



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:40 PM UTC

PDB ID : 6S0F / pdb_00006s0f
Title : Crystal structure of an inverting family GH156 exosialidase from uncultured bacterium pG7 in complex with 3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid
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Deposited on : 2019-06-14
Resolution : 2.00 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

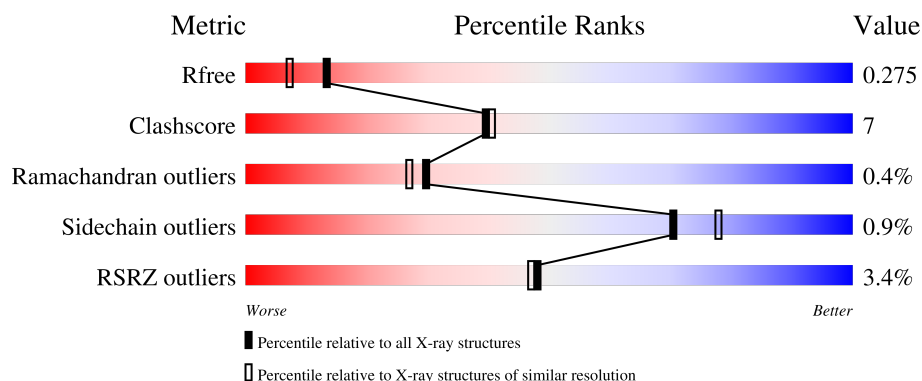
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	511	4% 81% 16% .
1	B	511	3% 79% 17% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	609	-	-	X	-
6	ACT	B	605	-	-	X	-

2 Entry composition [i](#)

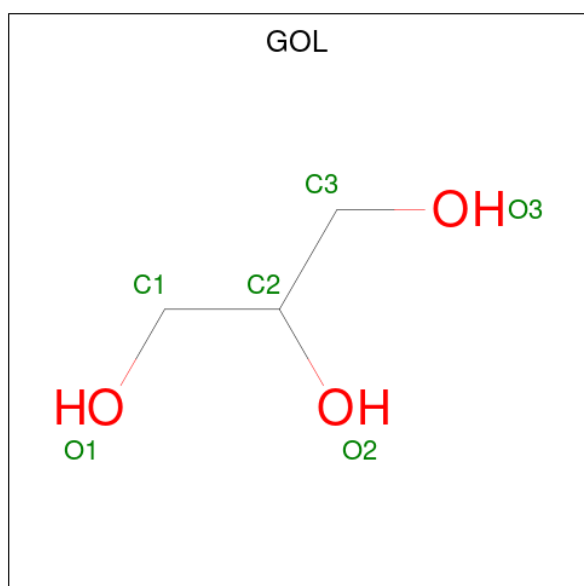
There are 7 unique types of molecules in this entry. The entry contains 8670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 exosialidase from uncultured bacterium pG7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	0
			4030	2569	728	715	18			
1	B	496	Total	C	N	O	S	0	3	0
			4028	2567	724	720	17			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



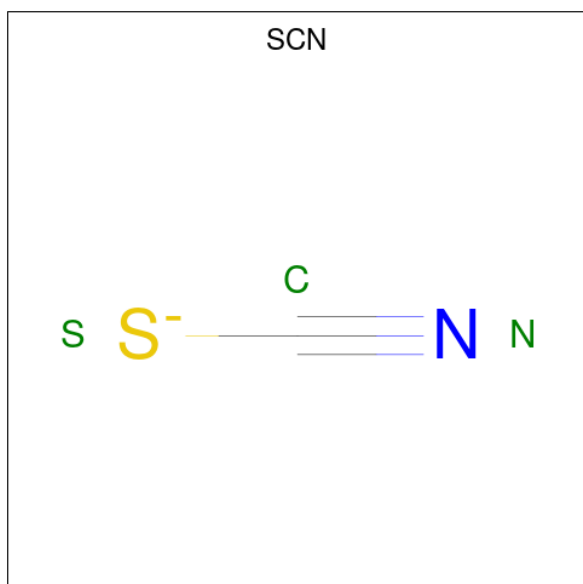
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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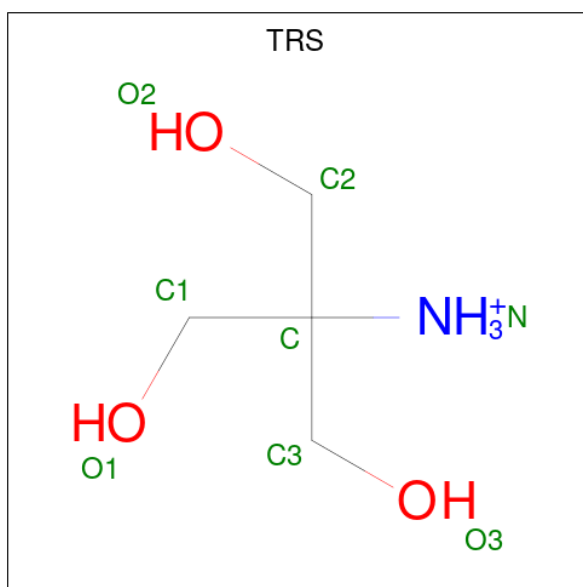
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



