



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:47 AM UTC

PDB ID : 1CVU / pdb_00001cvu
Title : CRYSTAL STRUCTURE OF ARACHIDONIC ACID BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on : 1999-08-24
Resolution : 2.40 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](#) ①) were used in the production of this report:

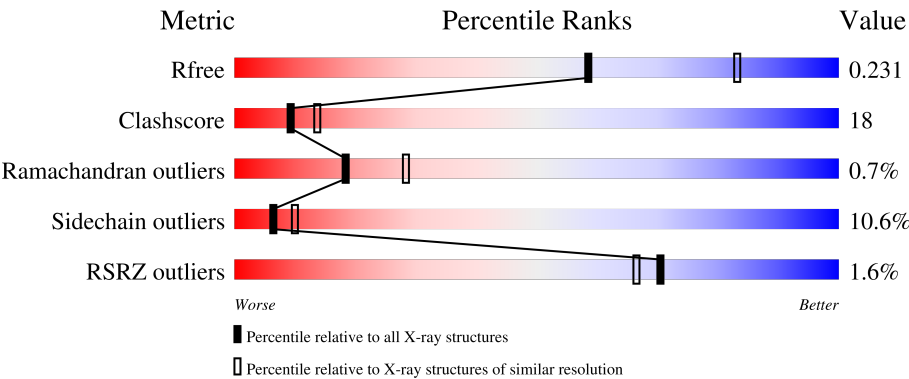
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	552	% 65% 27% 7%
1	B	552	% 63% 29% 8%
2	F	9	56% 44% 44% 11%
3	C	2	50% 50%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
4	D	4	 50% 50%
4	G	4	 25% 25% 50%

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	MAN	D	4	X	-	-	-
4	MAN	G	4	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 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 PROSTAGLANDIN H2 SYNTHASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	engineered mutation	UNP Q05769
A	333	LYS	ARG	engineered mutation	UNP Q05769
B	2310	GLN	ASN	engineered mutation	UNP Q05769
B	2333	LYS	ARG	engineered mutation	UNP Q05769

- Molecule 2 is a protein called PROTEIN (9-MER).

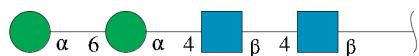
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	9	Total	C	N	O	0	0	0
			63	37	11	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



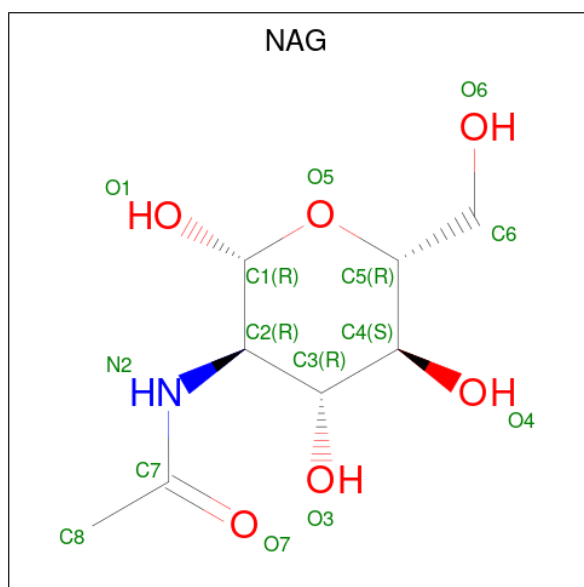
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



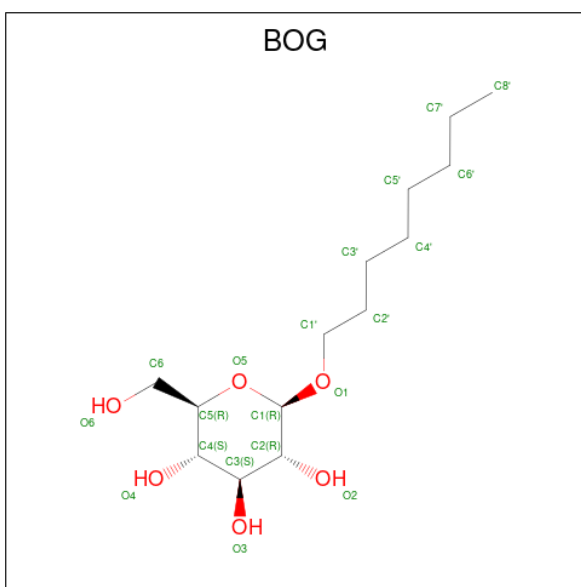
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



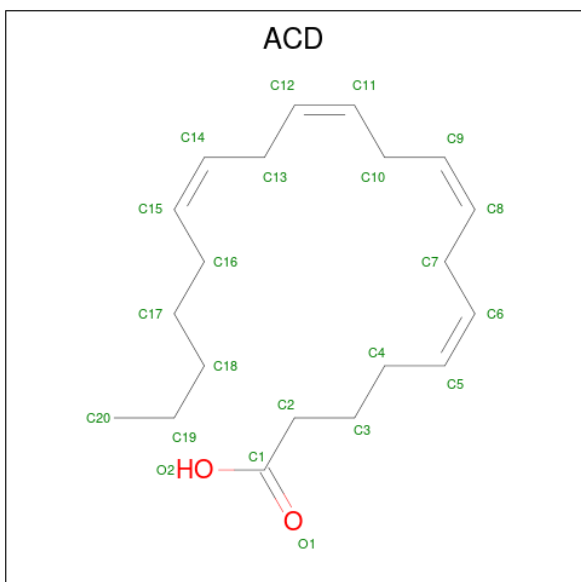
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is ARACHIDONIC ACID (CCD ID: ACD) (formula: $C_{20}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 22	C 20	O 2	0	0
7	B	1	Total 22	C 20	O 2	0	0

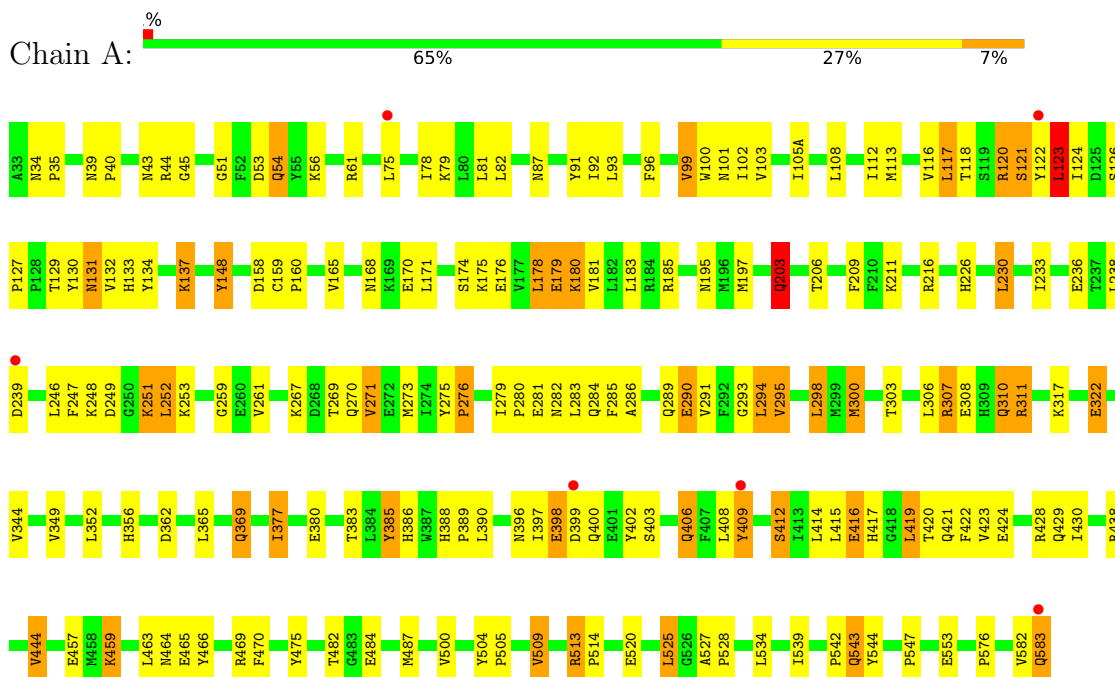
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	410	Total 410	O 410	0	0
8	B	361	Total 361	O 361	0	0

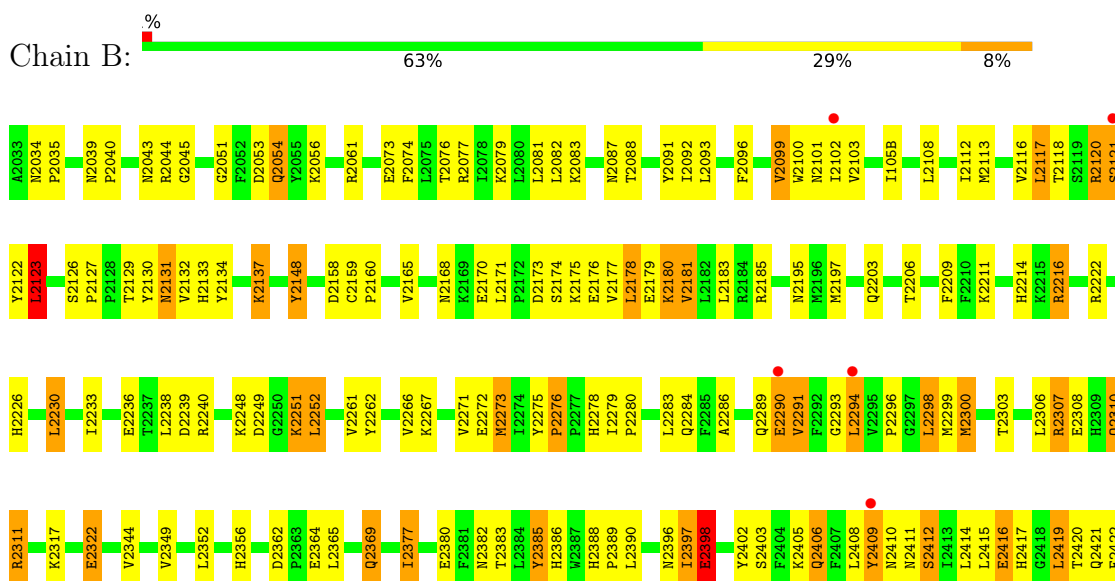
3 Residue-property plots

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: PROSTAGLANDIN H2 SYNTHASE-2

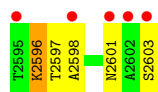


• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-2





• Molecule 2: PROTEIN (9-MER)



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



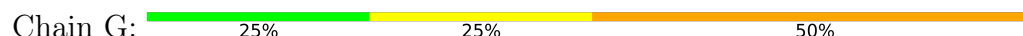
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.04Å 133.96Å 124.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 35.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (35.00-2.40) 96.2 (35.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.235 0.204 , 0.231	Depositor DCC
R_{free} test set	3887 reflections (6.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.0	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	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: BOG, MAN, ACD, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	1/4595 (0.0%)	0.98	14/6229 (0.2%)
1	B	0.56	0/4595	0.99	14/6229 (0.2%)
2	F	1.82	2/62 (3.2%)	1.55	2/82 (2.4%)
All	All	0.58	3/9252 (0.0%)	0.99	30/12540 (0.2%)

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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2603	SER	C-O	9.05	1.41	1.23
1	A	203	GLN	CD-OE1	6.98	1.36	1.23
2	F	2603	SER	C-OXT	-6.86	1.09	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-9.10	97.01	110.48
1	B	2148	TYR	N-CA-C	-8.70	97.60	110.48
2	F	2603	SER	CA-C-O	7.98	144.95	121.00
1	B	2276	PRO	N-CA-C	-7.16	101.97	110.70
2	F	2603	SER	N-CA-C	6.66	129.66	111.00
1	B	2130	TYR	N-CA-C	6.46	118.86	110.53
1	B	2251	LYS	N-CA-C	6.30	118.65	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LYS	N-CA-C	6.24	118.58	110.53
1	B	2123	LEU	N-CA-C	6.12	120.95	112.45
1	B	2356	HIS	N-CA-C	-6.10	105.67	113.23
1	B	2273	MET	N-CA-C	-6.05	97.91	110.80
1	A	356	HIS	N-CA-C	-6.03	105.75	113.23
1	B	2216	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	130	TYR	N-CA-C	5.92	118.16	110.53
1	A	45	GLY	N-CA-C	-5.90	105.15	111.93
1	B	2181	VAL	N-CA-C	5.89	118.86	113.20
1	A	123	LEU	N-CA-C	5.85	120.58	112.45
1	B	2197	MET	N-CA-C	-5.85	104.99	111.36
1	A	276	PRO	CA-C-N	5.67	125.78	119.32
1	A	276	PRO	C-N-CA	5.67	125.78	119.32
1	A	197	MET	N-CA-C	-5.58	105.28	111.36
1	A	159	CYS	CA-C-N	5.32	124.50	118.97
1	A	159	CYS	C-N-CA	5.32	124.50	118.97
1	B	2045	GLY	N-CA-C	-5.29	105.85	111.93
1	B	2398	GLU	CB-CA-C	-5.25	110.10	117.23
1	A	513	ARG	N-CA-C	-5.23	104.12	110.13
1	A	293	GLY	N-CA-C	-5.16	108.56	115.32
1	A	179	GLU	N-CA-C	5.10	116.53	111.07
1	B	2159	CYS	CA-C-N	5.04	124.22	118.97
1	B	2159	CYS	C-N-CA	5.04	124.22	118.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	TYR	Sidechain

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	4469	0	4373	159	0
1	B	4469	0	4373	171	0
2	F	63	0	65	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	0	0
3	E	28	0	25	0	0
4	D	50	0	42	3	0
4	G	50	0	42	5	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	60	0	84	6	0
6	B	40	0	56	6	0
7	A	22	0	31	0	0
7	B	22	0	31	0	0
8	A	410	0	0	8	0
8	B	361	0	0	11	0
All	All	10100	0	9173	334	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 18.

