



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:04 AM UTC

PDB ID : 7CBA / pdb_00007cba
Title : Crystal structure of snake venom phosphodiesterase (PDE) from Taiwan cobra (Naja atra atra) in complex with isorhamnetin and citrate
Authors : Lin, I.J.; Lin, C.C.; Wu, W.G.
Deposited on : 2020-06-11
Resolution : 2.90 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

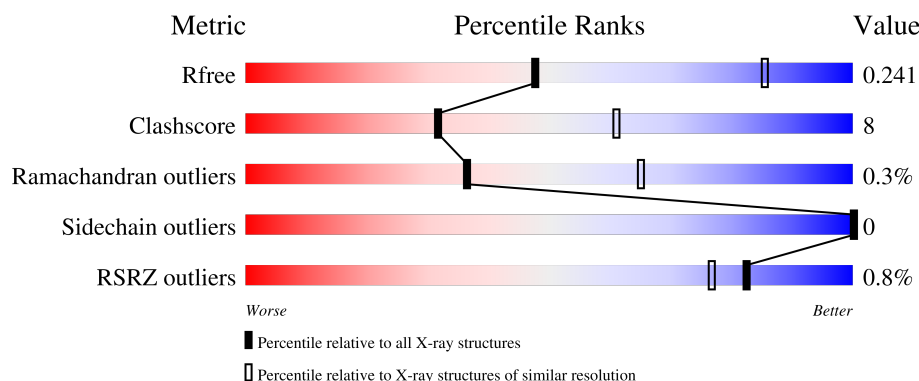
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	830	75% 17% 7%
1	B	830	75% 17% 7%
2	C	3	33% 67%
2	D	3	33% 67%

2 Entry composition [i](#)

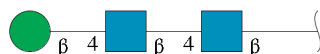
There are 7 unique types of molecules in this entry. The entry contains 12576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Venom phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			6156	3926	1038	1146	46			
1	B	768	Total	C	N	O	S	0	0	0
			6166	3936	1038	1146	46			

- Molecule 2 is an oligosaccharide called 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	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

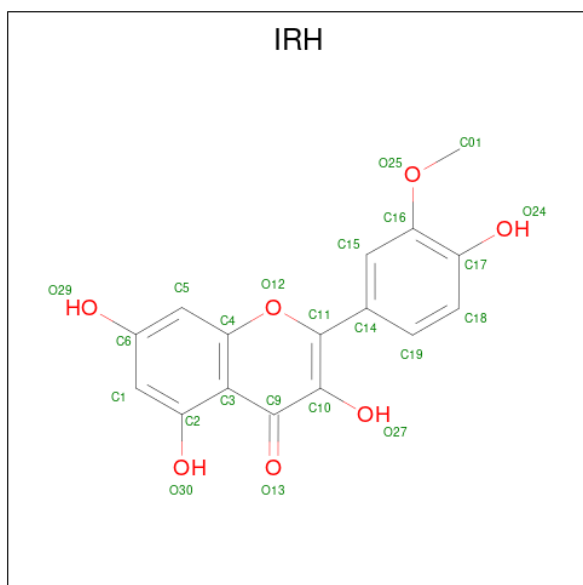
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is isorhamnetin (CCD ID: IRH) (formula: $C_{16}H_{12}O_7$) (labeled as "Ligand of Interest" by depositor).

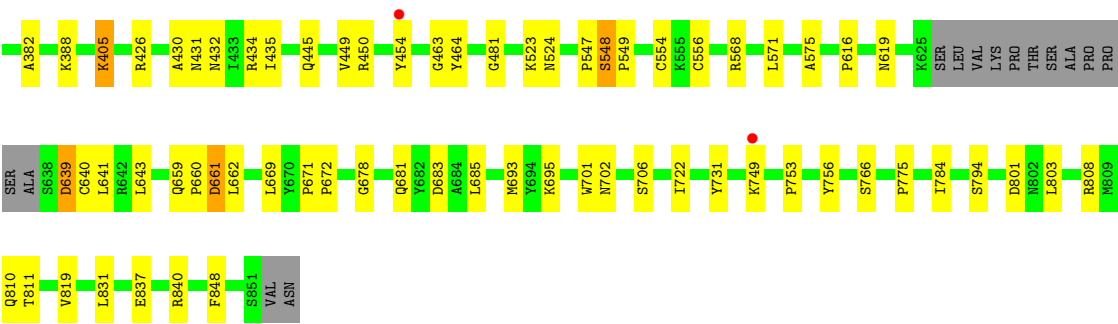


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 23 16 7	0	0
6	B	1	Total C O 23 16 7	0	0

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	B	1	Total	C	O	0	0
			13	6	7		



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



● Molecule 2: beta-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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.19Å 168.62Å 93.72Å 90.00° 105.93° 90.00°	Depositor
Resolution (Å)	28.30 – 2.90 28.30 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.30-2.90) 93.1 (28.30-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.242 0.189 , 0.241	Depositor DCC
R_{free} test set	2141 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: ZN, NAG, BMA, IRH, CIT, CA

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	0.33	1/6320 (0.0%)	0.55	4/8580 (0.0%)
1	B	0.37	1/6333 (0.0%)	0.60	10/8599 (0.1%)
All	All	0.35	2/12653 (0.0%)	0.57	14/17179 (0.1%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLN	CB-CG	5.44	1.68	1.52
1	B	86	LYS	CD-CE	5.24	1.68	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LYS	CB-CG-CD	-12.11	83.46	111.30
1	B	225	ARG	CD-NE-CZ	7.04	134.26	124.40
1	B	405	LYS	CB-CG-CD	-6.94	95.34	111.30
1	B	85	GLU	CA-C-N	-6.39	111.12	122.74
1	B	85	GLU	C-N-CA	-6.39	111.12	122.74
1	B	639	ASP	N-CA-C	6.39	118.12	111.03
1	A	535	GLN	CB-CA-C	6.38	119.79	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	GLN	CA-CB-CG	-6.34	101.42	114.10
1	A	535	GLN	N-CA-CB	-6.24	102.00	110.67
1	B	639	ASP	CB-CA-C	-5.80	101.96	110.95
1	A	105	CYS	CA-CB-SG	-5.38	102.03	114.40
1	B	283	LEU	CA-C-N	-5.18	113.30	122.26
1	B	283	LEU	C-N-CA	-5.18	113.30	122.26
1	B	250	PHE	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLN	Sidechain
1	A	535	GLN	Sidechain
1	B	524	ASN	Sidechain
1	B	639	ASP	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	6156	0	6012	106	0
1	B	6166	0	6021	98	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	56	0	52	1	0
3	B	42	0	39	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	23	0	0	0	0
6	B	23	0	0	1	0
7	A	13	0	4	4	0
7	B	13	0	5	1	0
All	All	12576	0	12201	200	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 8.