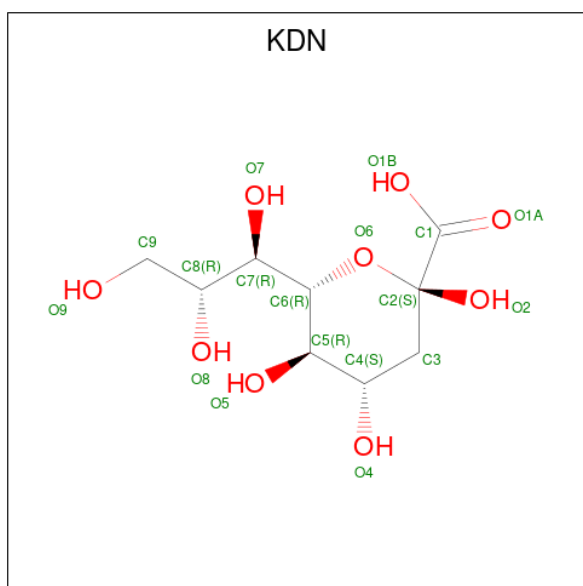
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



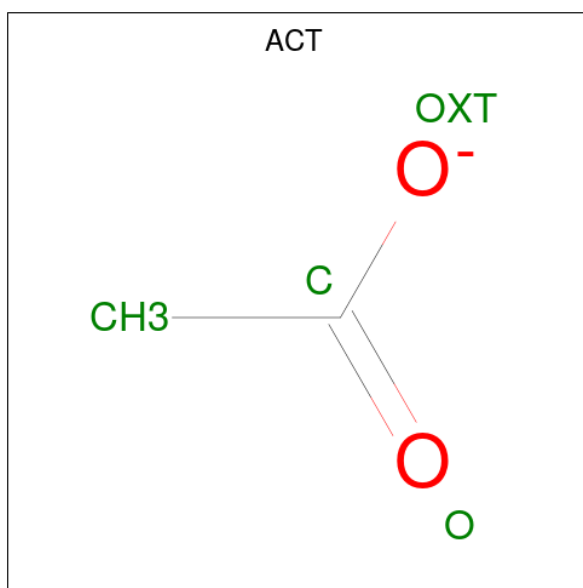
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is deamino-beta-neuraminic acid (CCD ID: KDN) (formula: C₉H₁₆O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			18	9	9		
5	B	1	Total	C	O	0	0
			18	9	9		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

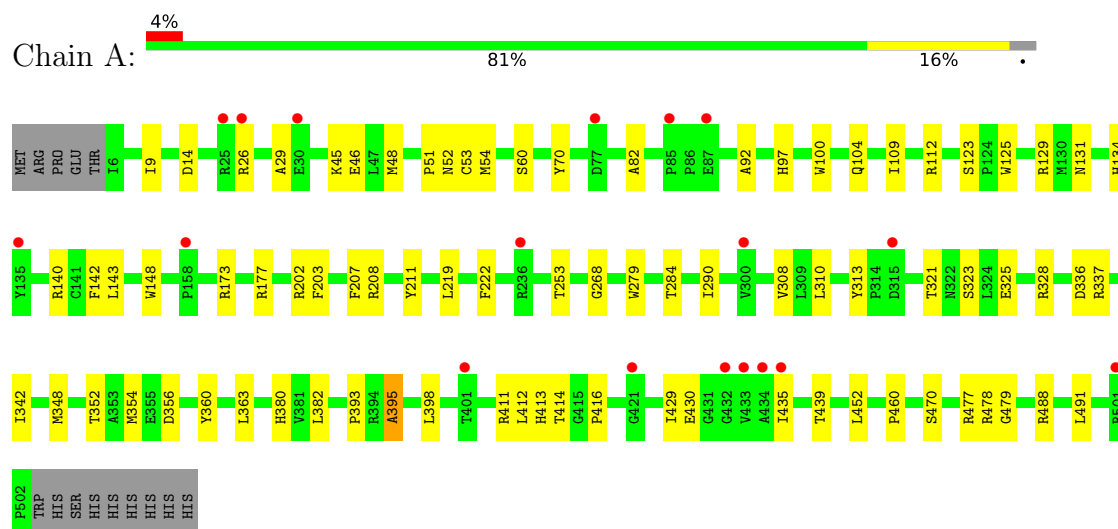
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	231	Total	O	0	0
			231	231		
7	B	256	Total	O	0	0
			256	256		