All (334) 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:300:MET:HE3	1:A:422:PHE:HB3	1.34	1.09
1:B:2300:MET:HE3	1:B:2422:PHE:HB3	1.33	1.07
1:B:2251:LYS:HD3	1:B:2310:GLN:HG3	1.49	0.92
1:A:251:LYS:HD3	1:A:310:GLN:HG3	1.51	0.89
1:B:2408:LEU:O	1:B:2409:TYR:HB2	1.74	0.87
1:B:2283:LEU:HD21	1:B:2415:LEU:HD12	1.55	0.85
1:A:543:GLN:OE1	1:A:543:GLN:HA	1.77	0.85
1:B:2209:PHE:HB2	1:B:2377:ILE:HD13	1.59	0.83
1:B:2240:ARG:NH2	1:B:2273:MET:HE2	1.93	0.83
1:B:2543:GLN:OE1	1:B:2543:GLN:HA	1.77	0.83
1:A:209:PHE:HB2	1:A:377:ILE:HD13	1.60	0.81
1:B:2293:GLY:HA2	1:B:2299:MET:HE3	1.64	0.79
1:A:246:LEU:HG	1:A:248:LYS:HG3	1.64	0.79
1:B:2216:ARG:NH1	4:G:2:NAG:C7	2.47	0.78
1:A:51:GLY:C	1:B:2322:GLU:HG2	2.10	0.77
1:A:75:LEU:HD11	1:A:79:LYS:HE3	1.68	0.76
1:B:2275:TYR:HB3	1:B:2279:ILE:HD13	1.68	0.76
1:A:322:GLU:HG2	1:B:2051:GLY:C	2.11	0.76
2:F:2597:THR:HG22	2:F:2601:ASN:HD22	1.52	0.75
1:B:2464:ASN:HD21	1:B:2475:TYR:H	1.36	0.74
2:F:2597:THR:CG2	2:F:2601:ASN:ND2	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2209:PHE:HB2	1:B:2377:ILE:CD1	2.19	0.71
1:A:464:ASN:HD21	1:A:475:TYR:H	1.37	0.71
2:F:2597:THR:HG23	2:F:2601:ASN:HD21	1.54	0.70
1:A:129:THR:HG22	1:A:137:LYS:HD3	1.72	0.70
1:B:2582:VAL:HG13	1:B:2583:GLN:OE1	1.91	0.70
1:B:2131:ASN:C	1:B:2131:ASN:HD22	2.00	0.70
2:F:2597:THR:HG23	2:F:2601:ASN:ND2	2.07	0.69
1:A:209:PHE:HB2	1:A:377:ILE:CD1	2.22	0.69
1:A:582:VAL:HG13	1:A:583:GLN:OE1	1.92	0.68
1:B:2129:THR:HG22	1:B:2137:LYS:HD3	1.76	0.68
1:A:131:ASN:C	1:A:131:ASN:HD22	2.00	0.67
1:A:412:SER:O	1:A:416:GLU:HB2	1.94	0.67
1:A:396:ASN:H	1:A:429:GLN:HE22	1.44	0.66
1:A:424:GLU:O	1:A:428:ARG:HG3	1.96	0.66
1:B:2276:PRO:O	1:B:2279:ILE:HD12	1.95	0.65
1:B:2061:ARG:HD2	8:B:3380:HOH:O	1.96	0.65
1:A:185:ARG:HH11	6:A:703:BOG:H4'1	1.61	0.64
1:B:2271:VAL:HG21	1:B:2286:ALA:HB1	1.77	0.64
1:A:469:ARG:HD2	1:A:469:ARG:O	1.98	0.64
1:A:398:GLU:OE1	1:A:417:HIS:HD2	1.81	0.63
1:B:2053:ASP:C	1:B:2054:GLN:HG3	2.23	0.63
1:B:2414:LEU:HD11	1:B:2419:LEU:HD22	1.81	0.63
1:A:75:LEU:HD12	1:A:75:LEU:O	1.99	0.63
1:B:2283:LEU:HD21	1:B:2415:LEU:CD1	2.26	0.62
1:B:2527:ALA:HB3	1:B:2528:PRO:HD3	1.82	0.62
1:B:2293:GLY:HA2	1:B:2299:MET:CE	2.29	0.62
1:B:2424:GLU:O	1:B:2428:ARG:HG3	1.99	0.62
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.82	0.62
1:B:2216:ARG:HG2	4:G:2:NAG:O7	1.98	0.62
1:A:543:GLN:HB2	8:A:3119:HOH:O	1.99	0.62
1:A:53:ASP:C	1:A:54:GLN:HG3	2.25	0.61
2:F:2597:THR:HG22	2:F:2601:ASN:ND2	2.14	0.61
1:B:2211:LYS:NZ	1:B:2236:GLU:HG2	2.15	0.61
1:A:251:LYS:CD	1:A:310:GLN:HG3	2.30	0.61
1:A:185:ARG:NH1	6:A:703:BOG:H4'1	2.16	0.61
1:A:444:VAL:O	1:A:444:VAL:HG13	1.99	0.61
1:A:273:MET:SD	1:A:290:GLU:HA	2.40	0.60
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.81	0.60
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.84	0.60
1:A:211:LYS:NZ	1:A:236:GLU:HG2	2.17	0.59
1:B:2203:GLN:HG2	1:B:2298:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:HG23	1:A:576:PRO:HG3	1.84	0.59
1:B:2398:GLU:OE2	1:B:2421:GLN:HG2	2.02	0.59
1:B:2251:LYS:CD	1:B:2310:GLN:HG3	2.29	0.59
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.85	0.59
1:B:2230:LEU:HD13	1:B:2233:ILE:HD12	1.84	0.58
1:B:2293:GLY:O	1:B:2411:ASN:ND2	2.30	0.58
1:B:2402:TYR:OH	1:B:2417:HIS:HE1	1.86	0.58
1:B:2280:PRO:HG2	1:B:2283:LEU:HD12	1.85	0.58
1:B:2482:THR:HG22	1:B:2509:VAL:HG13	1.86	0.58
1:A:203:GLN:OE1	6:A:704:BOG:H5'1	2.04	0.58
1:A:294:LEU:HA	1:A:409:TYR:CE2	2.37	0.58
1:B:2469:ARG:HD2	1:B:2469:ARG:O	2.03	0.58
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.69	0.58
1:B:2181:VAL:HG12	1:B:2487:MET:HG2	1.87	0.57
1:B:2108:LEU:O	1:B:2112:ILE:HG12	2.04	0.57
1:B:105(B):ILE:HG22	1:B:2108:LEU:H	1.68	0.57
4:D:2:NAG:H61	4:D:3:MAN:C1	2.35	0.57
1:B:2226:HIS:C	1:B:2377:ILE:HD12	2.30	0.57
1:B:2310:GLN:HG2	8:B:3241:HOH:O	2.04	0.56
1:A:226:HIS:C	1:A:377:ILE:HD12	2.30	0.56
1:B:2113:MET:HE3	1:B:2117:LEU:HD13	1.87	0.56
1:B:2148:TYR:HD1	1:B:2377:ILE:HG22	1.70	0.56
1:B:2364:GLU:HG3	8:B:3734:HOH:O	2.05	0.56
1:A:280:PRO:O	1:A:284:GLN:HG3	2.04	0.56
1:B:2383:THR:HA	1:B:2386:HIS:CD2	2.41	0.56
1:A:108:LEU:O	1:A:112:ILE:HG12	2.06	0.55
1:A:113:MET:HE3	1:A:117:LEU:HD13	1.88	0.55
1:A:543:GLN:O	1:B:2137:LYS:HE2	2.07	0.55
1:B:2444:VAL:HG13	1:B:2444:VAL:O	2.06	0.55
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.41	0.55
1:A:137:LYS:HE2	1:B:2543:GLN:O	2.06	0.55
1:B:2211:LYS:NZ	1:B:2236:GLU:CG	2.69	0.55
1:A:195:ASN:HB3	1:A:582:VAL:HG23	1.89	0.55
1:B:2120:ARG:HG2	1:B:2120:ARG:HH11	1.71	0.55
1:B:2500:VAL:HG12	1:B:2500:VAL:O	2.07	0.55
4:G:2:NAG:H61	4:G:3:MAN:C1	2.37	0.55
1:B:2396:ASN:H	1:B:2429:GLN:HE22	1.55	0.54
1:B:2470:PHE:CG	1:B:2525:LEU:HD22	2.42	0.54
1:B:2420:THR:HG23	1:B:2576:PRO:HG3	1.89	0.54
1:B:2412:SER:O	1:B:2416:GLU:HB2	2.06	0.54
1:B:2034:ASN:C	1:B:2034:ASN:HD22	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.71	0.54
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.43	0.53
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.70	0.53
2:F:2596:LYS:HD2	2:F:2597:THR:H	1.73	0.53
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.39	0.53
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.91	0.53
1:B:2575:CYS:SG	2:F:2598:ALA:HA	2.49	0.53
1:B:2148:TYR:CD1	1:B:2377:ILE:HG22	2.43	0.53
1:B:2203:GLN:OE1	6:B:2704:BOG:H5'1	2.09	0.53
1:B:2403:SER:OG	1:B:2406:GLN:HG3	2.09	0.53
1:B:2195:ASN:HB3	1:B:2582:VAL:HG23	1.90	0.52
1:B:2271:VAL:HG23	1:B:2271:VAL:O	2.08	0.52
1:B:2275:TYR:O	1:B:2276:PRO:C	2.52	0.52
1:B:2126:SER:HA	1:B:2127:PRO:C	2.34	0.52
1:B:2175:LYS:O	1:B:2179:GLU:HG3	2.10	0.52
1:A:34:ASN:HD22	1:A:34:ASN:C	2.17	0.52
1:A:75:LEU:CD1	1:A:79:LYS:HG3	2.40	0.51
1:B:2276:PRO:HD2	1:B:2279:ILE:CD1	2.39	0.51
1:A:175:LYS:O	1:A:179:GLU:HG3	2.11	0.51
1:B:2582:VAL:HG12	1:B:2582:VAL:O	2.11	0.51
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.74	0.51
1:A:269:THR:O	1:A:270:GLN:HB2	2.10	0.51
1:B:2083:LYS:HE2	8:B:3296:HOH:O	2.10	0.51
1:B:2296:PRO:HG3	1:B:2410:ASN:O	2.10	0.51
1:A:126:SER:HA	1:A:127:PRO:C	2.36	0.51
1:A:465:GLU:HA	1:A:465:GLU:OE1	2.10	0.51
1:B:2504:TYR:HB3	1:B:2505:PRO:HD3	1.92	0.51
1:B:2276:PRO:HB2	1:B:2278:HIS:CE1	2.46	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.94	0.50
1:B:2102:ILE:HG13	1:B:2103:VAL:N	2.27	0.50
1:A:261:VAL:O	1:A:307:ARG:NH1	2.44	0.50
1:A:513:ARG:NH2	1:A:520:GLU:HG3	2.27	0.50
1:A:280:PRO:HB2	1:A:282:ASN:OD1	2.11	0.50
1:A:383:THR:HA	1:A:386:HIS:CD2	2.47	0.50
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.95	0.50
1:B:2039:ASN:N	1:B:2040:PRO:CD	2.75	0.49
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.93	0.49
1:A:267:LYS:HD3	1:A:281:GLU:OE1	2.11	0.49
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.48	0.49
1:A:582:VAL:HG12	1:A:582:VAL:O	2.12	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2291:VAL:O	1:B:2294:LEU:HG	2.13	0.49
1:B:2131:ASN:HD21	1:B:2134:TYR:HD1	1.61	0.49
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.48	0.49
1:A:179:GLU:OE2	6:A:703:BOG:H1	2.13	0.48
1:A:403:SER:OG	1:A:406:GLN:HG2	2.13	0.48
1:B:2121:SER:O	1:B:2123:LEU:N	2.46	0.48
1:A:121:SER:O	1:A:123:LEU:N	2.46	0.48
1:A:306:LEU:HD23	1:A:306:LEU:C	2.37	0.48
1:A:131:ASN:HD21	1:A:134:TYR:HD1	1.60	0.48
1:B:2294:LEU:N	1:B:2294:LEU:HD23	2.27	0.48
1:A:132:VAL:HG13	1:A:133:HIS:CD2	2.49	0.48
1:A:39:ASN:N	1:A:40:PRO:CD	2.77	0.48
1:A:102:ILE:HG13	1:A:103:VAL:N	2.26	0.48
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.13	0.48
1:A:500:VAL:HG12	1:A:500:VAL:O	2.14	0.48
1:B:2073:GLU:O	1:B:2074:PHE:C	2.56	0.48
1:B:2174:SER:O	1:B:2178:LEU:HB2	2.13	0.48
1:B:2414:LEU:HA	1:B:2422:PHE:CE1	2.49	0.48
1:A:247:PHE:C	1:A:248:LYS:HG2	2.39	0.47
1:A:421:GLN:HG2	8:A:3103:HOH:O	2.15	0.47
1:B:2099:VAL:O	1:B:2102:ILE:HG12	2.14	0.47
1:A:131:ASN:ND2	1:A:134:TYR:H	2.12	0.47
1:B:2102:ILE:CG1	1:B:2103:VAL:N	2.77	0.47
1:A:99:VAL:O	1:A:102:ILE:HG12	2.14	0.47
1:A:174:SER:O	1:A:178:LEU:HB2	2.14	0.47