All (200) 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:B:661:ASP:O	1:B:662:LEU:HD12	1.64	0.96
1:B:449:VAL:HG11	1:B:454:TYR:HB2	1.64	0.79
1:B:659:GLN:OE1	1:B:662:LEU:HD11	1.83	0.78
1:A:99:CYS:HB2	1:A:105:CYS:SG	2.22	0.78
1:A:99:CYS:CB	1:A:105:CYS:SG	2.72	0.77
1:A:625:LYS:HG2	1:A:714:THR:HA	1.69	0.74
1:B:661:ASP:O	1:B:662:LEU:CD1	2.35	0.74
1:B:360:CYS:HA	1:B:363:LEU:HD13	1.68	0.73
1:A:432:ASN:HB3	1:A:435:ILE:HG13	1.70	0.73
1:A:501:CYS:HB3	1:A:506:LEU:HB2	1.69	0.72
1:B:370:PHE:CE2	1:B:405:LYS:HD3	2.28	0.68
1:B:99:CYS:SG	1:B:100:LEU:N	2.64	0.68
1:A:80:LYS:NZ	1:B:68:ILE:HG21	2.09	0.67
1:A:99:CYS:SG	1:A:100:LEU:N	2.67	0.67
1:A:400:GLU:HG3	1:A:419:LEU:HD11	1.76	0.66
1:B:87:ARG:NH1	1:B:98:ASP:O	2.31	0.64
1:A:93:CYS:SG	1:A:106:CYS:N	2.70	0.64
1:A:276:GLU:HG3	1:A:331:MET:HE1	1.79	0.64
1:B:68:ILE:HG23	1:B:71:LEU:HD12	1.79	0.63
1:A:450:ARG:NH1	1:A:451:ASN:OD1	2.32	0.63
1:B:122:ASP:OD2	1:B:337:LYS:NZ	2.31	0.63
1:B:660:PRO:O	1:B:661:ASP:HB2	1.99	0.62
1:A:112:ILE:HD12	1:A:113:CYS:SG	2.40	0.61
1:A:185:THR:HB	7:A:909:CIT:C1	2.31	0.61
1:A:462:HIS:HA	1:A:471:MET:HE1	1.83	0.61
1:B:245:LYS:NZ	1:B:291:ALA:O	2.34	0.61
1:B:556:CYS:SG	1:B:641:LEU:N	2.73	0.61
1:B:78:CYS:HB2	1:B:112:ILE:HD11	1.82	0.60
1:B:276:GLU:HG3	1:B:331:MET:HE1	1.84	0.60
1:B:643:LEU:H	1:B:643:LEU:HD23	1.67	0.59
1:A:183:THR:OG1	1:A:471:MET:HE3	2.02	0.59
1:A:185:THR:HG23	1:A:189:HIS:ND1	2.18	0.59
1:A:360:CYS:HA	1:A:363:LEU:HD13	1.84	0.59
1:A:185:THR:HG23	1:A:189:HIS:HD1	1.66	0.58
1:A:328:THR:HA	1:A:331:MET:HE3	1.85	0.58
1:A:373:VAL:HG13	1:A:375:PHE:CZ	2.40	0.57
1:A:161:MET:HE3	1:A:322:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:SER:HA	1:A:681:GLN:HG3	1.85	0.57
1:B:257:LYS:HD3	1:B:262:TYR:CE1	2.39	0.57
1:B:659:GLN:OE1	1:B:662:LEU:CD1	2.53	0.56
1:A:409:ARG:N	1:A:413:GLN:OE1	2.37	0.56
1:A:112:ILE:CD1	1:A:113:CYS:SG	2.94	0.56
1:B:206:ASN:ND2	7:B:908:CIT:O1	2.33	0.56
1:B:784:ILE:HD11	1:B:819:VAL:HG12	1.88	0.56
1:B:183:THR:OG1	1:B:463:GLY:N	2.39	0.55
1:B:360:CYS:HA	1:B:363:LEU:CD1	2.34	0.55
1:A:161:MET:HE2	1:A:164:ILE:HD12	1.89	0.55
1:A:362:ARG:NH1	1:A:445:GLN:HB3	2.22	0.55
1:B:432:ASN:HB3	1:B:435:ILE:HG13	1.89	0.55
1:A:247:ALA:O	1:A:297:SER:HA	2.07	0.54
1:B:157:TRP:CZ2	1:B:319:ILE:HD11	2.42	0.54
1:B:370:PHE:CD2	1:B:405:LYS:HD3	2.42	0.54
1:A:437:LYS:HB3	1:A:437:LYS:NZ	2.22	0.54
1:A:185:THR:OG1	7:A:909:CIT:O2	2.26	0.54
1:A:594:HIS:HE1	1:A:596:LYS:HE3	1.72	0.53
1:A:204:ILE:HG13	1:A:208:MET:SD	2.49	0.52
1:B:99:CYS:O	1:B:103:LYS:N	2.41	0.52
1:A:80:LYS:HZ1	1:B:68:ILE:HG21	1.74	0.52
1:A:170:CYS:HA	1:A:485:LYS:HG2	1.91	0.52
1:B:219:LEU:HA	1:B:224:MET:HE3	1.90	0.52
1:A:71:LEU:N	1:A:72:PRO:HD2	2.25	0.52
1:B:373:VAL:HG23	1:B:373:VAL:O	2.10	0.52
1:A:365:TYR:CD2	1:A:452:LYS:HA	2.45	0.52
1:B:775:PRO:HB3	1:B:831:LEU:HD22	1.91	0.52
1:A:79:ASN:ND2	1:A:82:ARG:HG3	2.26	0.51
1:B:249:TYR:CE1	1:B:278:ARG:HG2	2.46	0.51
1:B:426:ARG:HH21	1:B:811:THR:HB	1.75	0.51
1:B:157:TRP:HB3	1:B:160:LEU:HD12	1.92	0.51
1:A:723:SER:HB3	1:A:758:VAL:HG22	1.92	0.51
1:B:233:GLN:NE2	3:B:903:NAG:O7	2.37	0.50
1:A:658:TYR:CD2	1:A:666:PRO:HG3	2.46	0.50
1:B:93:CYS:SG	1:B:106:CYS:N	2.85	0.50
1:A:211:VAL:HG12	1:A:433:ILE:HG13	1.93	0.50
1:B:78:CYS:CB	1:B:112:ILE:HD11	2.42	0.50
1:B:68:ILE:O	1:B:68:ILE:HG22	2.11	0.50
1:A:794:SER:OG	1:A:808:ARG:HD2	2.11	0.50
1:A:816:VAL:HB	1:A:842:LYS:HA	1.93	0.50
1:B:662:LEU:O	1:B:695:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:OG	1:A:98:ASP:N	2.44	0.49
1:B:571:LEU:HB3	1:B:575:ALA:HB3	1.93	0.49
1:A:463:GLY:H	1:A:471:MET:CE	2.26	0.49
1:A:677:SER:HB2	1:A:681:GLN:NE2	2.28	0.49
1:A:358:ILE:HB	1:A:447:LEU:HD11	1.95	0.49
1:B:250:PHE:CE2	1:B:269:TYR:HA	2.47	0.49
1:A:365:TYR:HD2	1:A:451:ASN:O	1.96	0.48
1:B:216:ASN:O	1:B:223:ASN:ND2	2.46	0.48
1:A:319:ILE:O	1:A:323:GLN:HG3	2.14	0.48
1:B:71:LEU:N	1:B:72:PRO:HD2	2.29	0.48
1:A:160:LEU:HD23	1:B:320:LYS:HE2	1.95	0.48
1:B:801:ASP:HB2	1:B:803:LEU:HD22	1.95	0.48
1:A:766:SER:O	1:A:766:SER:OG	2.31	0.47
1:B:203:ILE:HA	1:B:208:MET:HE1	1.96	0.47
1:B:158:ASP:HB2	1:B:165:ASN:OD1	2.13	0.47
1:A:423:LEU:HD22	1:A:441:MET:HE3	1.95	0.47
1:A:641:LEU:HD23	1:A:655:CYS:SG	2.55	0.47
1:B:449:VAL:HG12	1:B:450:ARG:N	2.30	0.47
1:B:749:LYS:HG3	1:B:749:LYS:O	2.15	0.47
1:A:464:TYR:H	1:A:471:MET:HE2	1.80	0.47
1:A:199:GLU:HB2	1:A:430:ALA:O	2.15	0.46
1:A:594:HIS:HE1	1:A:596:LYS:CE	2.27	0.46
1:A:386:ARG:HH22	3:A:901:NAG:H5	1.80	0.46
1:A:186:PHE:HB2	1:A:206:ASN:OD1	2.16	0.46
1:A:370:PHE:CZ	1:A:402:ILE:HG23	2.51	0.46
1:A:658:TYR:CG	1:A:666:PRO:HG3	2.50	0.46
1:B:616:PRO:HG2	1:B:669:LEU:HD12	1.97	0.46
6:B:907:IRH:O13	6:B:907:IRH:O30	2.32	0.46
1:A:107:THR:HB	1:A:334:GLU:HB2	1.96	0.46
1:A:324:MET:O	1:A:328:THR:HG23	2.16	0.46