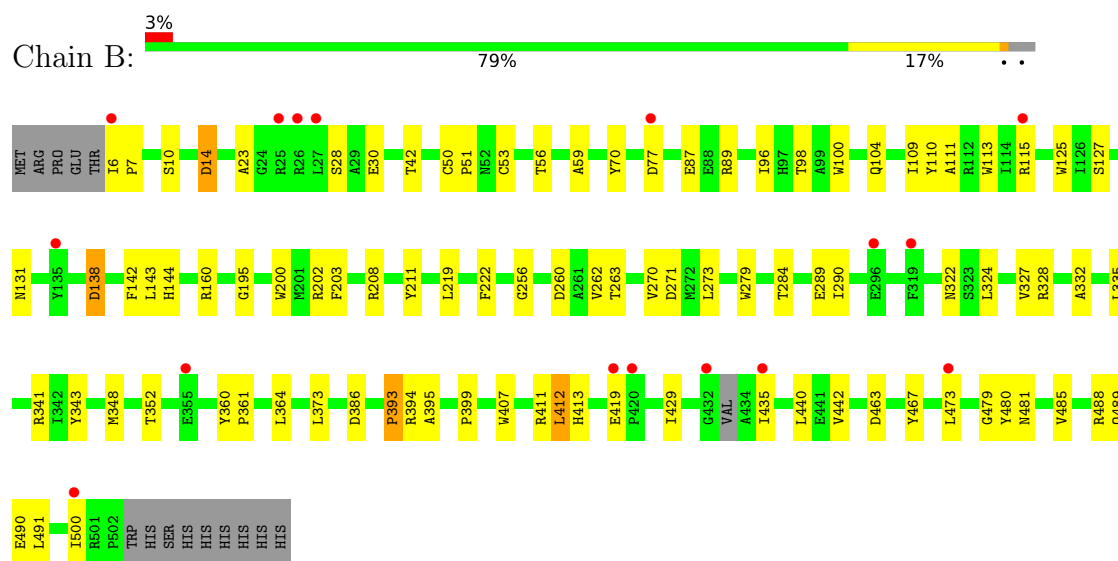
3 Residue-property plots [i](#)

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

- Molecule 1: exosialidase from uncultured bacterium pG7



- Molecule 1: exosialidase from uncultured bacterium pG7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.66Å 78.92Å 112.99Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	112.58 – 2.00 112.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (112.58-2.00) 99.8 (112.58-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.217 , 0.265 0.230 , 0.275	Depositor DCC
R_{free} test set	3867 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8670	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KDN, SCN, ACT, GOL, TRS