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.48	0.47
1:B:2306:LEU:C	1:B:2306:LEU:HD23	2.38	0.47
1:B:2465:GLU:HA	1:B:2465:GLU:OE1	2.14	0.47
1:A:211:LYS:HZ3	1:A:236:GLU:CG	2.26	0.47
1:A:43:ASN:O	1:A:44:ARG:HB2	2.15	0.47
1:A:273:MET:HG3	1:A:285:PHE:O	2.14	0.47
1:A:294:LEU:HD23	1:A:295:VAL:HG23	1.97	0.47
1:A:295:VAL:CG2	1:A:298:LEU:HD22	2.44	0.47
1:A:547:PRO:HB3	1:A:553:GLU:OE1	2.14	0.47
1:B:2211:LYS:HZ3	1:B:2236:GLU:CG	2.27	0.47
1:B:2240:ARG:HH22	1:B:2273:MET:HE2	1.75	0.47
1:B:2513:ARG:NH2	1:B:2520:GLU:HG3	2.30	0.47
1:B:2176:GLU:O	1:B:2180:LYS:HG3	2.15	0.46
1:B:2249:ASP:OD2	1:B:2317:LYS:HE2	2.15	0.46
1:B:2569:CYS:SG	2:F:2597:THR:HG22	2.55	0.46
1:A:303:THR:O	1:A:307:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2308:GLU:CD	1:B:2311:ARG:HH11	2.23	0.46
1:A:102:ILE:CG1	1:A:103:VAL:N	2.78	0.46
1:B:2262:TYR:CZ	1:B:2415:LEU:HD23	2.50	0.46
1:B:2386:HIS:CE1	6:B:2704:BOG:H1'2	2.51	0.46
1:A:176:GLU:O	1:A:180:LYS:HG3	2.16	0.46
1:B:2380:GLU:HG2	1:B:2466:TYR:CE1	2.51	0.46
1:B:2132:VAL:HG13	1:B:2133:HIS:CD2	2.51	0.46
1:A:308:GLU:CD	1:A:311:ARG:HH11	2.24	0.46
1:B:2397:ILE:HD12	1:B:2422:PHE:CZ	2.51	0.46
1:A:226:HIS:HA	1:A:377:ILE:HD12	1.98	0.46
1:B:2290:GLU:H	1:B:2290:GLU:HG3	1.39	0.45
1:B:2419:LEU:O	1:B:2423:VAL:HG23	2.15	0.45
1:A:252:LEU:O	1:A:310:GLN:NE2	2.49	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.79	0.45
1:B:105(B):ILE:CG2	1:B:2108:LEU:HB2	2.46	0.45
1:B:2388:HIS:N	1:B:2389:PRO:CD	2.79	0.45
1:B:2547:PRO:HB3	1:B:2553:GLU:OE1	2.16	0.45
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.99	0.45
1:B:2383:THR:HA	1:B:2386:HIS:HD2	1.80	0.45
1:B:2464:ASN:HD22	1:B:2464:ASN:HA	1.61	0.45
1:B:2088:THR:HA	6:B:2702:BOG:H1'2	1.98	0.45
1:B:2131:ASN:ND2	1:B:2134:TYR:H	2.15	0.45
1:A:61:ARG:NH1	1:B:2542:PRO:O	2.50	0.45
1:B:2362:ASP:HB3	1:B:2365:LEU:HG	1.99	0.45
1:B:2397:ILE:HD12	1:B:2422:PHE:CE1	2.52	0.45
1:A:168:ASN:C	1:A:170:GLU:N	2.74	0.45
1:A:459:LYS:HE2	1:A:459:LYS:HB3	1.63	0.45
1:B:2073:GLU:O	1:B:2076:THR:HB	2.16	0.45
1:B:2226:HIS:HA	1:B:2377:ILE:HD12	1.98	0.45
1:A:388:HIS:C	1:A:390:LEU:N	2.75	0.45
1:A:582:VAL:O	1:A:583:GLN:C	2.60	0.45
1:A:276:PRO:HG2	1:A:279:ILE:HD11	1.98	0.45
1:B:2120:ARG:HD2	1:B:2120:ARG:HA	1.81	0.45
1:B:2298:LEU:HD12	1:B:2298:LEU:HA	1.86	0.45
1:A:419:LEU:O	1:A:423:VAL:HG23	2.16	0.44
1:B:2252:LEU:O	1:B:2310:GLN:NE2	2.49	0.44
1:B:2294:LEU:HB3	1:B:2409:TYR:CD2	2.51	0.44
1:A:61:ARG:NH2	8:A:3003:HOH:O	2.49	0.44
1:B:2226:HIS:CA	1:B:2377:ILE:HD12	2.47	0.44
1:A:78:ILE:O	1:A:82:LEU:HD13	2.17	0.44
1:B:2276:PRO:HD2	1:B:2279:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:NAG:C6	4:D:3:MAN:C1	2.96	0.44
1:A:91:TYR:C	1:A:91:TYR:CD2	2.95	0.44
1:B:2081:LEU:C	1:B:2082:LEU:HD12	2.43	0.44
1:B:2091:TYR:C	1:B:2091:TYR:CD2	2.96	0.44
1:B:2168:ASN:C	1:B:2170:GLU:N	2.74	0.44
4:G:2:NAG:C6	4:G:3:MAN:C1	2.95	0.44
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.99	0.44
1:A:249:ASP:OD2	1:A:317:LYS:HE2	2.18	0.44
1:B:2178:LEU:HD22	1:B:2183:LEU:HG	1.99	0.44
1:B:2308:GLU:OE1	1:B:2311:ARG:NH1	2.51	0.44
1:B:2434:VAL:C	1:B:2435:ALA:O	2.59	0.44
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.48	0.44
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.53	0.44
1:B:2180:LYS:HD3	1:B:2490:GLU:OE2	2.17	0.44
1:B:2459:LYS:HE2	1:B:2459:LYS:HB3	1.63	0.44
1:A:105(A):ILE:O	1:A:108:LEU:N	2.51	0.43
1:A:294:LEU:HD23	1:A:295:VAL:CG2	2.48	0.43
1:B:2203:GLN:CG	1:B:2298:LEU:HD11	2.48	0.43
1:B:2216:ARG:HH11	4:G:2:NAG:C7	2.27	0.43
1:B:2405:LYS:HD2	8:B:3692:HOH:O	2.17	0.43
1:B:2088:THR:HG23	6:B:2702:BOG:H3'2	1.99	0.43
1:B:2266:VAL:HG23	1:B:2284:GLN:O	2.17	0.43
1:A:362:ASP:HB3	1:A:365:LEU:HG	2.00	0.43
1:A:124:ILE:HB	8:A:3495:HOH:O	2.18	0.43
1:B:2043:ASN:O	1:B:2044:ARG:HB2	2.18	0.43
1:B:2303:THR:O	1:B:2307:ARG:HD3	2.19	0.43
1:A:34:ASN:HD22	1:A:35:PRO:N	2.16	0.43
1:A:542:PRO:O	1:B:2061:ARG:NH1	2.51	0.43
1:B:2034:ASN:HD22	1:B:2035:PRO:N	2.16	0.43
1:B:2100:TRP:HA	1:B:2100:TRP:CE3	2.53	0.43
1:B:2214:HIS:HD2	8:B:3233:HOH:O	2.02	0.43
1:B:2388:HIS:C	1:B:2390:LEU:N	2.76	0.43
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.19	0.43
1:A:226:HIS:CA	1:A:377:ILE:HD12	2.48	0.43
8:A:3106:HOH:O	1:B:2543:GLN:HB2	2.17	0.43
1:B:2344:VAL:O	1:B:2349:VAL:HG23	2.19	0.43
1:B:2582:VAL:O	1:B:2583:GLN:C	2.61	0.43
1:A:553:GLU:OE1	1:A:553:GLU:HA	2.19	0.43
1:A:118:THR:HG22	1:A:369:GLN:HG2	2.00	0.43
1:B:2538:PRO:HD3	8:B:3638:HOH:O	2.17	0.43
1:A:179:GLU:O	1:A:185:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2087:ASN:HB3	6:B:2702:BOG:H3	2.01	0.42
1:B:2222:ARG:HD3	8:B:3289:HOH:O	2.19	0.42
1:A:276:PRO:HG2	1:A:279:ILE:HG13	2.01	0.42
1:B:2083:LYS:HE3	8:B:3661:HOH:O	2.18	0.42
1:B:105(B):ILE:O	1:B:2108:LEU:N	2.52	0.42
1:B:105(B):ILE:CD1	1:B:2108:LEU:HD12	2.48	0.42
1:A:131:ASN:HD22	1:A:134:TYR:H	1.67	0.42
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.49	0.42
1:B:2118:THR:HG22	1:B:2369:GLN:HG2	2.01	0.42
1:B:2160:PRO:HG2	1:B:2165:VAL:HA	2.01	0.42
1:B:2583:GLN:CD	1:B:2583:GLN:N	2.77	0.42
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.82	0.42
1:A:183:LEU:O	1:A:438:ARG:HB3	2.20	0.42
1:A:275:TYR:HD2	1:A:279:ILE:HD12	1.84	0.42
1:A:283:LEU:HD21	1:A:415:LEU:HD12	2.02	0.42
1:A:396:ASN:H	1:A:429:GLN:NE2	2.15	0.42
1:A:400:GLN:HB2	1:A:402:TYR:CE2	2.55	0.42
1:A:81:LEU:C	1:A:82:LEU:HD12	2.45	0.42
1:A:216:ARG:HH12	4:D:1:NAG:H3	1.84	0.42
1:A:294:LEU:HA	1:A:409:TYR:CD2	2.55	0.42
1:A:464:ASN:ND2	1:A:475:TYR:H	2.11	0.42
1:B:2470:PHE:CD2	1:B:2525:LEU:HD22	2.53	0.42
1:A:280:PRO:HG2	1:A:283:LEU:HB2	2.02	0.42
1:A:398:GLU:HB3	1:A:399:ASP:H	1.68	0.42
1:B:2513:ARG:HD2	8:B:3249:HOH:O	2.19	0.42
1:B:2553:GLU:OE1	1:B:2553:GLU:HA	2.18	0.42
1:A:259:GLY:N	8:A:3216:HOH:O	2.53	0.42
1:A:402:TYR:HA	1:A:406:GLN:OE1	2.20	0.42
1:A:539:ILE:HA	1:A:544:TYR:HB3	2.02	0.42
1:B:2096:PHE:HB3	1:B:2099:VAL:HG13	2.01	0.41
1:B:2261:VAL:O	1:B:2307:ARG:NH1	2.50	0.41
1:A:276:PRO:HD2	1:A:279:ILE:HD12	2.02	0.41
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.84	0.41
1:B:2082:LEU:HD12	1:B:2082:LEU:N	2.36	0.41
1:B:2382:ASN:HD21	6:B:2704:BOG:H61	1.84	0.41
1:B:2464:ASN:ND2	1:B:2475:TYR:H	2.10	0.41
1:A:175:LYS:HG3	8:A:3497:HOH:O	2.20	0.41
1:B:2074:PHE:O	1:B:2077:ARG:HB2	2.20	0.41
1:A:96:PHE:HB3	1:A:99:VAL:HG13	2.01	0.41
1:A:158:ASP:OD2	1:A:158:ASP:C	2.64	0.41
1:A:253:LYS:HD3	8:A:3621:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:C	1:A:390:LEU:H	2.27	0.41
1:B:2500:VAL:O	1:B:2500:VAL:CG1	2.68	0.41
1:B:2554:VAL:HB	8:B:3346:HOH:O	2.19	0.41
1:A:322:GLU:H	1:A:322:GLU:HG3	1.47	0.41
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.55	0.41
1:A:87:ASN:HB3	6:A:702:BOG:H3	2.03	0.41
1:A:290:GLU:H	1:A:290:GLU:HG3	1.40	0.41
1:A:470:PHE:CD2	1:A:525:LEU:HD22	2.56	0.41
1:B:2158:ASP:C	1:B:2158:ASP:OD2	2.63	0.41
1:B:2173:ASP:O	1:B:2177:VAL:HG23	2.21	0.41
1:B:2179:GLU:O	1:B:2185:ARG:NH2	2.54	0.41
1:B:2388:HIS:C	1:B:2390:LEU:H	2.28	0.41
1:B:2398:GLU:OE1	1:B:2421:GLN:CD	2.64	0.41
1:A:583:GLN:CD	1:A:583:GLN:N	2.78	0.41
1:B:2206:THR:HG21	1:B:2385:TYR:CE2	2.55	0.41
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.86	0.40
1:A:131:ASN:C	1:A:131:ASN:ND2	2.72	0.40
1:A:386:HIS:CE1	6:A:704:BOG:H1'2	2.56	0.40
1:A:457:GLU:C	1:A:459:LYS:H	2.28	0.40
1:B:2131:ASN:HD22	1:B:2134:TYR:H	1.69	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:B:2092:ILE:HA	1:B:2096:PHE:HE1	1.86	0.40
1:B:2185:ARG:HE	1:B:2438:ARG:HD3	1.86	0.40
1:A:344:VAL:O	1:A:349:VAL:HG23	2.22	0.40
1:B:2183:LEU:HD23	1:B:2183:LEU:HA	1.84	0.40
1:B:2452:ILE:O	1:B:2456:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	522 (95%)	24 (4%)	4 (1%)	18	28
1	B	550/552 (100%)	516 (94%)	30 (6%)	4 (1%)	18	28
2	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1107/1113 (100%)	1045 (94%)	54 (5%)	8 (1%)	18	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	B	2121	SER
1	B	2122	TYR
1	A	514	PRO
1	B	2514	PRO
1	A	398	GLU
1	B	2435	ALA