1:A:594:HIS:CG	1:A:595:SER:N	2.83	0.46
1:A:614:LEU:O	1:A:653:GLN:NE2	2.48	0.46
1:A:238:THR:HG22	1:A:506:LEU:HD13	1.97	0.46
1:A:107:THR:HG21	1:A:331:MET:HG2	1.97	0.46
1:B:223:ASN:OD1	1:B:223:ASN:N	2.48	0.46
1:A:90:ASN:OD1	1:A:90:ASN:N	2.39	0.46
1:B:212:LYS:HB3	1:B:212:LYS:HE3	1.70	0.45
1:B:375:PHE:O	1:B:388:LYS:HE3	2.16	0.45
1:A:462:HIS:CA	1:A:471:MET:HE1	2.44	0.45
1:A:548:SER:OG	1:A:549:PRO:HD3	2.16	0.45
1:B:110:LYS:HB3	1:B:110:LYS:HE3	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TRP:HH2	1:B:274:PRO:HG2	1.80	0.45
1:B:659:GLN:HG3	1:B:662:LEU:HD22	1.97	0.45
1:A:719:LEU:HD23	1:A:762:SER:HB3	1.98	0.45
1:A:247:ALA:HB2	1:A:265:ILE:HD12	1.99	0.45
1:B:678:GLY:O	1:B:681:GLN:HG2	2.17	0.45
1:A:533:LYS:O	1:A:535:GLN:HG3	2.17	0.45
1:B:205:ASP:OD1	1:B:206:ASN:N	2.49	0.45
1:A:120:LEU:HD21	1:A:162:PRO:HB2	1.99	0.45
1:A:185:THR:HB	7:A:909:CIT:O1	2.17	0.45
1:B:362:ARG:HE	1:B:445:GLN:HB3	1.82	0.45
1:B:794:SER:OG	1:B:808:ARG:HD2	2.16	0.45
1:B:568:ARG:NH1	1:B:683:ASP:OD2	2.50	0.45
1:B:831:LEU:HA	1:B:831:LEU:HD23	1.86	0.45
1:A:664:ILE:HD12	1:A:745:VAL:HG12	1.98	0.44
1:A:185:THR:CB	7:A:909:CIT:C1	2.96	0.44
1:B:640:CYS:HB3	1:B:685:LEU:HD13	1.98	0.44
1:B:702:ASN:O	1:B:706:SER:OG	2.32	0.44
1:A:80:LYS:CE	1:B:68:ILE:HG21	2.47	0.44
1:A:211:VAL:HG13	1:A:212:LYS:HD3	1.98	0.44
1:A:437:LYS:HB3	1:A:437:LYS:HZ1	1.82	0.44
1:A:593:GLN:NE2	1:A:823:THR:O	2.51	0.44
1:B:118:SER:HB3	1:B:121:LYS:H	1.82	0.44
1:B:481:GLY:C	1:B:523:LYS:H	2.26	0.44
1:B:547:PRO:HD2	1:B:643:LEU:HD11	1.99	0.44
1:B:303:GLU:CD	1:B:307:THR:HG1	2.24	0.44
1:A:120:LEU:HD12	1:A:166:LYS:HD2	2.00	0.44
1:A:649:THR:O	1:A:652:SER:OG	2.22	0.43
1:B:753:PRO:HG2	1:B:756:TYR:CZ	2.53	0.43
1:B:157:TRP:CE2	1:B:319:ILE:HD11	2.54	0.43
1:A:304:PRO:HG3	1:A:322:LEU:HD21	2.00	0.43
1:A:554:CYS:HB3	1:A:641:LEU:O	2.18	0.43
1:A:693:MET:HE1	1:A:701:TRP:CD1	2.54	0.43
1:A:804:TRP:CD1	1:A:804:TRP:H	2.37	0.43
1:B:199:GLU:HB2	1:B:430:ALA:O	2.19	0.43
1:A:695:LYS:HE3	1:A:696:GLU:HG2	2.01	0.43
1:A:370:PHE:HZ	1:A:402:ILE:HG23	1.83	0.43
1:A:99:CYS:SG	1:A:100:LEU:HG	2.59	0.43
1:A:568:ARG:O	1:A:571:LEU:HD21	2.18	0.43
1:A:79:ASN:HD21	1:A:82:ARG:HG3	1.83	0.42
1:B:78:CYS:SG	1:B:106:CYS:HB2	2.58	0.42
1:B:236:TRP:CD1	1:B:263:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:MET:HE1	1:B:701:TRP:CE2	2.54	0.42
1:A:184:LYS:HE3	1:A:462:HIS:O	2.19	0.42
1:B:96:SER:OG	1:B:97:GLU:N	2.53	0.42
1:B:67:ASP:C	1:B:69:CYS:H	2.28	0.42
1:B:208:MET:HE3	1:B:229:TRP:CE3	2.54	0.42
1:B:431:ASN:HB2	1:B:731:TYR:O	2.18	0.42
1:A:158:ASP:OD1	1:A:159:THR:N	2.52	0.42
1:B:208:MET:HG3	1:B:217:PHE:HB3	2.02	0.42
1:B:247:ALA:O	1:B:297:SER:HA	2.20	0.42
1:A:400:GLU:H	1:A:400:GLU:CD	2.27	0.42
1:B:382:ALA:HB2	1:B:463:GLY:O	2.20	0.42
1:A:215:GLN:NE2	1:A:223:ASN:OD1	2.53	0.41
1:A:707:THR:C	1:A:710:PRO:HD2	2.45	0.41
1:B:837:GLU:OE2	1:B:840:ARG:NH2	2.53	0.41
1:A:706:SER:OG	1:A:707:THR:N	2.52	0.41
1:B:319:ILE:O	1:B:323:GLN:HG3	2.19	0.41
1:B:183:THR:HG23	1:B:464:TYR:O	2.20	0.41
1:A:247:ALA:HA	1:A:265:ILE:O	2.19	0.41
1:A:320:LYS:NZ	1:B:159:THR:HG21	2.36	0.41
1:A:568:ARG:NH1	1:A:683:ASP:OD2	2.54	0.41
1:B:229:TRP:HA	1:B:434:ARG:HH22	1.85	0.41
1:A:341:LEU:HB3	1:A:345:VAL:HG23	2.01	0.41
1:A:392:LYS:HB3	1:A:392:LYS:HE3	1.79	0.41
1:A:625:LYS:HG3	1:A:717:ASN:HA	2.01	0.41
1:A:749:LYS:HD3	1:A:749:LYS:HA	1.90	0.41
1:B:284:LYS:O	1:B:284:LYS:HG3	2.21	0.41
1:B:554:CYS:HB3	1:B:641:LEU:O	2.21	0.41
1:B:766:SER:O	1:B:766:SER:OG	2.35	0.41
1:A:784:ILE:HD13	1:A:822:LEU:HD12	2.02	0.41
1:B:132:CYS:SG	1:B:133:PRO:HD2	2.61	0.41
1:B:168:LYS:HG3	1:B:173:HIS:CG	2.56	0.41
1:B:449:VAL:HG12	1:B:450:ARG:H	1.85	0.41
1:A:96:SER:OG	1:A:97:GLU:N	2.54	0.40
1:B:810:GLN:HG2	1:B:848:PHE:CD2	2.56	0.40
1:A:178:ARG:NH2	1:A:845:LEU:HB3	2.36	0.40
1:A:593:GLN:HB3	1:A:735:PHE:CZ	2.57	0.40
1:B:548:SER:OG	1:B:549:PRO:CD	2.69	0.40
1:B:619:ASN:O	1:B:722:ILE:HA	2.21	0.40
1:B:257:LYS:HD3	1:B:262:TYR:HE1	1.86	0.40
1:B:671:PRO:HA	1:B:672:PRO:HD3	1.98	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	760/830 (92%)	713 (94%)	46 (6%)	1 (0%)	48	77
1	B	762/830 (92%)	712 (93%)	46 (6%)	4 (0%)	24	54
All	All	1522/1660 (92%)	1425 (94%)	92 (6%)	5 (0%)	36	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	B	250	PHE
1	B	661	ASP
1	B	548	SER
1	B	133	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	694/752 (92%)	694 (100%)	0	100	100
1	B	694/752 (92%)	694 (100%)	0	100	100
All	All	1388/1504 (92%)	1388 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	79	ASN
1	A	215	GLN
1	A	535	GLN
1	A	583	ASN
1	A	594	HIS
1	A	747	ASN
1	A	791	ASN
1	B	74	GLN
1	B	79	ASN
1	B	226	ASN
1	B	338	GLN
1	B	478	HIS
1	B	524	ASN
1	B	611	GLN
1	B	720	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 ⓘ