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	1.19	5/4153 (0.1%)	1.45	8/5650 (0.1%)
1	B	1.22	6/4153 (0.1%)	1.44	10/5649 (0.2%)
All	All	1.20	11/8306 (0.1%)	1.45	18/11299 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	ARG	C-O	6.79	1.32	1.24
1	B	393	PRO	C-O	-6.25	1.16	1.23
1	A	325	GLU	C-O	5.86	1.30	1.24
1	B	412	LEU	C-O	5.84	1.30	1.24
1	B	111	ALA	C-O	5.60	1.30	1.24
1	A	478	ARG	C-O	5.52	1.30	1.23
1	B	332	ALA	C-O	5.50	1.30	1.24
1	A	92	ALA	C-O	5.36	1.30	1.24
1	B	53	CYS	C-O	5.19	1.30	1.24
1	B	138	ASP	C-O	5.02	1.29	1.23
1	A	328	ARG	C-O	5.01	1.29	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	284	THR	N-CA-C	-5.95	105.98	113.18
1	A	53	CYS	N-CA-C	-5.93	103.06	108.75
1	A	142	PHE	CA-C-O	-5.83	114.36	120.55
1	B	70	TYR	CA-C-O	-5.67	114.22	120.69
1	B	56	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	26	ARG	CB-CA-C	5.53	119.15	110.19
1	B	373	LEU	N-CA-C	-5.51	106.39	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	THR	CA-CB-OG1	-5.41	101.48	109.60
1	B	110	TYR	CA-C-O	-5.40	114.70	120.42
1	A	60	SER	CA-C-O	-5.35	115.73	121.56
1	B	284	THR	N-CA-C	-5.28	106.69	113.23
1	A	109	ILE	CA-C-O	-5.27	115.57	121.05
1	B	463	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	222	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	395	ALA	CA-C-O	-5.12	114.86	120.70
1	B	14	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	481	ASN	CB-CA-C	5.03	118.81	109.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4030	0	3936	50	0
1	B	4028	0	3922	58	0
2	A	36	0	48	8	0
2	B	24	0	32	6	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
4	A	8	0	12	5	0
5	A	18	0	5	0	0
5	B	18	0	5	0	0
6	B	12	0	9	4	0
7	A	231	0	0	2	0
7	B	256	0	0	10	0
All	All	8670	0	7969	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (108) 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:177:ARG:HD2	4:A:603:TRS:H11	1.51	0.91
6:B:602:ACT:H2	7:B:865:HOH:O	1.74	0.86
2:B:608:GOL:H32	7:B:826:HOH:O	1.80	0.80
1:B:262:VAL:HG23	2:B:603:GOL:H2	1.66	0.77
2:A:608:GOL:H11	1:B:480:TYR:HB2	1.69	0.74
1:A:177:ARG:CD	4:A:603:TRS:H11	2.19	0.72
1:A:52:ASN:O	1:A:129:ARG:HG3	1.91	0.71
2:B:608:GOL:C3	7:B:826:HOH:O	2.39	0.68
1:A:177:ARG:HD2	4:A:603:TRS:C1	2.25	0.67
1:A:413:HIS:CE1	1:A:479:GLY:HA2	2.31	0.66
1:A:411:ARG:C	1:A:412:LEU:HD12	2.21	0.65
1:A:354[A]:MET:HE1	1:A:363:LEU:HD13	1.79	0.65
1:B:87:GLU:HG2	7:B:806:HOH:O	1.96	0.64
1:B:411:ARG:C	1:B:412:LEU:HD12	2.23	0.62
1:B:290:ILE:HG12	7:B:826:HOH:O	1.99	0.61
1:B:413:HIS:CE1	1:B:479:GLY:HA2	2.37	0.59
1:A:70:TYR:OH	1:A:97:HIS:HD2	1.85	0.59
1:A:45:LYS:HZ3	2:A:609:GOL:C3	2.17	0.58
1:B:429:ILE:HD13	1:B:491:LEU:HD13	1.86	0.57
1:A:268:GLY:HA2	7:A:726:HOH:O	2.07	0.55
1:A:45:LYS:NZ	2:A:609:GOL:C3	2.70	0.55
1:B:490:GLU:O	1:B:491:LEU:HD23	2.08	0.54
1:A:14:ASP:OD1	1:A:14:ASP:C	2.51	0.54
2:A:605:GOL:H32	1:B:256:GLY:CA	2.38	0.54
1:B:262:VAL:HG23	2:B:603:GOL:C2	2.39	0.53
1:B:429:ILE:HD11	1:B:440:LEU:HD11	1.90	0.53
1:B:473:LEU:HD13	1:B:473:LEU:O	2.08	0.53
1:B:14:ASP:OD2	1:B:348:MET:HE1	2.10	0.52
1:B:442:VAL:HG22	1:B:485:VAL:HG12	1.90	0.52
1:A:134:HIS:NE2	2:A:607:GOL:H2	2.25	0.52
1:B:77:ASP:HB2	1:B:89:ARG:NH1	2.24	0.52
1:A:354[A]:MET:HE3	1:A:360:TYR:HD1	1.75	0.52
1:A:45:LYS:NZ	2:A:609:GOL:H32	2.25	0.51
1:A:100:TRP:CZ2	1:A:104:GLN:HG3	2.46	0.51
1:B:138:ASP:O	1:B:144:HIS:NE2	2.42	0.51
1:B:394:ARG:NH1	7:B:718:HOH:O	2.44	0.50
1:A:70:TYR:OH	1:A:97:HIS:CD2	2.65	0.49