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	492/492 (100%)	441 (90%)	51 (10%)	7	10
1	B	492/492 (100%)	439 (89%)	53 (11%)	6	9
2	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
All	All	991/991 (100%)	886 (89%)	105 (11%)	6	10

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	56	LYS
1	A	93	LEU
1	A	99	VAL
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	123	LEU
1	A	131	ASN
1	A	137	LYS
1	A	171	LEU
1	A	178	LEU
1	A	180	LYS
1	A	203	GLN
1	A	230	LEU
1	A	238	LEU
1	A	239	ASP
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL
1	A	294	LEU
1	A	295	VAL
1	A	298	LEU
1	A	300	MET
1	A	307	ARG
1	A	310	GLN
1	A	311	ARG
1	A	322	GLU
1	A	352	LEU
1	A	369	GLN
1	A	377	ILE
1	A	385	TYR
1	A	397	ILE
1	A	406	GLN
1	A	408	LEU
1	A	412	SER
1	A	416	GLU
1	A	419	LEU
1	A	430	ILE
1	A	444	VAL
1	A	459	LYS
1	A	463	LEU
1	A	484	GLU
1	A	509	VAL

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Mol	Chain	Res	Type
1	A	525	LEU
1	A	534	LEU
1	A	543	GLN
1	A	583	GLN
1	B	2054	GLN
1	B	2056	LYS
1	B	2079	LYS
1	B	2093	LEU
1	B	2099	VAL
1	B	2101	ASN
1	B	2116	VAL
1	B	2117	LEU
1	B	2120	ARG
1	B	2123	LEU
1	B	2131	ASN
1	B	2137	LYS
1	B	2171	LEU
1	B	2178	LEU
1	B	2180	LYS
1	B	2230	LEU
1	B	2238	LEU
1	B	2239	ASP
1	B	2248	LYS
1	B	2252	LEU
1	B	2267	LYS
1	B	2272	GLU
1	B	2289	GLN
1	B	2290	GLU
1	B	2291	VAL
1	B	2294	LEU
1	B	2298	LEU
1	B	2300	MET
1	B	2307	ARG
1	B	2310	GLN
1	B	2311	ARG
1	B	2322	GLU
1	B	2352	LEU
1	B	2369	GLN
1	B	2377	ILE
1	B	2385	TYR
1	B	2397	ILE
1	B	2398	GLU

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Mol	Chain	Res	Type
1	B	2406	GLN
1	B	2409	TYR
1	B	2412	SER
1	B	2416	GLU
1	B	2419	LEU
1	B	2444	VAL
1	B	2459	LYS
1	B	2463	LEU
1	B	2484	GLU
1	B	2509	VAL
1	B	2525	LEU
1	B	2534	LEU
1	B	2543	GLN
1	B	2578	THR
1	B	2583	GLN
2	F	2596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	131	ASN
1	A	214	HIS
1	A	386	HIS
1	A	417	HIS
1	A	429	GLN
1	A	454	GLN
1	A	464	ASN
1	B	2034	ASN
1	B	2131	ASN
1	B	2242	HIS
1	B	2386	HIS
1	B	2400	GLN
1	B	2417	HIS
1	B	2429	GLN
1	B	2454	GLN
1	B	2464	ASN
1	B	2581	ASN
1	B	2583	GLN
2	F	2601	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 ⓘ

12 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	C	1	3,1	14,14,15	0.82	0	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	0.93	0	17,19,21	0.96	1 (5%)
4	NAG	D	1	1,4	14,14,15	0.38	0	17,19,21	0.67	0
4	NAG	D	2	4	14,14,15	2.10	2 (14%)	17,19,21	4.21	4 (23%)
4	MAN	D	3	4	11,11,12	1.32	2 (18%)	15,15,17	1.56	2 (13%)
4	MAN	D	4	4	11,11,12	2.24	3 (27%)	15,15,17	1.05	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.84	0	17,19,21	0.67	0
3	NAG	E	2	3	14,14,15	0.89	0	17,19,21	0.93	0
4	NAG	G	1	1,4	14,14,15	0.69	0	17,19,21	0.92	0
4	NAG	G	2	4	14,14,15	1.32	2 (14%)	17,19,21	4.10	6 (35%)
4	MAN	G	3	4	11,11,12	1.14	1 (9%)	15,15,17	1.42	2 (13%)
4	MAN	G	4	4	11,11,12	2.28	3 (27%)	15,15,17	1.08	2 (13%)

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	C	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	1/1/4/5	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	MAN	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	1/1/4/5	1/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C8-C7	5.80	1.62	1.50
4	D	4	MAN	C2-C3	4.49	1.59	1.52
4	D	2	NAG	C1-C2	-4.48	1.46	1.52
4	G	4	MAN	C2-C3	4.31	1.59	1.52
4	G	4	MAN	O5-C5	3.91	1.51	1.43
4	G	4	MAN	C4-C5	3.90	1.61	1.53
4	D	4	MAN	C4-C5	3.90	1.61	1.53
4	D	4	MAN	O5-C5	3.53	1.50	1.43
4	G	2	NAG	C8-C7	3.39	1.57	1.50
4	D	3	MAN	C6-C5	2.59	1.60	1.51
4	G	3	MAN	C6-C5	2.34	1.59	1.51
4	G	2	NAG	C1-C2	-2.26	1.49	1.52
4	D	3	MAN	C1-C2	2.11	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C1-C2-N2	12.53	130.17	110.43
4	D	2	NAG	C1-C2-N2	11.88	129.16	110.43
4	D	2	NAG	C8-C7-N2	-10.88	98.08	116.12
4	G	2	NAG	C8-C7-N2	-9.17	100.90	116.12
4	G	2	NAG	O7-C7-C8	-5.07	113.02	122.05
4	D	2	NAG	O7-C7-C8	-4.96	113.23	122.05
4	D	3	MAN	C1-O5-C5	4.25	117.89	112.19
4	G	3	MAN	C1-O5-C5	3.40	116.75	112.19
4	D	3	MAN	O6-C6-C5	2.92	121.28	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	MAN	O6-C6-C5	2.88	121.14	111.33
4	D	2	NAG	C2-N2-C7	-2.63	119.38	122.90
4	G	2	NAG	C1-O5-C5	2.38	115.38	112.19
4	G	2	NAG	C2-N2-C7	-2.20	119.95	122.90
4	D	4	MAN	O2-C2-C1	-2.15	104.29	109.22
4	G	2	NAG	O5-C1-C2	-2.15	107.96	111.29
4	G	4	MAN	O5-C1-C2	2.15	115.92	110.79
4	G	4	MAN	O2-C2-C1	-2.08	104.47	109.22
3	C	2	NAG	C1-C2-N2	2.02	113.61	110.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	4	MAN	C1
4	G	4	MAN	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	3	MAN	C4-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	G	3	MAN	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
4	D	3	MAN	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

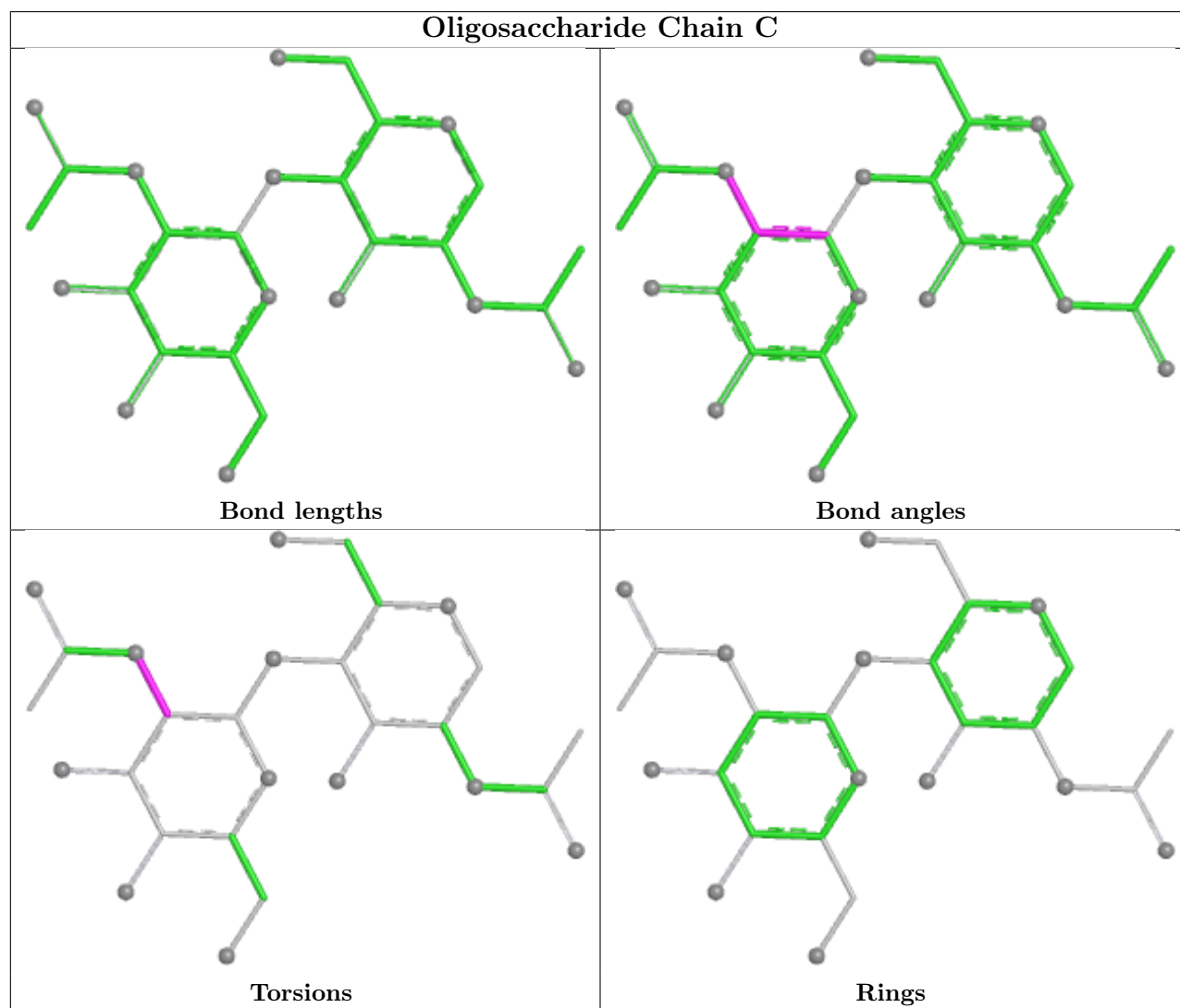
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
4	G	3	MAN	2	0