6 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	C	1	1,2	14,14,15	0.34	0	17,19,21	0.74	0
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	0.73	1 (5%)
2	BMA	C	3	2	11,11,12	1.25	1 (9%)	15,15,17	0.79	0
2	NAG	D	1	1,2	14,14,15	0.25	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	2	2	14,14,15	1.15	1 (7%)	17,19,21	0.84	1 (5%)
2	BMA	D	3	2	11,11,12	0.81	0	15,15,17	0.62	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	-4.04	1.36	1.43
2	C	3	BMA	C4-C3	2.14	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	2.60	115.66	112.19
2	C	2	NAG	C1-O5-C5	2.35	115.33	112.19
2	D	1	NAG	C1-O5-C5	2.16	115.08	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

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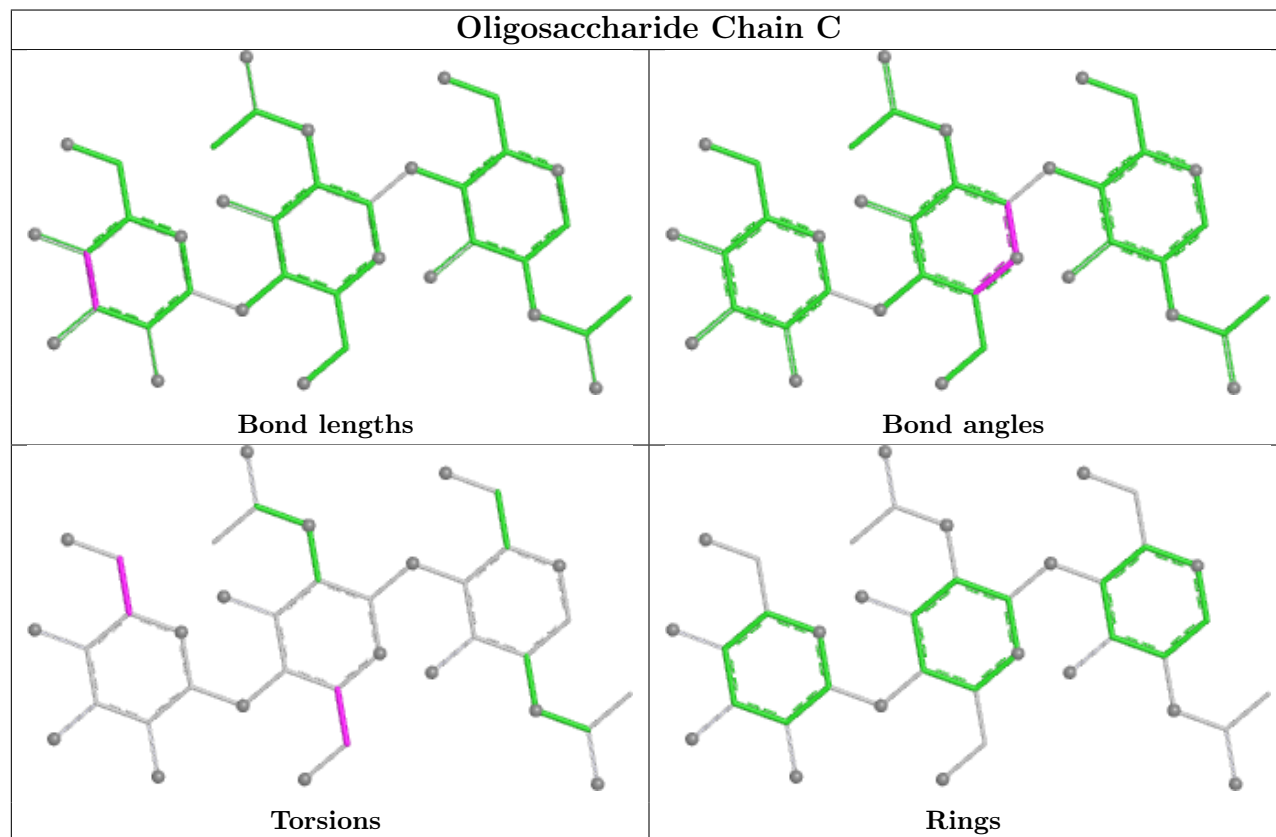
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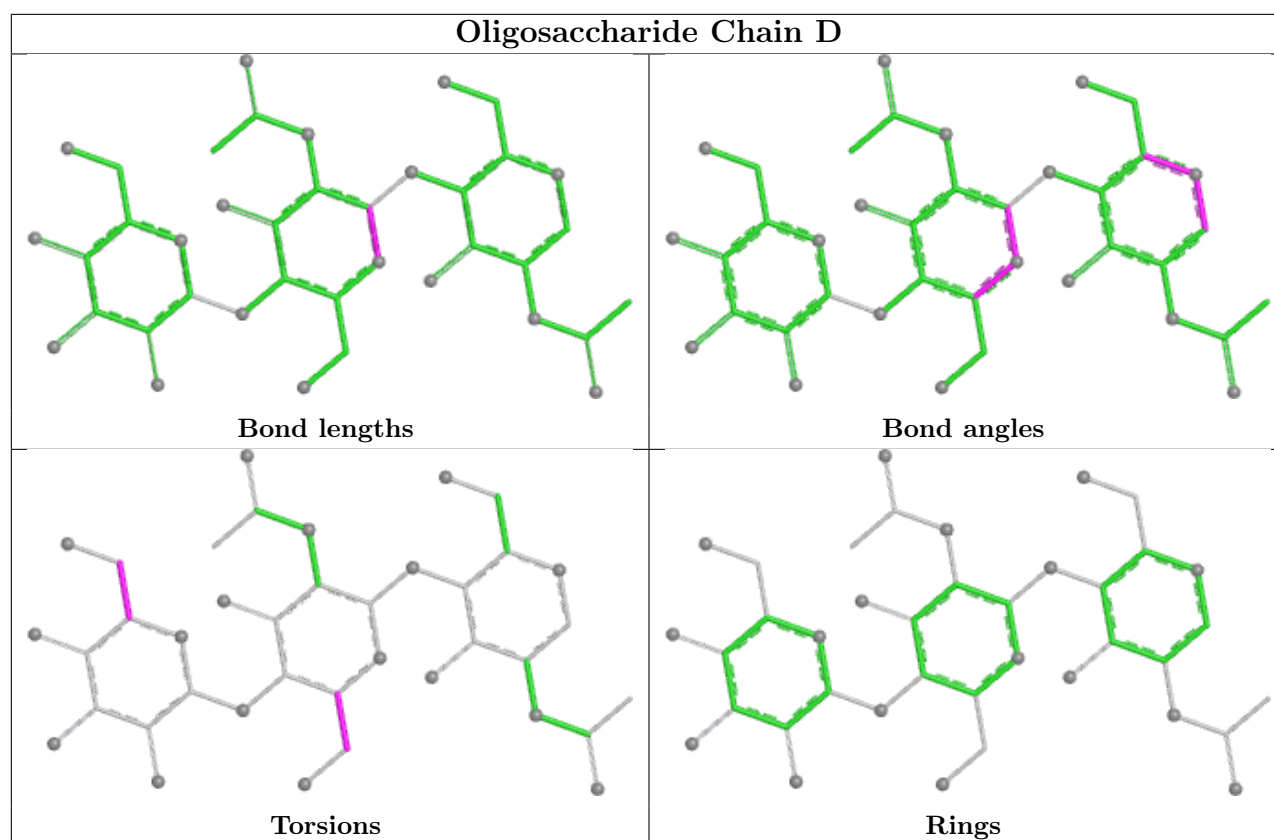
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	IRH	B	907	-	25,25,25	1.61	4 (16%)	37,37,37	2.20	8 (21%)
6	IRH	A	908	-	25,25,25	1.74	4 (16%)	37,37,37	2.28	8 (21%)
3	NAG	A	904	1	14,14,15	0.46	0	17,19,21	0.64	0
3	NAG	A	903	1	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	A	902	1	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
3	NAG	A	901	1	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	B	901	1	14,14,15	0.27	0	17,19,21	0.53	0
7	CIT	A	909	4	12,12,12	1.32	1 (8%)	17,17,17	1.56	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	902	1	14,14,15	0.18	0	17,19,21	0.64	1 (5%)
7	CIT	B	908	4	12,12,12	1.17	0	17,17,17	1.21	2 (11%)
3	NAG	B	903	1	14,14,15	0.23	0	17,19,21	0.52	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
6	IRH	B	907	-	-	2/6/6/6	0/3/3/3
6	IRH	A	908	-	-	2/6/6/6	0/3/3/3
3	NAG	A	904	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	4/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	NAG	B	901	1	-	1/6/23/26	0/1/1/1
7	CIT	A	909	4	-	0/16/16/16	-
3	NAG	B	902	1	-	2/6/23/26	0/1/1/1
7	CIT	B	908	4	-	7/16/16/16	-
3	NAG	B	903	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	908	IRH	C10-C11	5.41	1.41	1.36
6	B	907	IRH	C14-C11	-4.41	1.40	1.47
6	A	908	IRH	C14-C11	-4.34	1.40	1.47
6	B	907	IRH	C10-C11	4.17	1.40	1.36
6	B	907	IRH	C3-C9	-2.90	1.39	1.46
6	B	907	IRH	C10-C9	-2.72	1.39	1.46
6	A	908	IRH	C10-C9	-2.52	1.39	1.46
6	A	908	IRH	C3-C9	-2.48	1.40	1.46
7	A	909	CIT	C2-C3	-2.38	1.51	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	908	IRH	C01-O25-C16	7.56	128.60	117.51
6	B	907	IRH	C01-O25-C16	7.07	127.88	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	907	IRH	O25-C16-C17	6.99	125.03	114.55
6	A	908	IRH	O25-C16-C17	6.18	123.81	114.55
6	B	907	IRH	O25-C16-C15	-4.34	116.59	124.08
6	A	908	IRH	O12-C11-C14	4.16	116.71	110.87
6	A	908	IRH	O25-C16-C15	-4.00	117.19	124.08
6	A	908	IRH	O12-C4-C5	3.87	121.31	115.83
7	A	909	CIT	O6-C6-C3	3.77	120.38	113.14
7	A	909	CIT	C3-C2-C1	-3.30	104.90	113.92
6	B	907	IRH	O12-C4-C5	3.30	120.50	115.83
7	B	908	CIT	O6-C6-C3	3.20	119.28	113.14
6	A	908	IRH	O12-C11-C10	-2.88	117.46	120.19
6	B	907	IRH	O12-C11-C14	2.63	114.55	110.87
3	A	902	NAG	C1-O5-C5	2.62	115.70	112.19
6	B	907	IRH	O30-C2-C3	-2.59	116.35	121.14
6	A	908	IRH	C2-C3-C4	2.48	119.77	117.41
6	B	907	IRH	C14-C15-C16	2.42	122.85	119.60
6	A	908	IRH	C15-C14-C11	2.31	123.91	120.65
6	B	907	IRH	O12-C4-C3	-2.13	119.10	121.19
7	B	908	CIT	C3-C2-C1	-2.11	108.16	113.92
3	B	902	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	908	IRH	C17-C16-O25-C01
6	B	907	IRH	C17-C16-O25-C01
6	A	908	IRH	C15-C16-O25-C01
6	B	907	IRH	C15-C16-O25-C01
3	A	901	NAG	O5-C5-C6-O6
3	A	901	NAG	C4-C5-C6-O6
3	B	902	NAG	O5-C5-C6-O6
3	B	902	NAG	C4-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6
3	A	903	NAG	C8-C7-N2-C2
3	A	903	NAG	O7-C7-N2-C2
3	A	902	NAG	C4-C5-C6-O6
7	B	908	CIT	C6-C3-C4-C5
7	B	908	CIT	O7-C3-C4-C5
3	A	903	NAG	C4-C5-C6-O6
7	B	908	CIT	C2-C3-C4-C5
3	A	903	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	908	CIT	C4-C3-C6-O5
7	B	908	CIT	C2-C3-C6-O6
7	B	908	CIT	C4-C3-C6-O6
7	B	908	CIT	C2-C3-C6-O5
3	B	901	NAG	C4-C5-C6-O6

