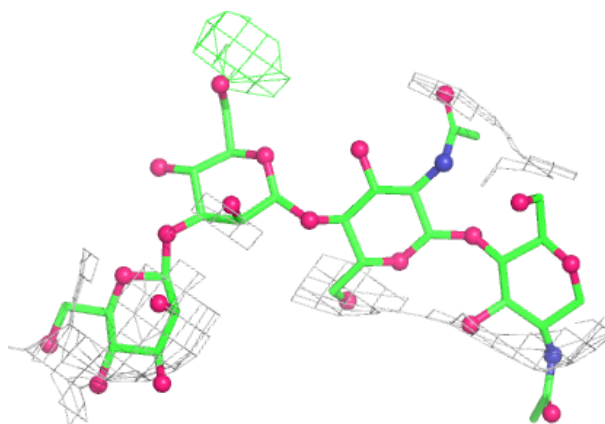
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	1	14/15	0.77	0.14	167,167,167,167	0
2	NAG	E	1	14/15	0.82	0.09	227,227,227,227	0
2	NAG	H	2	14/15	0.82	0.07	294,294,294,294	0
2	NAG	G	1	14/15	0.91	0.06	211,211,211,211	0

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.

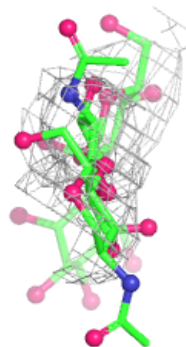
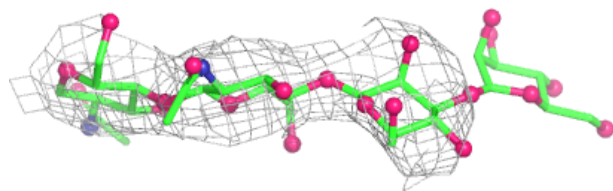
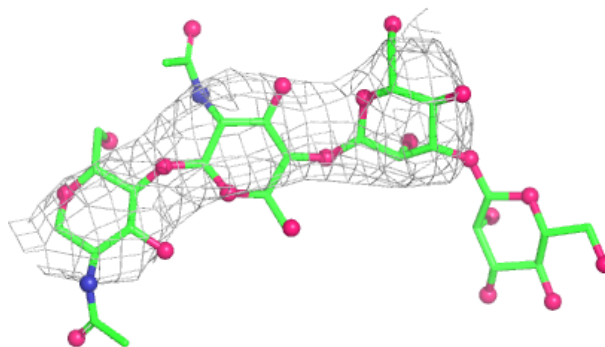