1:A:177:ARG:NE	4:A:603:TRS:H11	2.26	0.49
1:A:354[A]:MET:CE	1:A:363:LEU:HD13	2.41	0.49
1:B:260:ASP:OD2	1:B:263:THR:OG1	2.25	0.49
1:A:382:LEU:HD23	1:A:398:LEU:HD11	1.95	0.49
1:B:399:PRO:CG	2:B:607:GOL:H31	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:HD13	1:A:491:LEU:HD13	1.93	0.49
2:A:608:GOL:H11	1:B:480:TYR:CB	2.41	0.49
1:A:207:PHE:HZ	1:A:219:LEU:HG	1.79	0.48
1:B:160:ARG:O	1:B:160:ARG:HG3	2.12	0.48
1:A:435:ILE:HB	1:A:439:THR:HB	1.95	0.48
1:B:435:ILE:HG12	1:B:467:TYR:CZ	2.49	0.47
1:A:477:ARG:NH1	1:B:211:TYR:CE2	2.83	0.47
1:B:7:PRO:HG2	1:B:335:LEU:HD22	1.95	0.47
1:B:348:MET:HE3	1:B:352:THR:HB	1.97	0.47
1:B:270:VAL:HG21	1:B:273:LEU:HD21	1.97	0.47
1:B:28:SER:HB2	1:B:30[B]:GLU:OE2	2.15	0.46
1:B:59:ALA:O	6:B:605:ACT:H1	2.16	0.46
1:B:59:ALA:HB3	6:B:605:ACT:OXT	2.15	0.46
1:B:488:ARG:N	1:B:488:ARG:HD2	2.31	0.46
1:B:96:ILE:HD11	1:B:142:PHE:CD2	2.51	0.46
1:B:10:SER:OG	1:B:341:ARG:HG2	2.16	0.46
1:B:109:ILE:HD11	1:B:113:TRP:CZ2	2.51	0.46
1:B:419:GLU:HG3	7:B:892:HOH:O	2.16	0.46
1:B:271:ASP:OD1	6:B:606:ACT:H2	2.16	0.45
1:A:208:ARG:HB2	1:A:211:TYR:CD1	2.52	0.45
1:A:336:ASP:HB2	1:A:416:PRO:HD3	1.98	0.45
1:B:473:LEU:HD13	1:B:473:LEU:C	2.41	0.45
1:A:100:TRP:CE2	1:A:104:GLN:HG3	2.52	0.45
1:A:393:PRO:HB2	1:B:395:ALA:HB1	1.97	0.45
1:B:429:ILE:HD12	1:B:435:ILE:HG21	1.98	0.45
1:B:125:TRP:CD2	1:B:195:GLY:HA3	2.52	0.45
1:A:290:ILE:HG12	7:A:704:HOH:O	2.17	0.44
1:A:395:ALA:HB1	1:B:393:PRO:HB2	1.99	0.44
1:B:324:LEU:HD21	1:B:328:ARG:NH2	2.32	0.44
1:B:360:TYR:N	1:B:361:PRO:CD	2.81	0.44
1:A:45:LYS:HZ2	2:A:609:GOL:H32	1.83	0.44
1:A:9:ILE:HA	1:A:342:ILE:O	2.18	0.44
1:A:29:ALA:HB1	1:A:112:ARG:CZ	2.47	0.44
1:B:115:ARG:HD3	7:B:814:HOH:O	2.18	0.43
1:B:100:TRP:CZ2	1:B:104:GLN:HG3	2.52	0.43
1:A:380:HIS:CE1	1:A:414:THR:HA	2.54	0.43
1:B:42:THR:HB	1:B:364:LEU:O	2.17	0.43
1:B:208:ARG:HG2	7:B:784:HOH:O	2.18	0.43
1:A:354[A]:MET:HE3	1:A:360:TYR:CD1	2.53	0.43
1:A:202:ARG:HA	1:A:203:PHE:HA	1.81	0.43
1:A:488:ARG:N	1:A:488:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CE2	1:B:195:GLY:HA3	2.54	0.43
1:B:322:ASN:HB3	1:B:327:VAL:HG23	2.01	0.43
1:A:348:MET:HE3	1:A:352:THR:HB	2.01	0.42
1:B:10:SER:O	1:B:343:TYR:HA	2.18	0.42
1:B:6:ILE:N	7:B:729:HOH:O	2.52	0.42
1:A:308:VAL:HG22	1:A:321:THR:HB	2.00	0.42
1:A:452:LEU:HD11	1:A:470:SER:HB2	2.02	0.42
1:B:360:TYR:O	1:B:364:LEU:HG	2.20	0.42
1:A:46:GLU:HG3	1:A:123:SER:HB3	2.02	0.42
1:A:48:MET:HE3	1:A:125:TRP:CD2	2.55	0.42
1:B:7:PRO:O	1:B:341:ARG:HD3	2.20	0.42
1:B:14:ASP:OD1	1:B:14:ASP:C	2.63	0.42
1:A:337:ARG:CG	1:A:413:HIS:CE1	3.03	0.41
1:A:313:TYR:OH	1:A:430:GLU:OE2	2.35	0.41
1:B:200:TRP:CH2	1:B:219:LEU:HD22	2.56	0.41
1:B:407:TRP:HB2	2:B:601:GOL:H32	2.02	0.41
1:A:222:PHE:HA	4:A:603:TRS:H31	2.03	0.41
1:B:50:CYS:HA	1:B:127:SER:O	2.20	0.41
1:B:202:ARG:HA	1:B:203:PHE:HA	1.85	0.41
1:A:310:LEU:HD23	1:A:460:PRO:HG2	2.02	0.41
1:A:54:MET:HE1	1:A:148:TRP:CD1	2.57	0.40
1:A:82:ALA:HB3	1:A:140:ARG:HH22	1.86	0.40
1:A:323:SER:HA	1:A:356:ASP:OD1	2.21	0.40
1:B:23:ALA:HA	1:B:98:THR:OG1	2.22	0.40
1:A:412:LEU:HD12	1:A:412:LEU:N	2.35	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	497/511 (97%)	480 (97%)	15 (3%)	2 (0%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	495/511 (97%)	480 (97%)	13 (3%)	2 (0%)	30	27
All	All	992/1022 (97%)	960 (97%)	28 (3%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	TRP
1	A	279	TRP
1	A	131	ASN
1	B	131	ASN