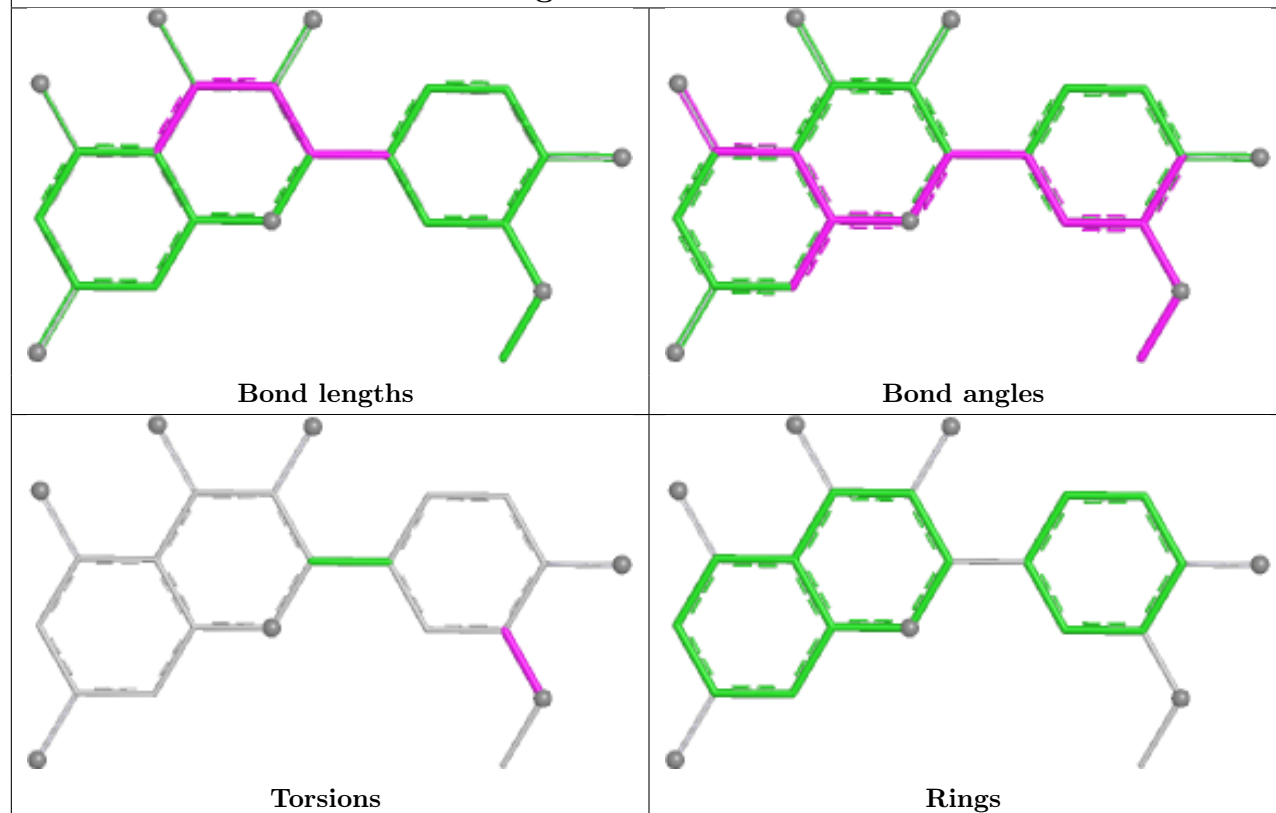
There are no ring outliers.

5 monomers are involved in 8 short contacts:

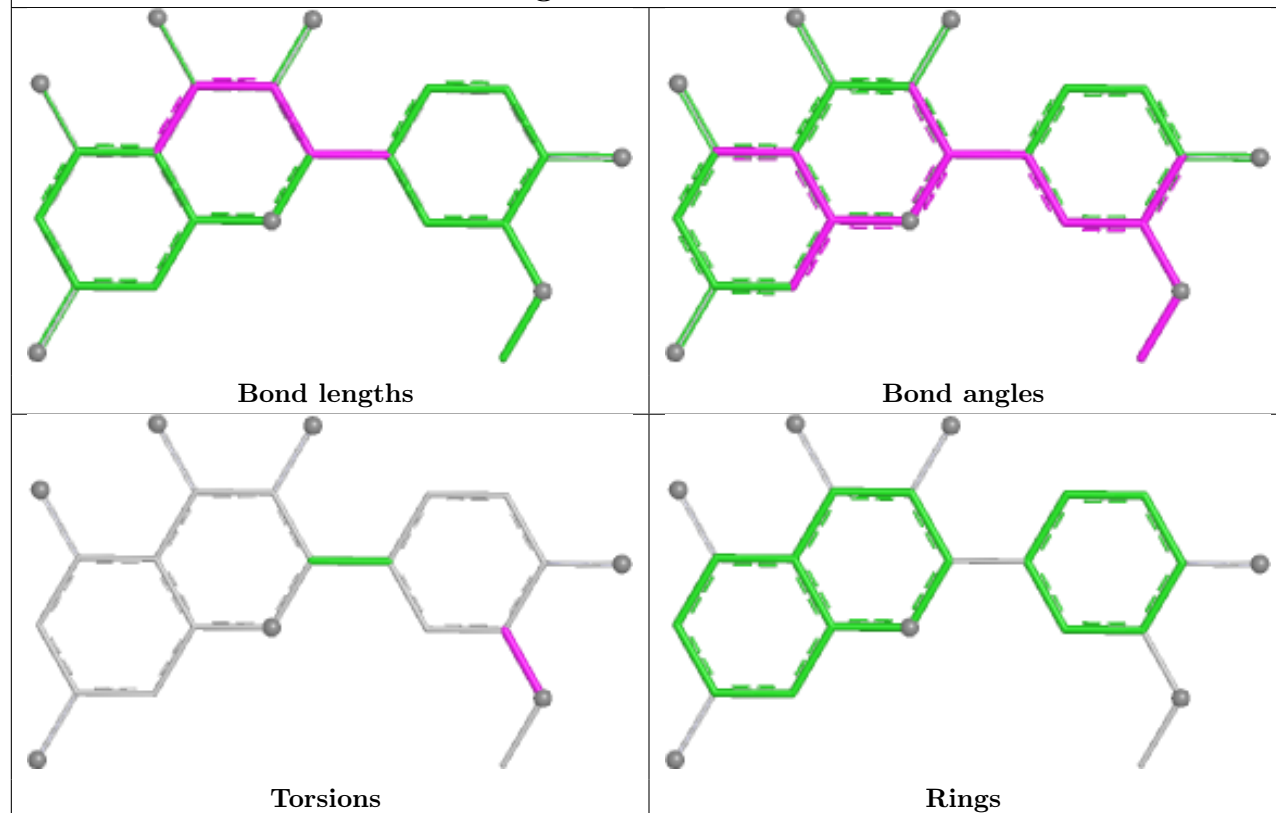
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	907	IRH	1	0
3	A	901	NAG	1	0
7	A	909	CIT	4	0
7	B	908	CIT	1	0
3	B	903	NAG	1	0