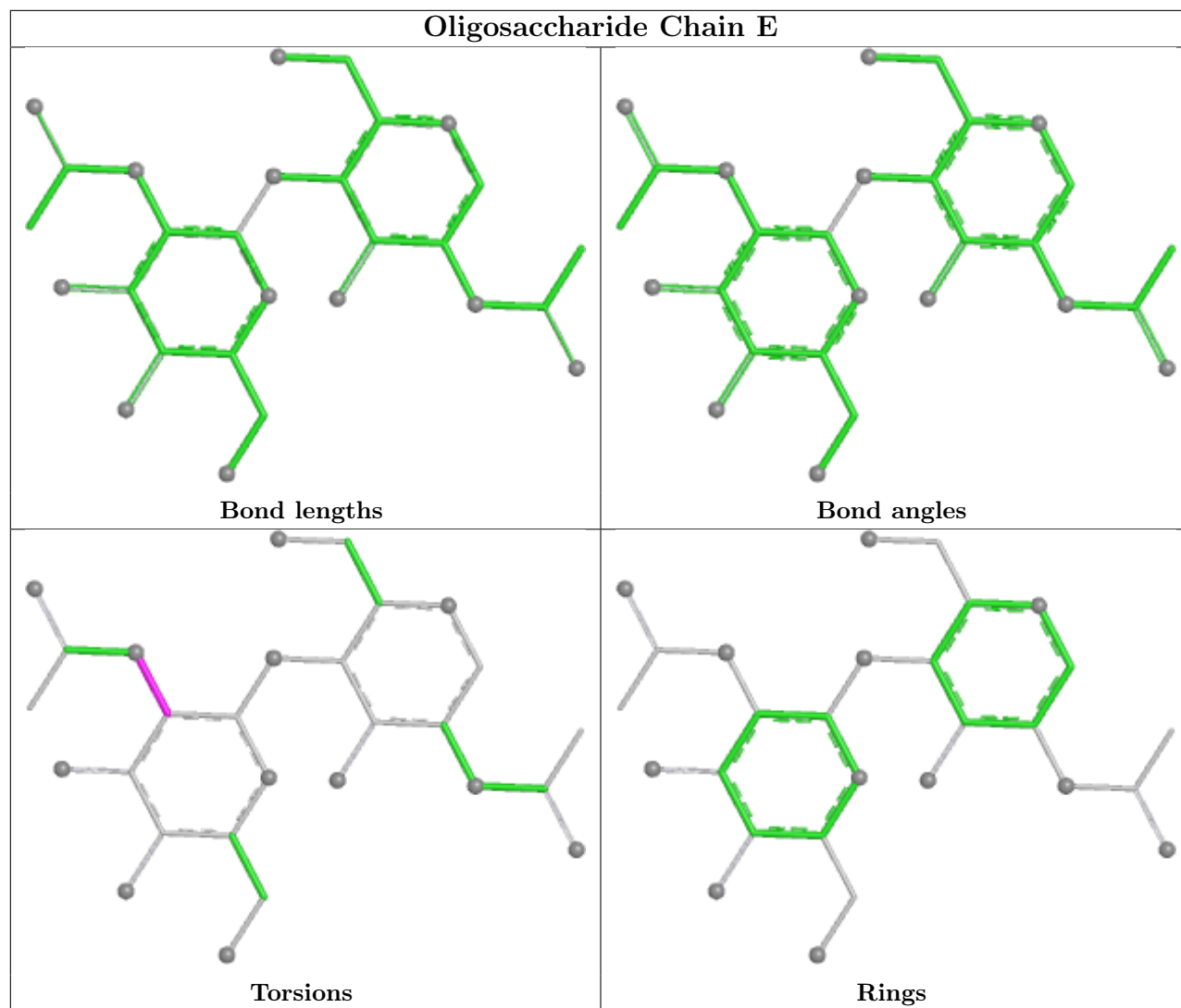
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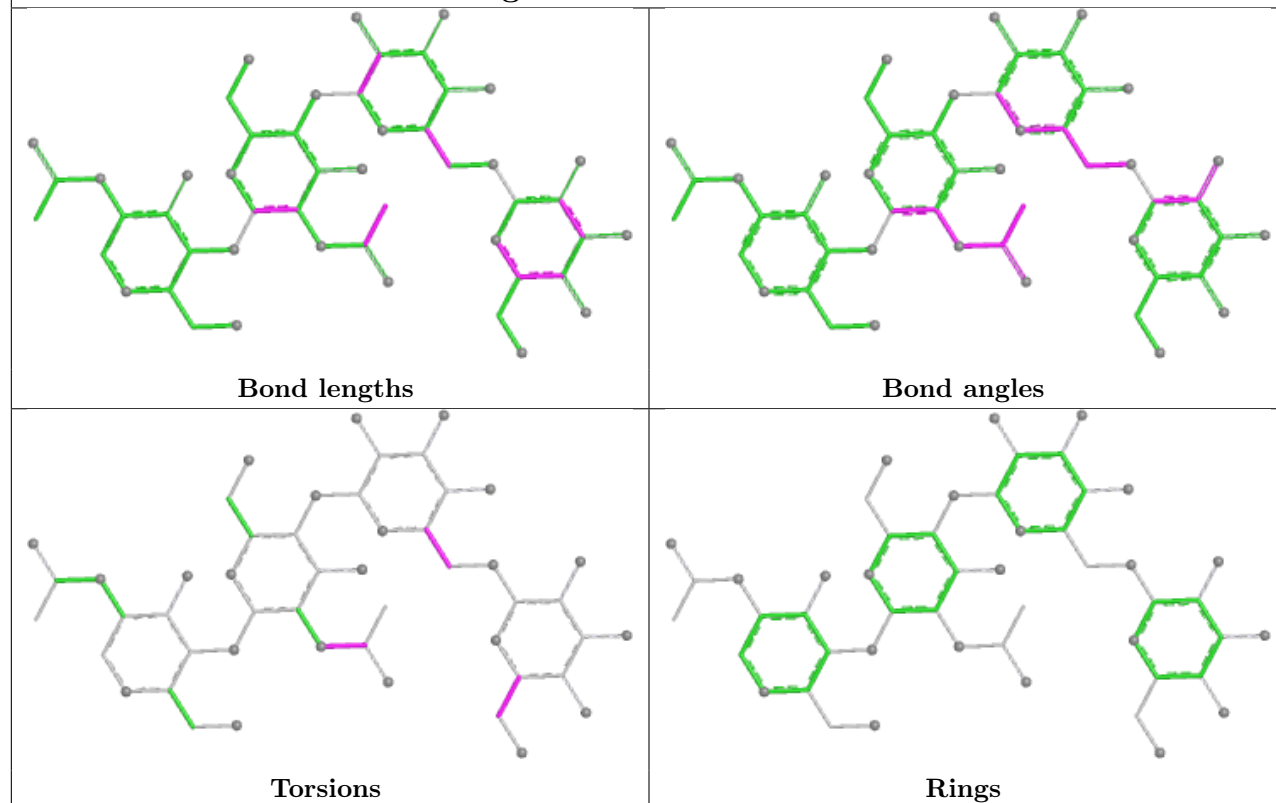
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	MAN	2	0
4	G	2	NAG	5	0
4	D	1	NAG	1	0

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

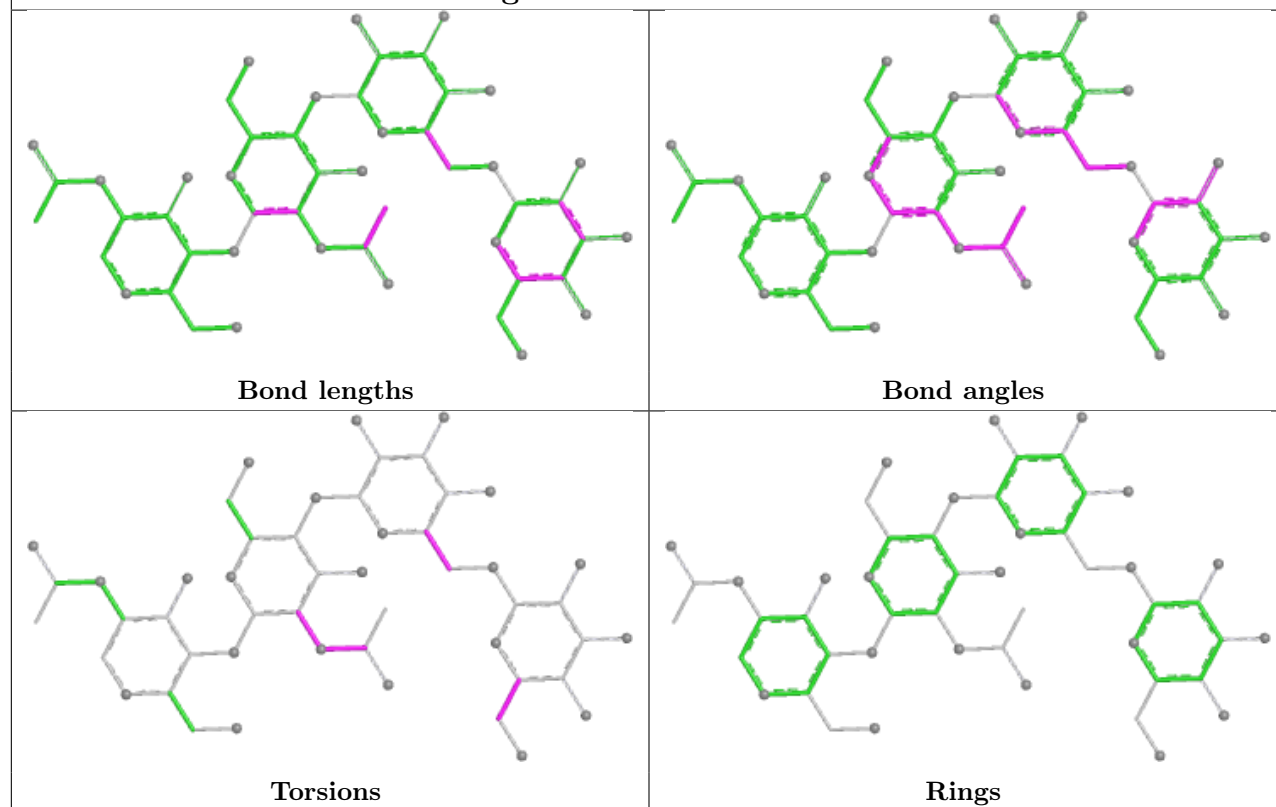




Oligosaccharide Chain D



Oligosaccharide Chain G



5.6 Ligand geometry

9 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$
5	NAG	A	681	1	14,14,15	0.91	1 (7%)	17,19,21	1.07	1 (5%)
6	BOG	B	2704	-	20,20,20	0.84	2 (10%)	25,25,25	0.66	0
7	ACD	B	2701	-	21,21,21	0.69	0	21,21,21	0.67	0
6	BOG	A	704	-	20,20,20	0.93	2 (10%)	25,25,25	0.66	0
6	BOG	B	2702	-	20,20,20	0.68	0	25,25,25	0.61	0
7	ACD	A	701	-	21,21,21	0.80	0	21,21,21	0.78	1 (4%)
6	BOG	A	702	-	20,20,20	0.84	2 (10%)	25,25,25	0.66	0
5	NAG	B	2681	1	14,14,15	0.83	0	17,19,21	1.08	1 (5%)
6	BOG	A	703	-	20,20,20	0.91	0	25,25,25	0.67	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
5	NAG	A	681	1	-	0/6/23/26	0/1/1/1
6	BOG	B	2704	-	-	5/11/31/31	0/1/1/1
7	ACD	B	2701	-	-	4/19/19/19	-
6	BOG	A	704	-	-	6/11/31/31	0/1/1/1
6	BOG	B	2702	-	-	4/11/31/31	0/1/1/1
7	ACD	A	701	-	-	6/19/19/19	-
6	BOG	A	702	-	-	2/11/31/31	0/1/1/1
5	NAG	B	2681	1	-	0/6/23/26	0/1/1/1
6	BOG	A	703	-	-	4/11/31/31	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	704	BOG	O1-C1	2.44	1.44	1.40
5	A	681	NAG	C1-C2	2.42	1.55	1.52
6	A	704	BOG	O5-C1	2.32	1.47	1.41
6	B	2704	BOG	O1-C1	2.24	1.43	1.40
6	B	2704	BOG	O5-C1	2.20	1.47	1.41
6	A	702	BOG	O1-C1	2.03	1.43	1.40
6	A	702	BOG	O5-C1	2.02	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2681	NAG	C8-C7-N2	-2.75	111.56	116.12
5	A	681	NAG	C8-C7-N2	2.20	119.77	116.12
7	A	701	ACD	O2-C1-C2	2.08	120.58	114.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2701	ACD	C12-C13-C14-C15
6	A	704	BOG	C4-C5-C6-O6
6	A	704	BOG	O5-C5-C6-O6
6	A	702	BOG	C4-C5-C6-O6
6	A	702	BOG	O5-C5-C6-O6
6	A	704	BOG	O5-C1-O1-C1'
6	A	704	BOG	O1-C1'-C2'-C3'
6	A	703	BOG	C3'-C4'-C5'-C6'
7	A	701	ACD	C16-C17-C18-C19
6	A	703	BOG	C2-C1-O1-C1'
6	B	2702	BOG	O1-C1'-C2'-C3'
6	B	2702	BOG	C3'-C4'-C5'-C6'
7	B	2701	ACD	C15-C16-C17-C18
6	B	2704	BOG	C3'-C4'-C5'-C6'
6	B	2702	BOG	C4-C5-C6-O6
6	A	704	BOG	C3'-C4'-C5'-C6'
7	A	701	ACD	C15-C16-C17-C18
6	B	2704	BOG	O1-C1'-C2'-C3'
6	A	703	BOG	C2'-C1'-O1-C1
6	A	704	BOG	C2'-C1'-O1-C1
7	A	701	ACD	C12-C13-C14-C15
6	A	703	BOG	O5-C1-O1-C1'
6	B	2702	BOG	O5-C5-C6-O6