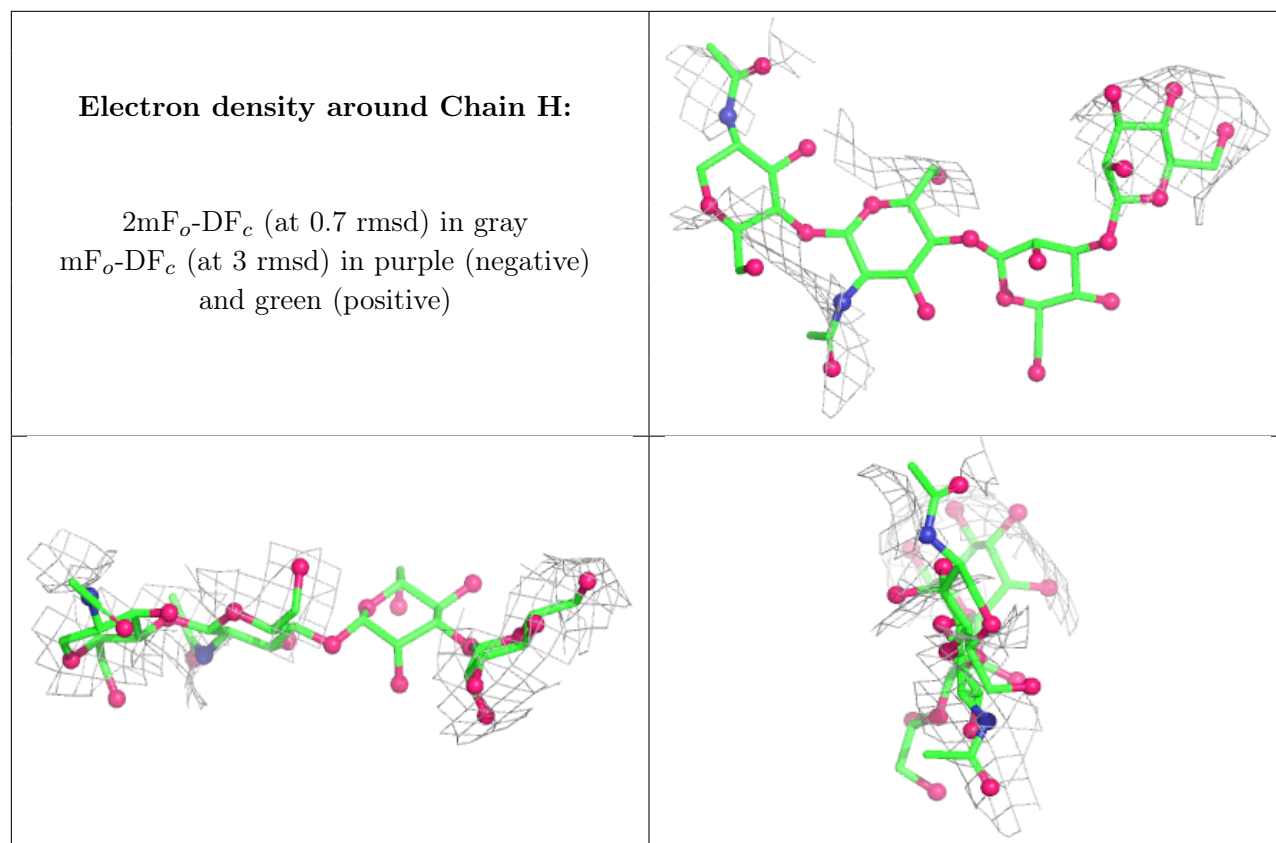
Electron density around Chain F:

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

**Electron density around Chain G:**

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





6.4 Ligands [i](#)

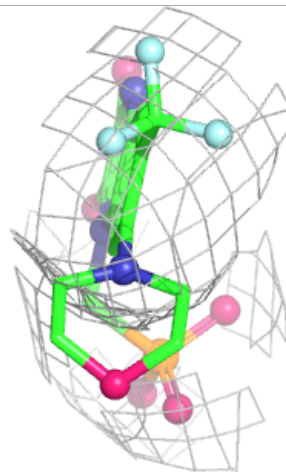
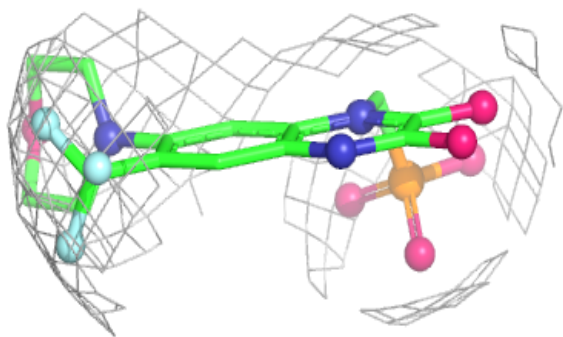
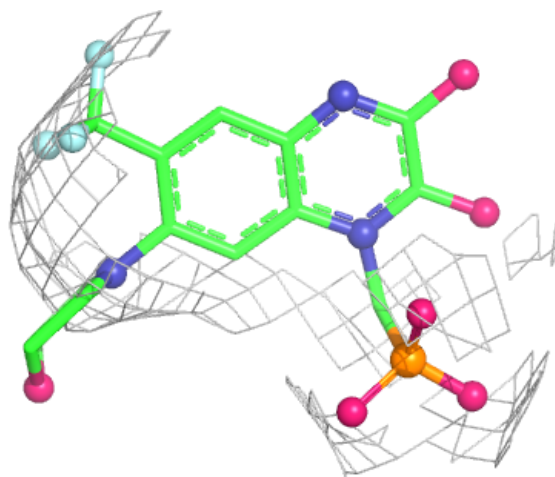
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZK1	D	901	27/27	0.89	0.12	136,136,136,136	0
3	ZK1	B	901	27/27	0.90	0.08	236,236,236,236	0
3	ZK1	A	901	27/27	0.90	0.10	138,138,138,138	0
3	ZK1	C	901	27/27	0.92	0.10	137,137,137,137	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.