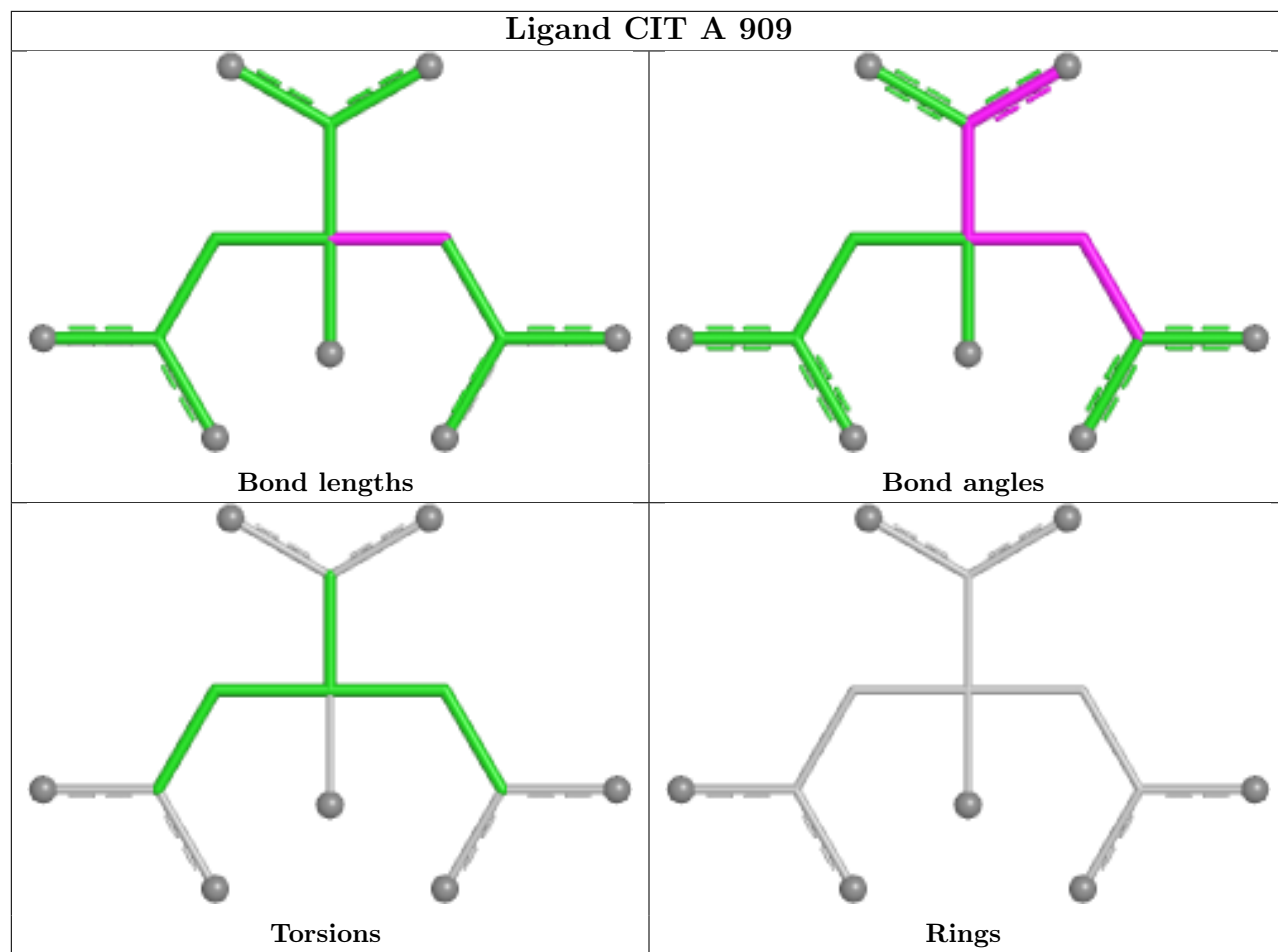
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

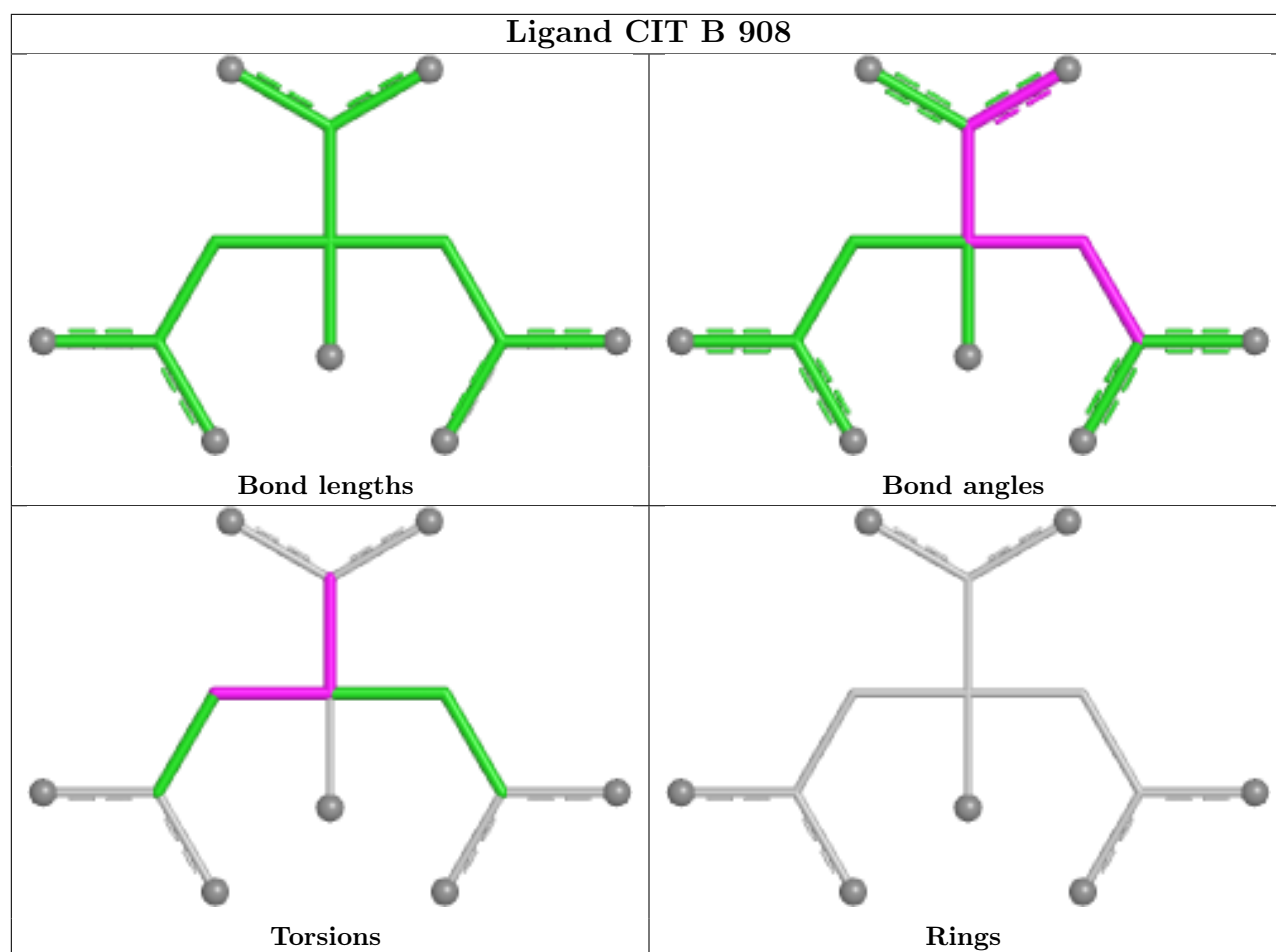
Ligand IRH B 907



Ligand IRH A 908







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	768/830 (92%)	-0.28	7 (0%) 81 75	25, 46, 78, 101	0
1	B	768/830 (92%)	-0.29	5 (0%) 84 79	24, 44, 79, 102	0
All	All	1536/1660 (92%)	-0.29	12 (0%) 82 77	24, 45, 78, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	3.6
1	B	125	ALA	3.3
1	A	594	HIS	3.1
1	A	738	TYR	3.1
1	B	454	TYR	2.9
1	B	83	CYS	2.6
1	B	749	LYS	2.5
1	A	125	ALA	2.3
1	A	105	CYS	2.3
1	A	849	ILE	2.1
1	B	70	VAL	2.1
1	A	773	CYS	2.0