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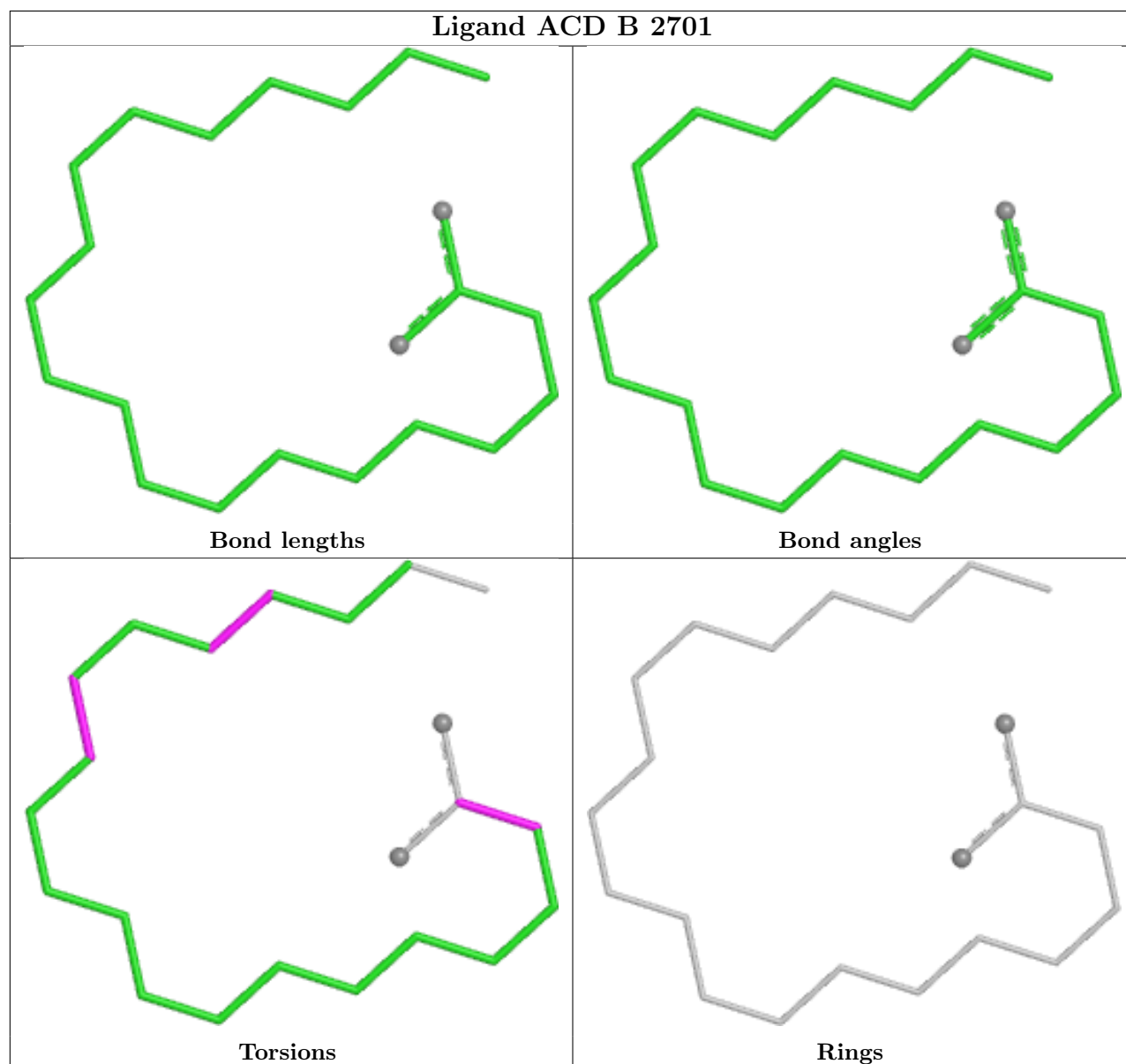
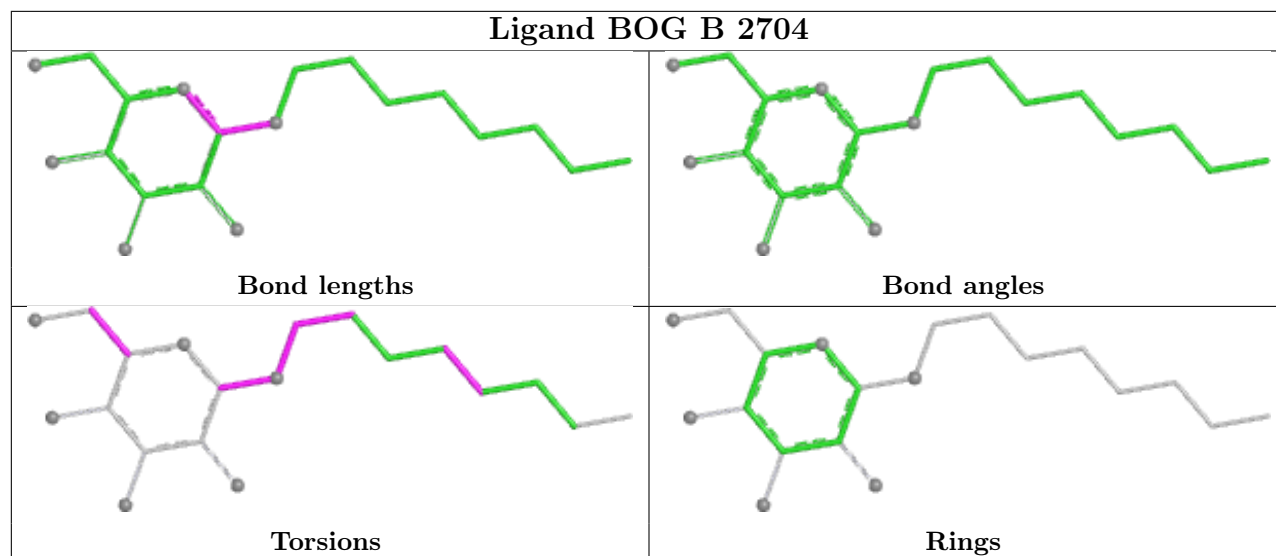
Mol	Chain	Res	Type	Atoms
7	A	701	ACD	C14-C15-C16-C17
7	B	2701	ACD	O1-C1-C2-C3
6	B	2704	BOG	C4-C5-C6-O6
7	B	2701	ACD	O2-C1-C2-C3
7	A	701	ACD	O1-C1-C2-C3
6	B	2704	BOG	C2'-C1'-O1-C1
7	A	701	ACD	O2-C1-C2-C3
6	B	2704	BOG	O5-C1-O1-C1'

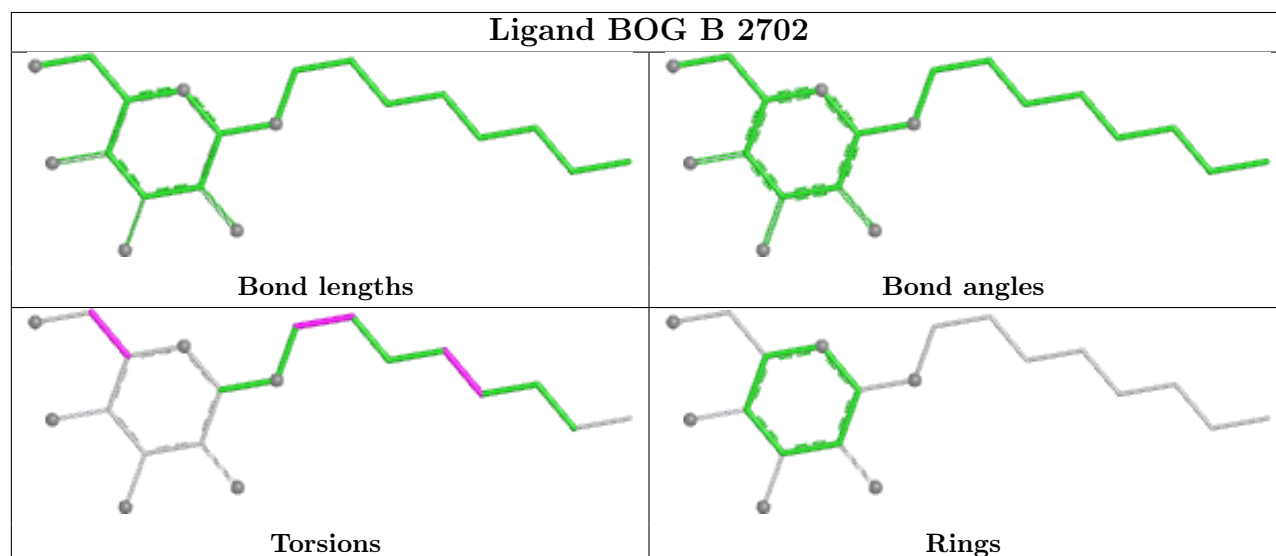
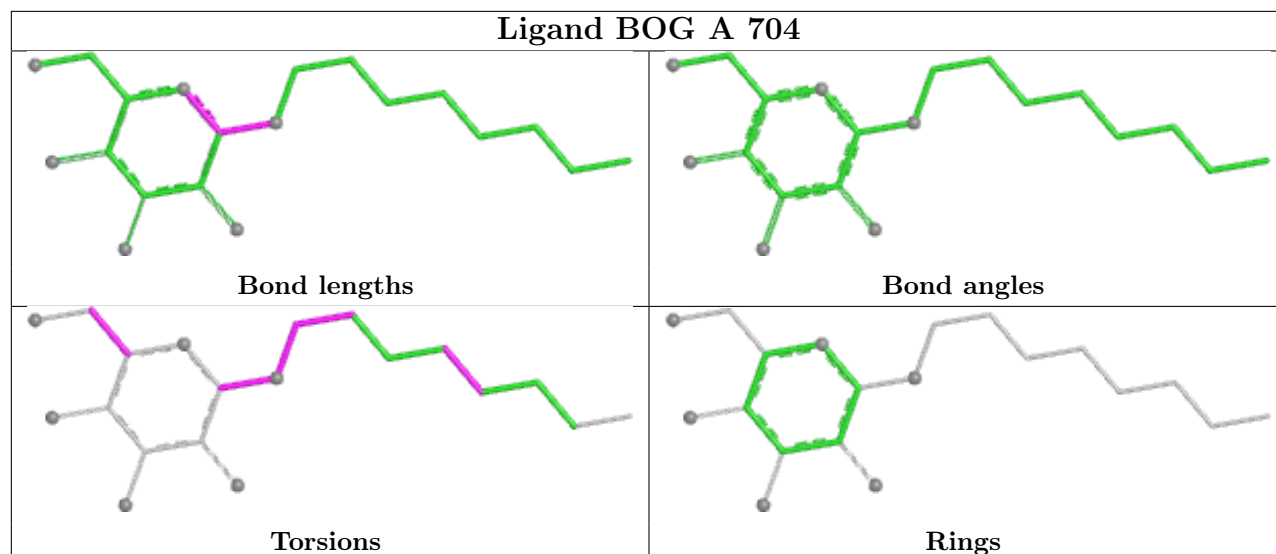
There are no ring outliers.

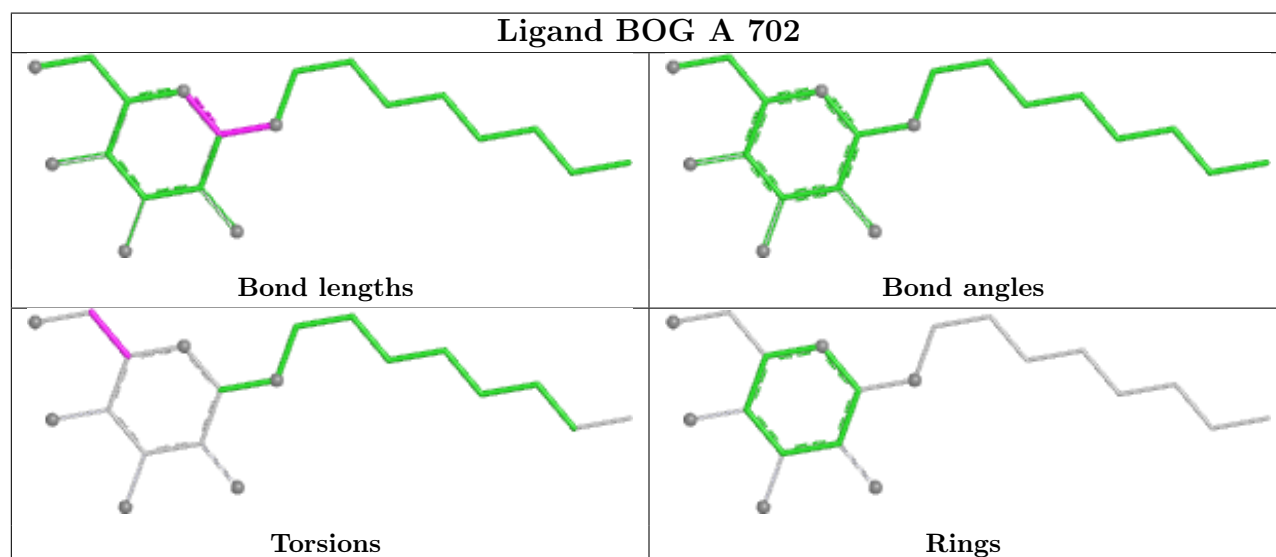
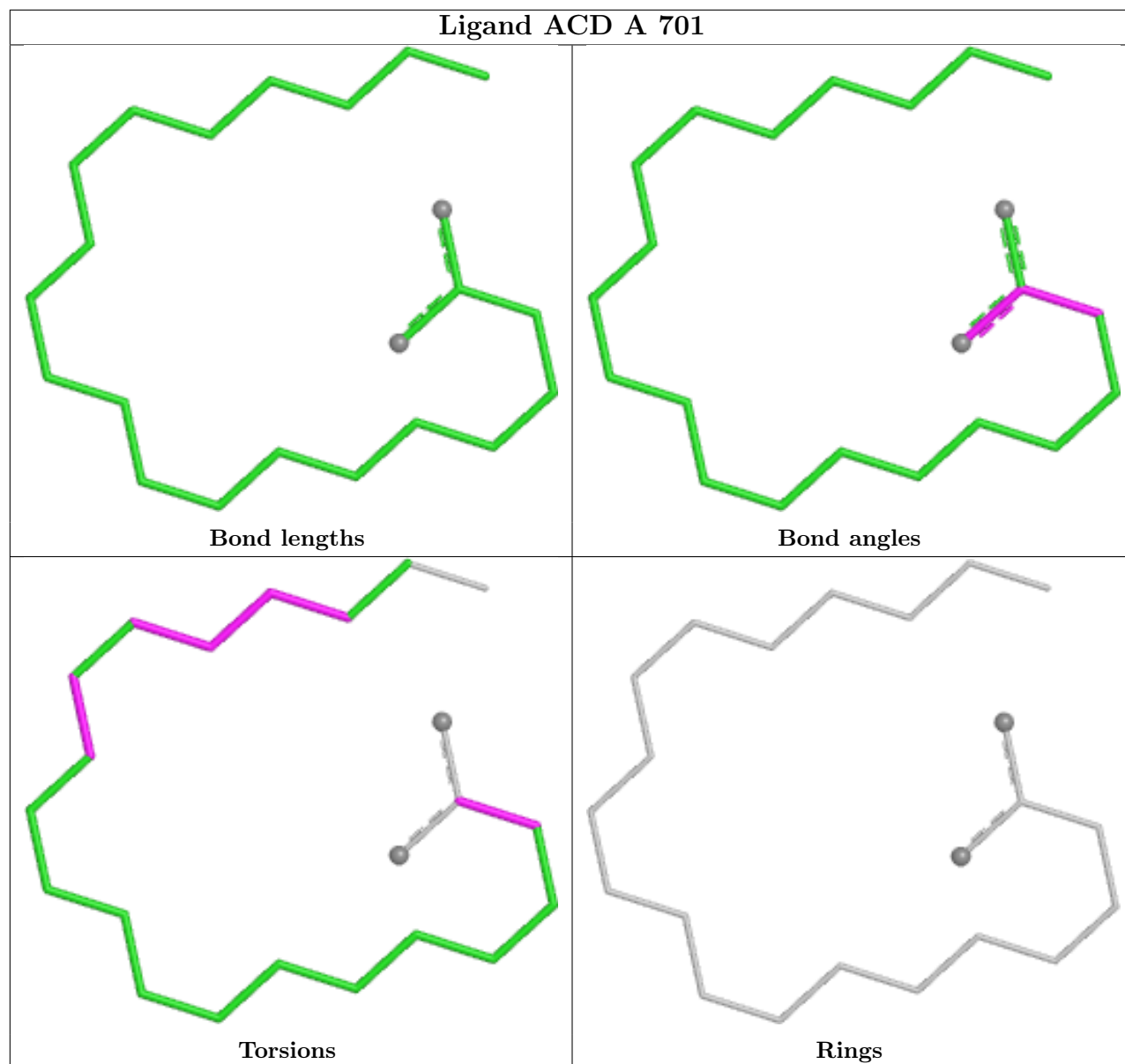
5 monomers are involved in 12 short contacts:

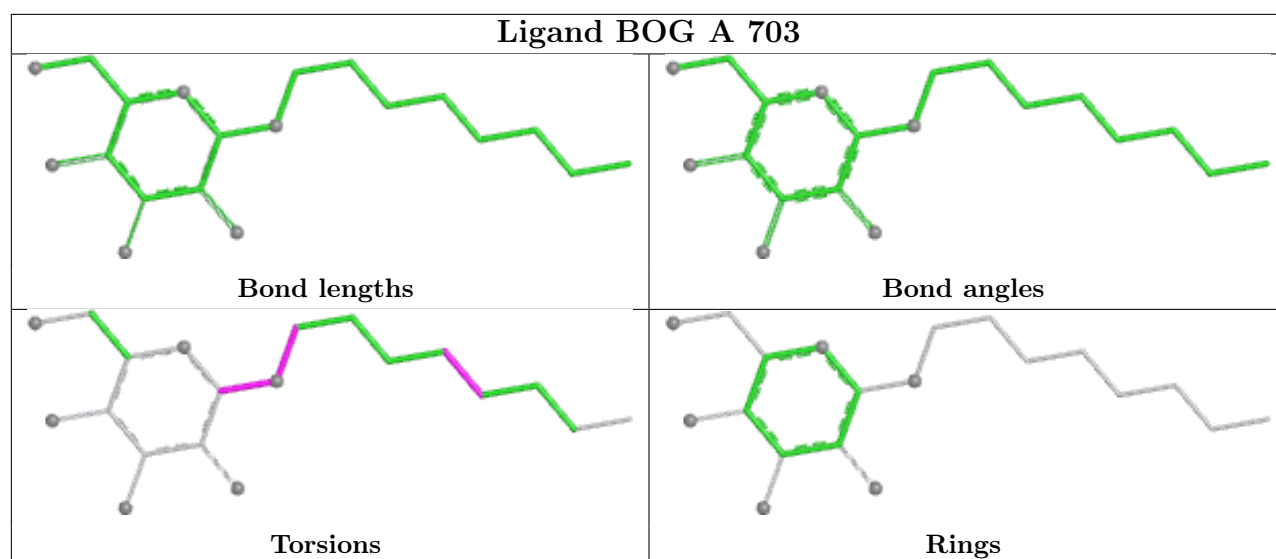
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2704	BOG	3	0
6	A	704	BOG	2	0
6	B	2702	BOG	3	0
6	A	702	BOG	1	0
6	A	703	BOG	3	0

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	552/552 (100%)	-0.22	6 (1%) 78 74	14, 26, 43, 56	0
1	B	552/552 (100%)	-0.15	7 (1%) 75 71	12, 27, 46, 61	0
2	F	9/9 (100%)	2.18	5 (55%) 0 0	52, 55, 66, 71	0
All	All	1113/1113 (100%)	-0.17	18 (1%) 70 66	12, 27, 46, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2409	TYR	6.2
2	F	2603	SER	5.3
1	A	399	ASP	4.6
1	B	2583	GLN	3.3
1	B	2582	VAL	2.7
1	A	75	LEU	2.6
1	B	2121	SER	2.6
1	B	2294	LEU	2.5
1	A	583	GLN	2.4
1	A	122	TYR	2.3
2	F	2601	ASN	2.2
2	F	2598	ALA	2.2
2	F	2595	THR	2.1
1	B	2102	ILE	2.0
1	A	239	ASP	2.0
1	A	409	TYR	2.0
2	F	2602	ALA	2.0
1	B	2290	GLU	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 ⓘ

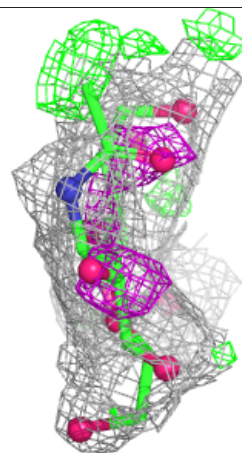
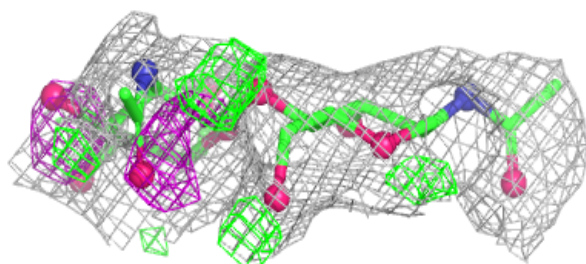
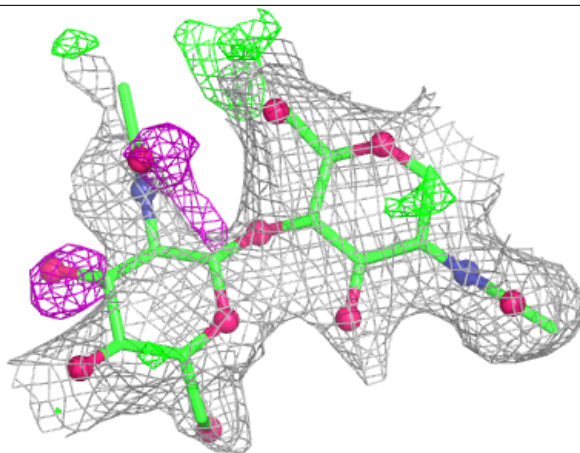
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	1	14/15	-	-	44,50,53,58	0
3	NAG	C	2	14/15	-	-	64,67,70,72	0
4	MAN	G	4	11/12	0.11	0.22	78,80,82,82	0
4	MAN	G	3	11/12	0.30	0.19	66,67,72,76	0
4	NAG	D	2	14/15	0.42	0.20	46,52,55,57	0
4	NAG	G	2	14/15	0.68	0.15	49,55,57,62	0
4	MAN	D	3	11/12	-	-	60,62,65,67	0
4	MAN	D	4	11/12	-	-	70,71,72,72	0
3	NAG	E	2	14/15	0.72	0.17	68,71,74,75	0
4	NAG	D	1	14/15	0.78	0.12	28,30,33,39	0
4	NAG	G	1	14/15	0.91	0.10	27,29,34,41	0
3	NAG	E	1	14/15	0.94	0.08	52,54,58,64	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.

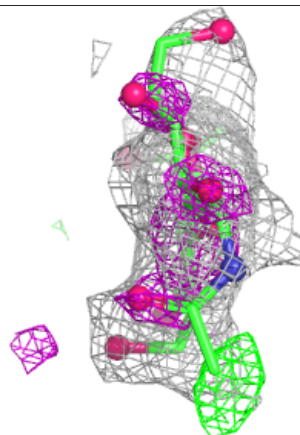
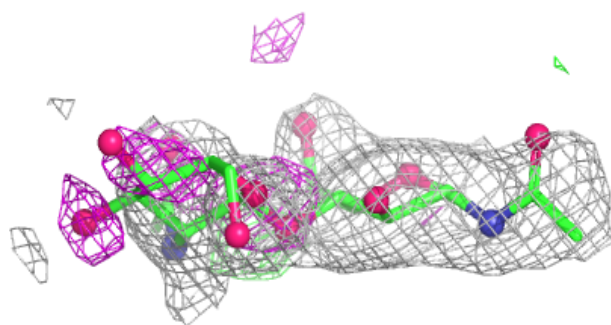
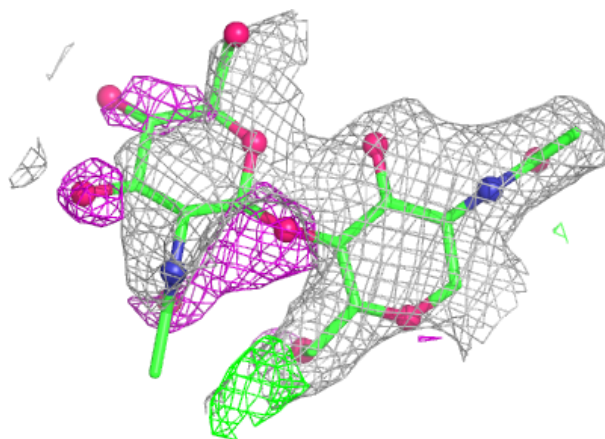
Electron density around Chain C:

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

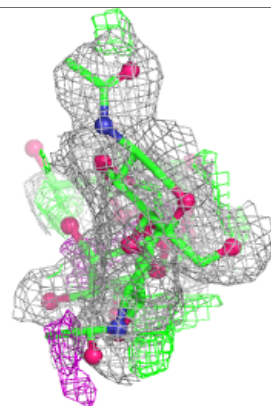
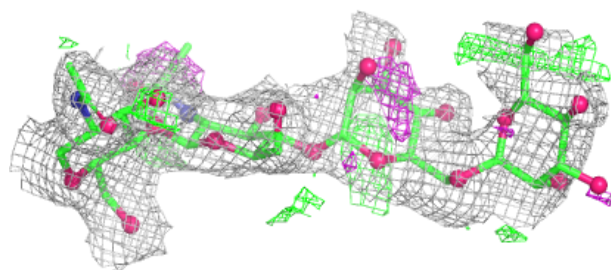
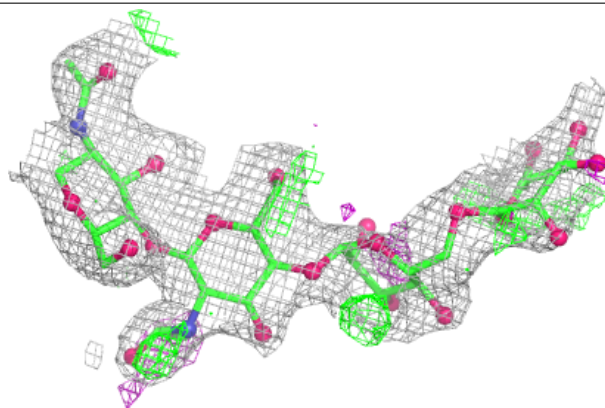