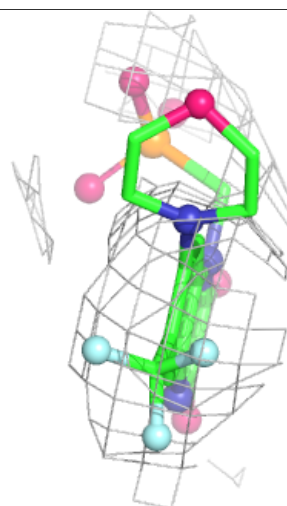
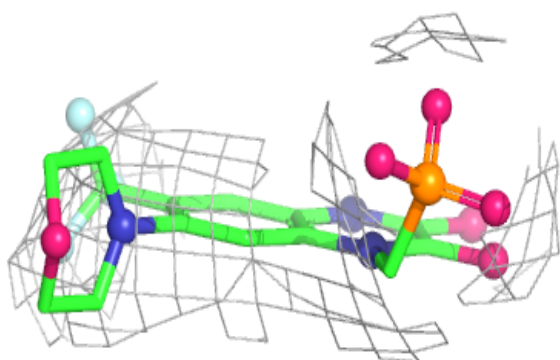
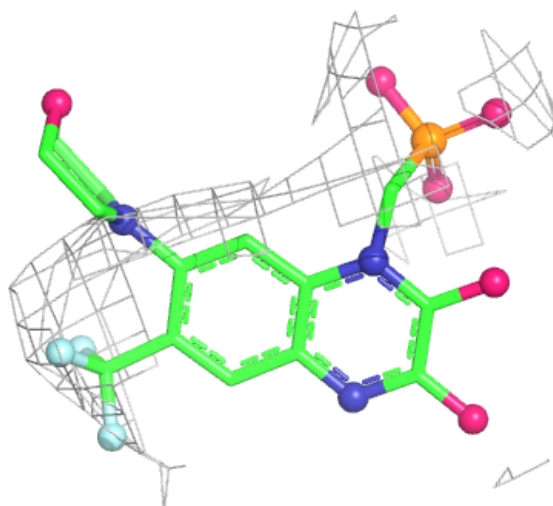
Electron density around ZK1 D 901:

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



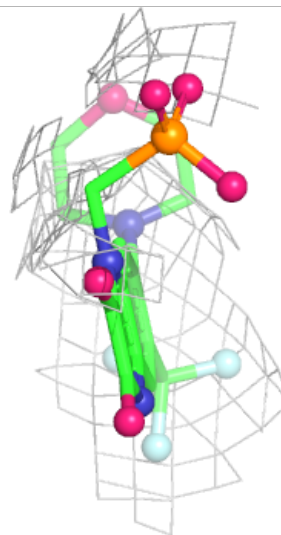
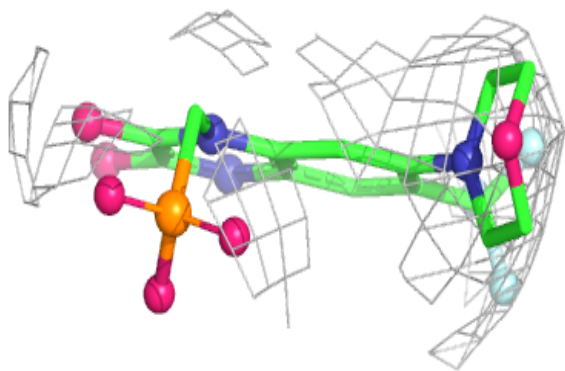
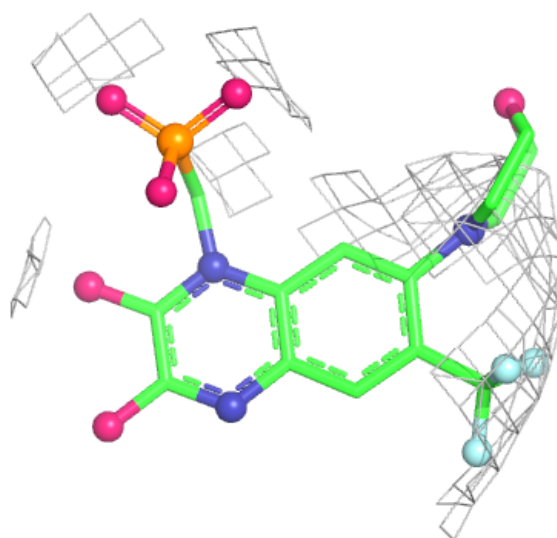
Electron density around ZK1 B 901:

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



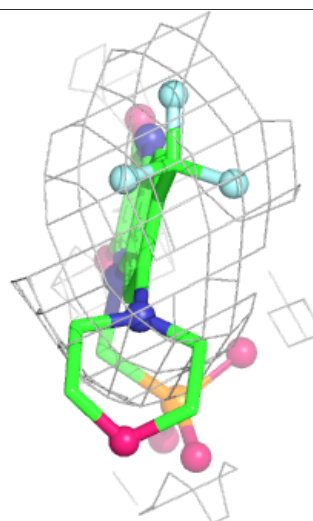
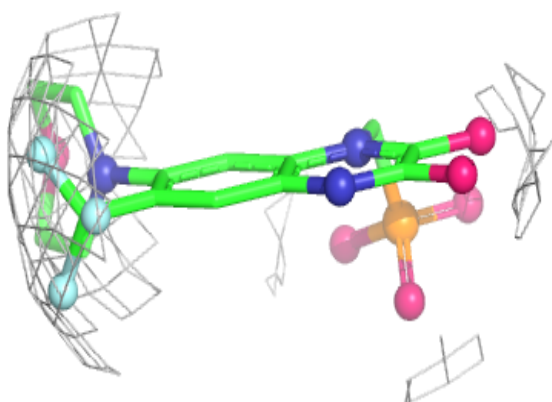
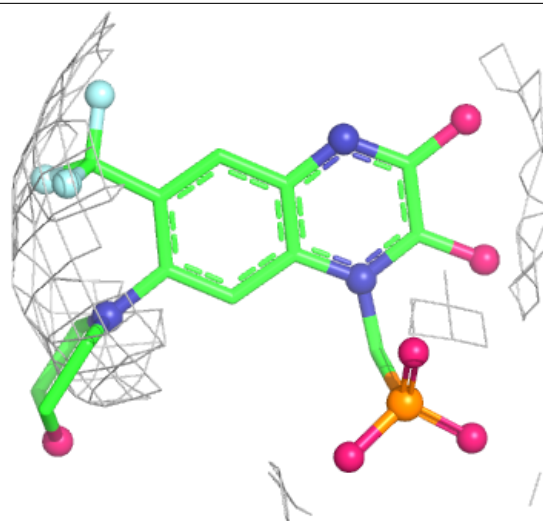
Electron density around ZK1 A 901:

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



Electron density around ZK1 C 901:

$2mF_o-DF_c$ (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.