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

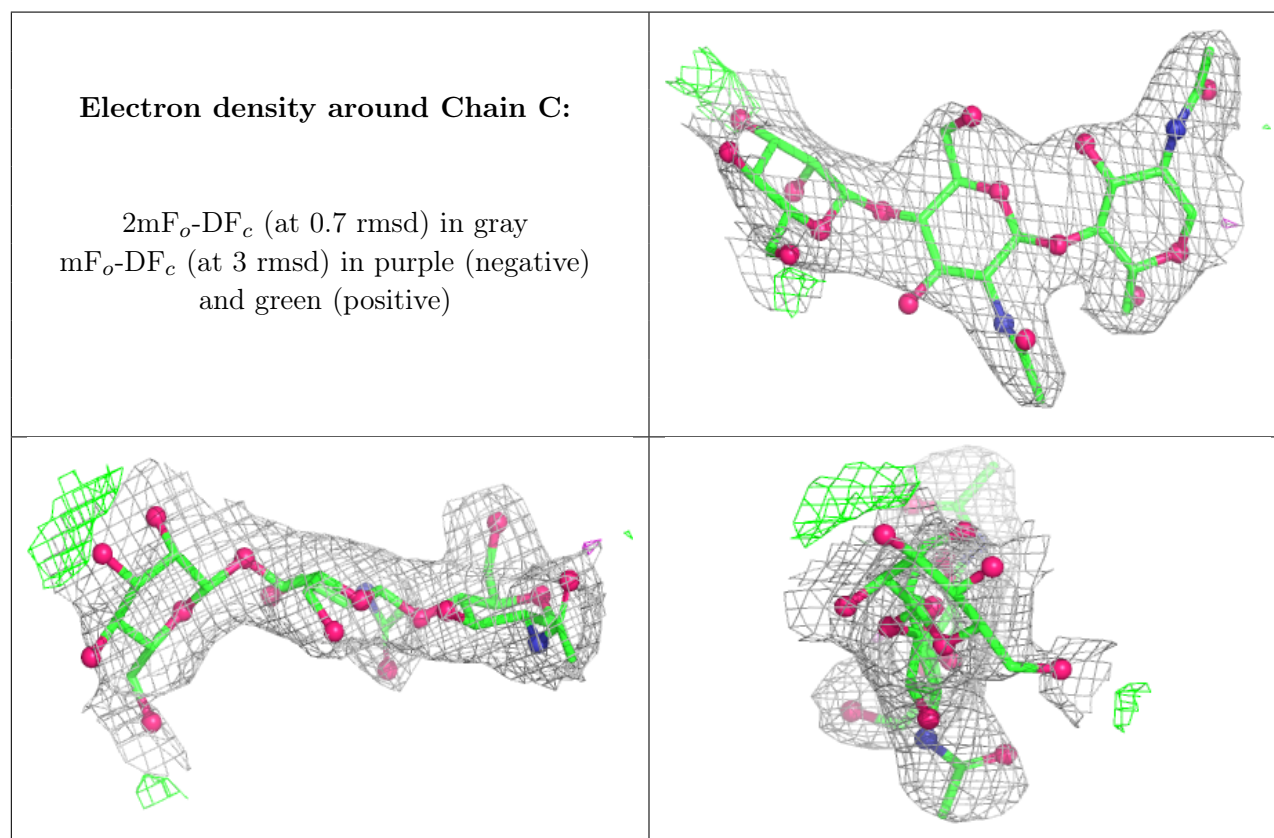
There are no non-standard protein/DNA/RNA residues in this entry.

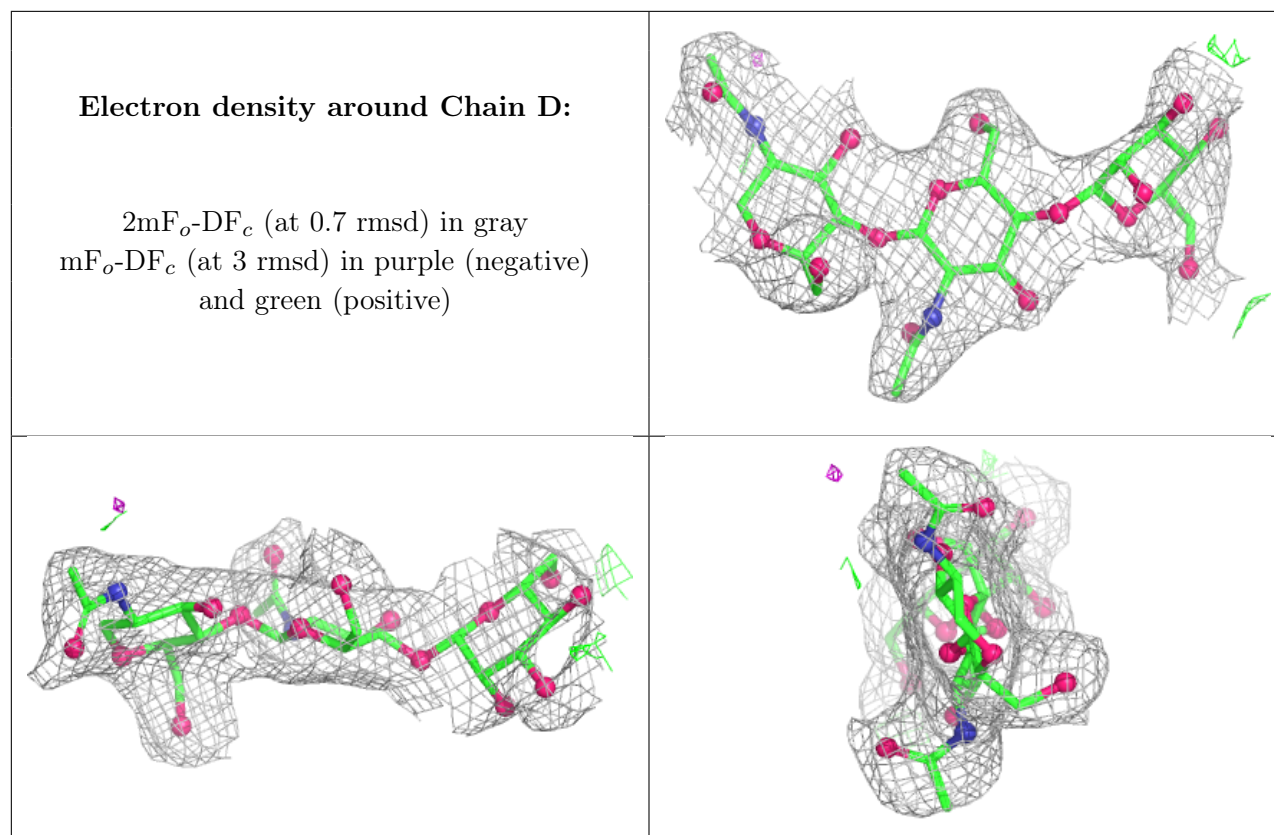
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	C	3	11/12	0.66	0.11	65,82,87,89	0
2	BMA	D	3	11/12	0.69	0.11	73,76,84,87	0
2	NAG	C	2	14/15	0.90	0.09	43,56,69,73	0
2	NAG	D	2	14/15	0.94	0.06	37,43,54,63	0
2	NAG	C	1	14/15	0.96	0.06	27,33,39,47	0
2	NAG	D	1	14/15	0.96	0.06	27,32,38,40	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	903	14/15	0.64	0.12	75,81,88,91	0
3	NAG	B	902	14/15	0.72	0.11	62,82,89,90	0
6	IRH	A	908	23/23	0.73	0.16	48,59,69,83	0
3	NAG	A	901	14/15	0.82	0.10	57,66,72,73	0
6	IRH	B	907	23/23	0.82	0.14	51,62,69,79	0
3	NAG	A	902	14/15	0.83	0.10	58,77,83,85	0
3	NAG	B	901	14/15	0.90	0.08	63,69,73,77	0
3	NAG	B	903	14/15	0.91	0.08	34,40,44,47	0
7	CIT	B	908	13/13	0.91	0.11	47,55,60,61	0
7	CIT	A	909	13/13	0.93	0.09	52,57,62,67	0
3	NAG	A	904	14/15	0.94	0.08	23,34,40,47	0
5	CA	A	907	1/1	0.94	0.10	64,64,64,64	0
5	CA	B	906	1/1	0.97	0.08	57,57,57,57	0
4	ZN	A	906	1/1	0.99	0.03	51,51,51,51	0