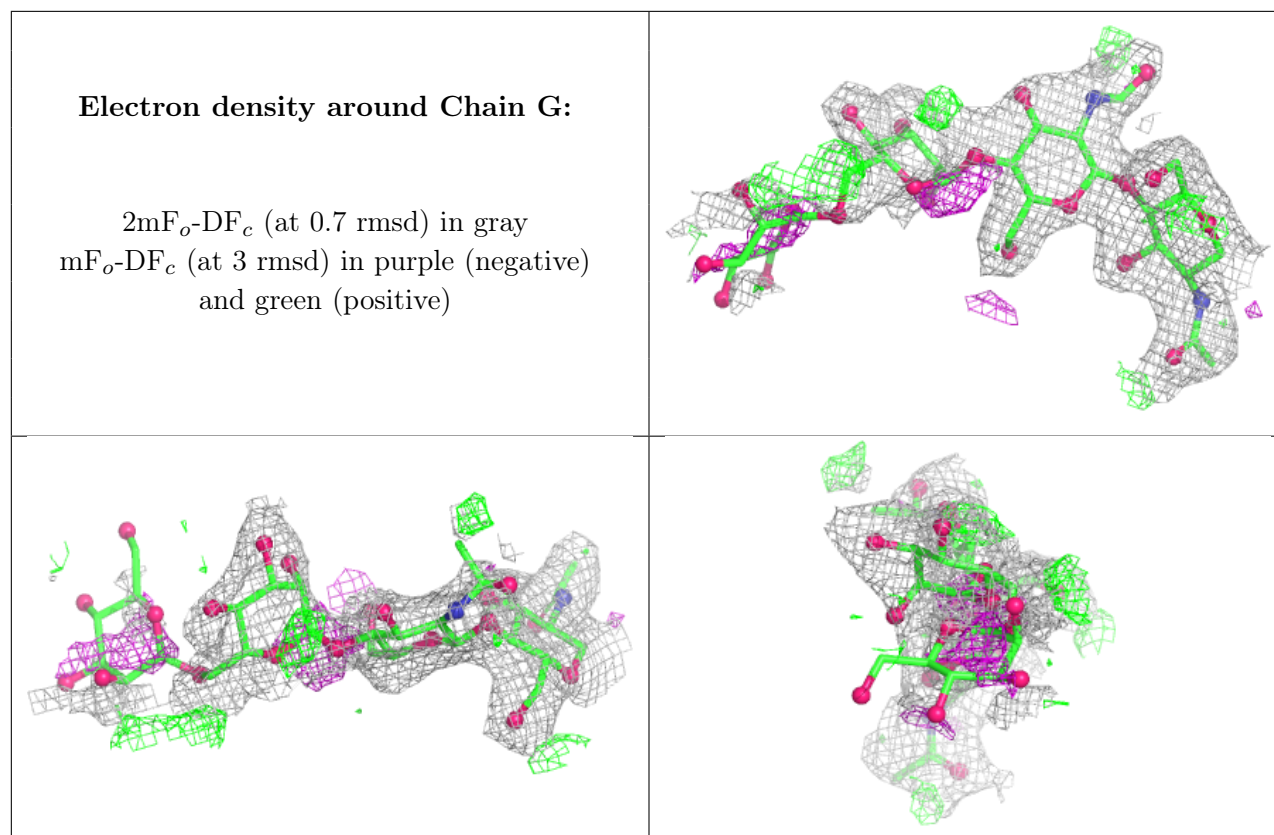
Electron density around Chain E:

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

**Electron density around Chain D:**

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





6.4 Ligands [i](#)

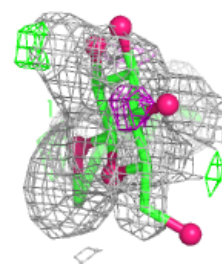
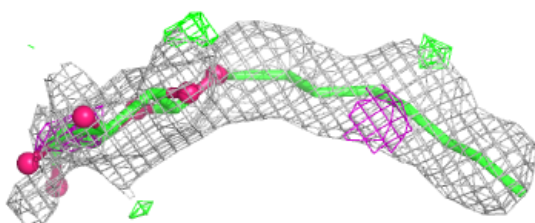
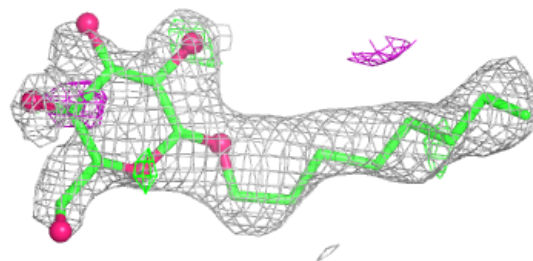
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	2681	14/15	0.41	0.22	68,70,71,72	0
5	NAG	A	681	14/15	0.67	0.16	58,61,64,66	0
6	BOG	A	704	20/20	0.72	0.18	42,63,65,67	0
6	BOG	B	2704	20/20	0.75	0.17	32,61,64,65	0
6	BOG	A	702	20/20	0.76	0.14	38,50,54,54	0
6	BOG	B	2702	20/20	0.83	0.12	40,45,47,47	0
6	BOG	A	703	20/20	0.87	0.11	33,44,46,47	0
7	ACD	A	701	22/22	0.94	0.08	18,22,28,31	0
7	ACD	B	2701	22/22	0.94	0.08	19,25,29,32	0

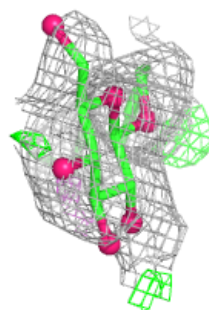
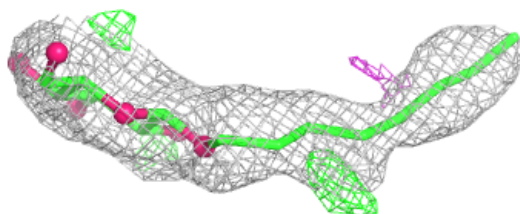
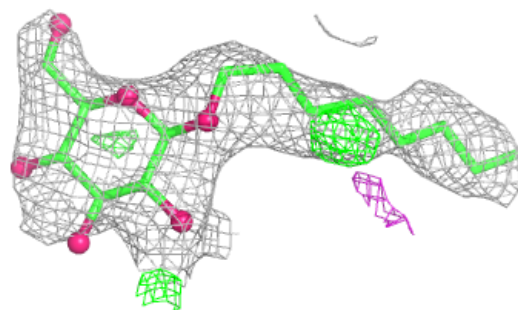
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 704:

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

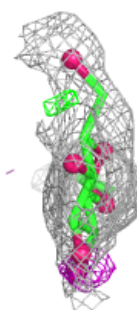
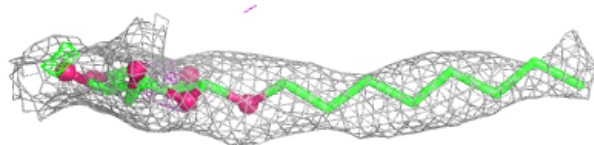
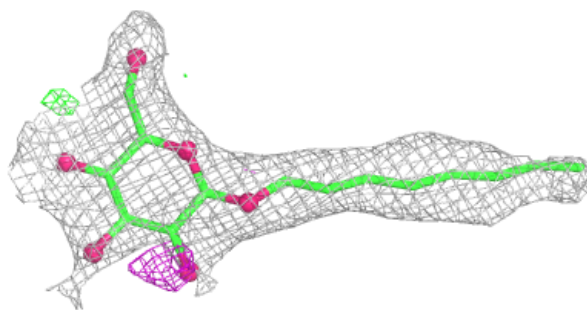
**Electron density around BOG B 2704:**

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

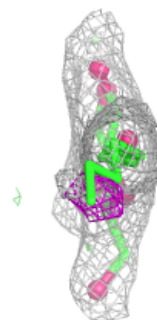
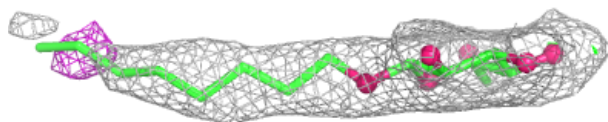
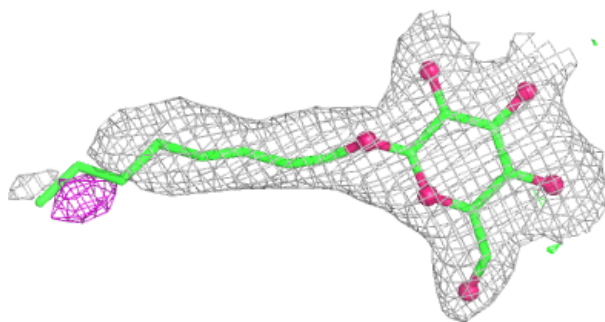


Electron density around BOG A 702:

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

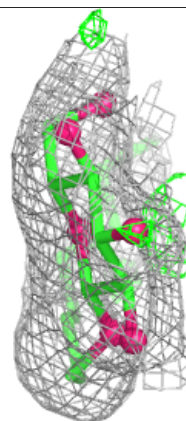
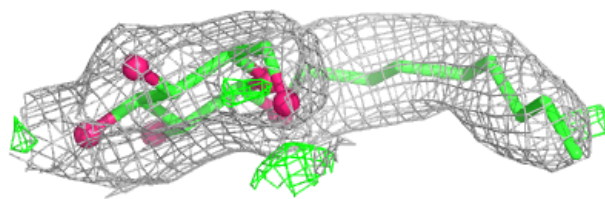
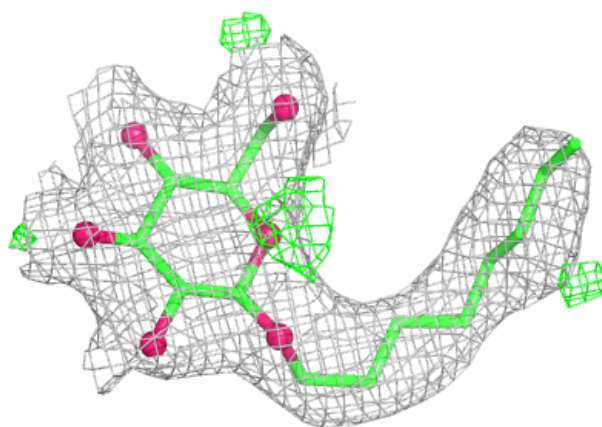
**Electron density around BOG B 2702:**

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



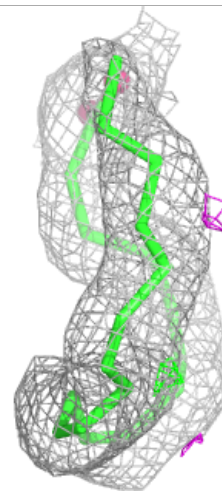
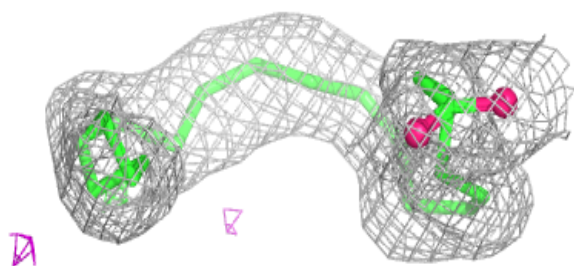
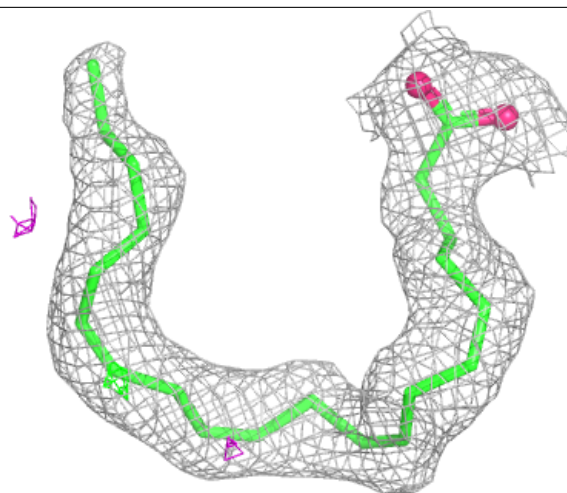
Electron density around BOG A 703:

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



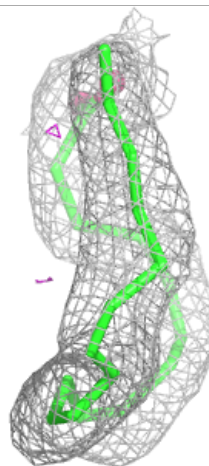
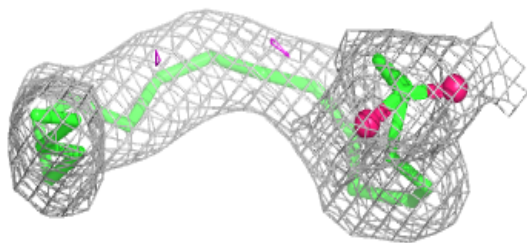
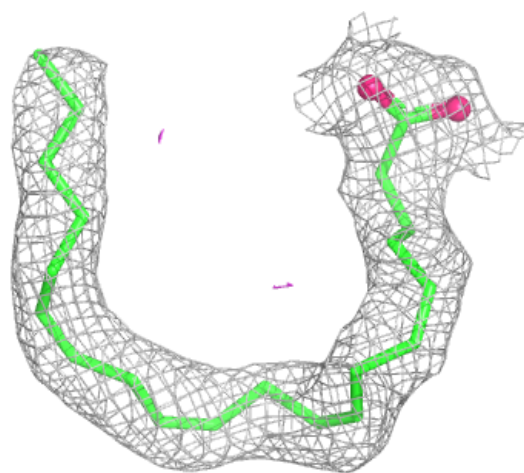
Electron density around ACD A 701:

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



Electron density around ACD B 2701:

$2mF_o-DF_c$ (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.