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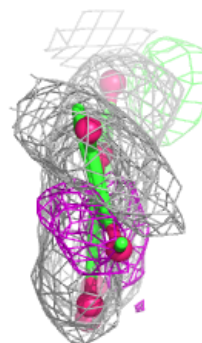
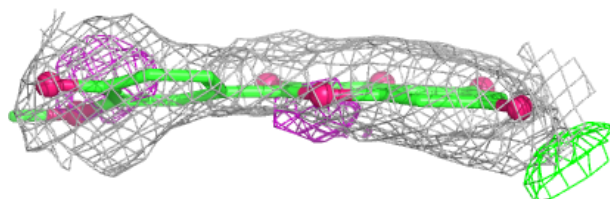
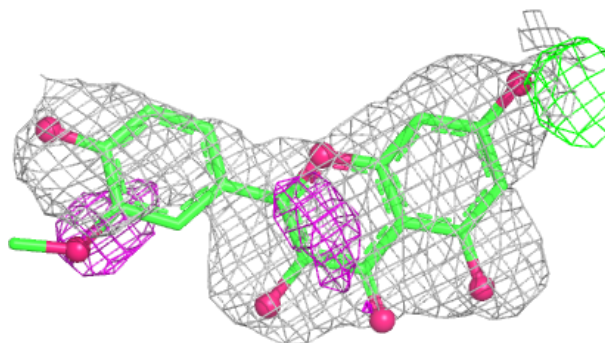
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	905	1/1	0.99	0.02	47,47,47,47	0
4	ZN	B	904	1/1	1.00	0.01	42,42,42,42	0
4	ZN	A	905	1/1	1.00	0.02	37,37,37,37	0

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.

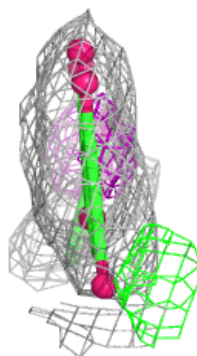
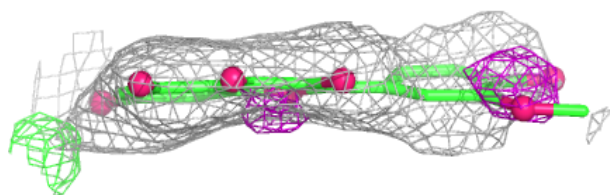
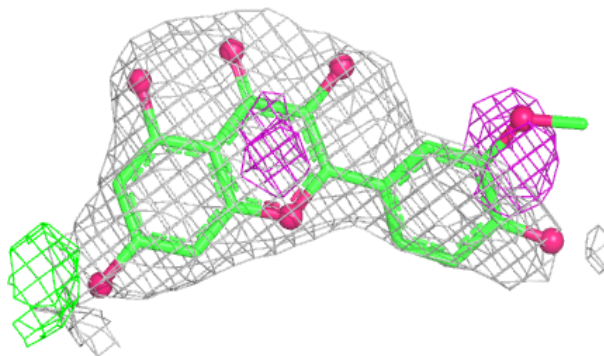
Electron density around IRH A 908:

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

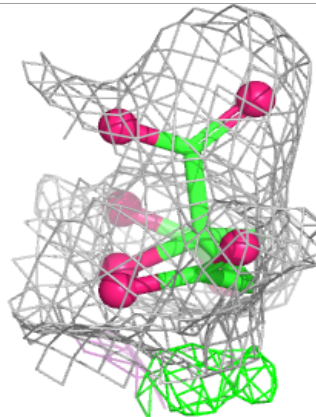
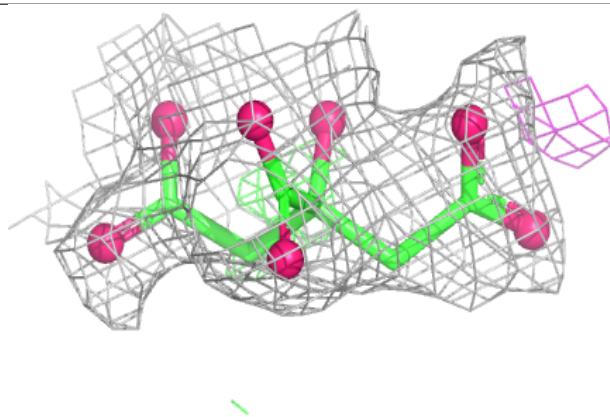
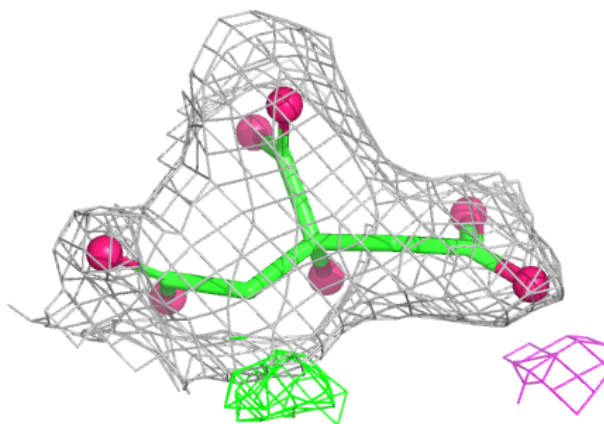


Electron density around IRH B 907:

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

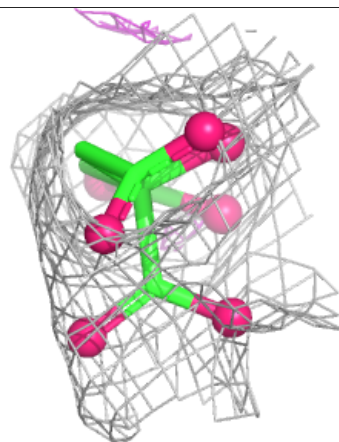
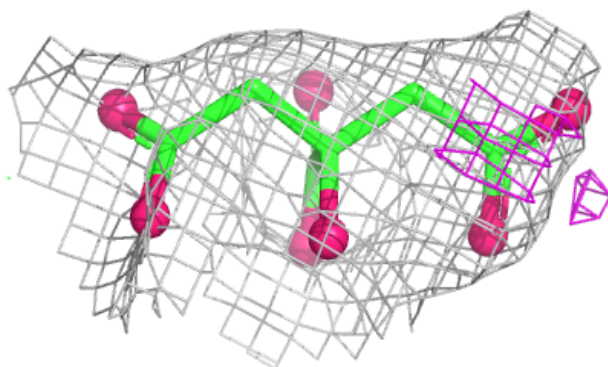
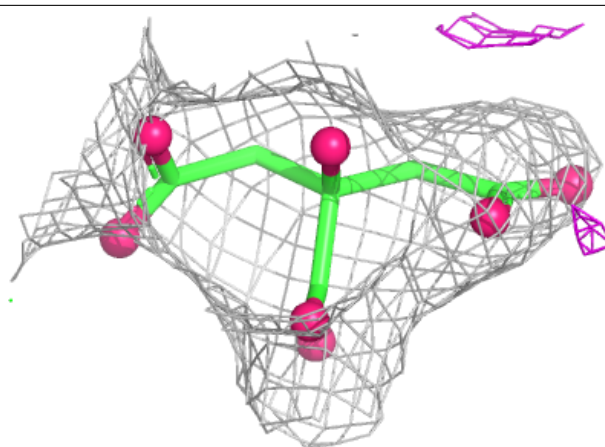
**Electron density around CIT B 908:**

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



Electron density around CIT A 909:

$2mF_o-DF_c$ (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.