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	414/426 (97%)	412 (100%)	2 (0%)	81	87
1	B	414/426 (97%)	409 (99%)	5 (1%)	63	70
All	All	828/852 (97%)	821 (99%)	7 (1%)	70	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PRO
1	A	143	LEU
1	B	51	PRO
1	B	143	LEU
1	B	289	GLU
1	B	489	GLN
1	B	500	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	104	GLN
1	A	413	HIS
1	B	322	ASN
1	B	346	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
2	GOL	A	601	-	5,5,5	0.17	0	5,5,5	0.63	0
2	GOL	A	607	-	5,5,5	0.16	0	5,5,5	0.37	0
5	KDN	B	609	-	18,18,18	1.24	1 (5%)	21,27,27	2.46	7 (33%)
6	ACT	B	605	-	3,3,3	1.26	0	3,3,3	0.61	0
3	SCN	A	606	-	1,2,2	0.37	0	0,1,1	-	-
3	SCN	B	604	-	1,2,2	0.10	0	0,1,1	-	-
2	GOL	A	605	-	5,5,5	0.19	0	5,5,5	0.53	0
2	GOL	B	601	-	5,5,5	0.11	0	5,5,5	0.36	0
2	GOL	B	607	-	5,5,5	0.18	0	5,5,5	0.31	0
3	SCN	A	602	-	1,2,2	0.77	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	608	-	5,5,5	0.38	0	5,5,5	0.35	0
2	GOL	B	603	-	5,5,5	0.15	0	5,5,5	0.33	0
6	ACT	B	602	-	3,3,3	1.13	0	3,3,3	0.69	0
2	GOL	A	604	-	5,5,5	0.08	0	5,5,5	0.70	0
2	GOL	A	608	-	5,5,5	0.24	0	5,5,5	0.45	0
5	KDN	A	610	-	18,18,18	1.44	2 (11%)	21,27,27	1.80	6 (28%)
2	GOL	A	609	-	5,5,5	0.19	0	5,5,5	0.38	0
4	TRS	A	603	-	7,7,7	0.37	0	9,9,9	1.06	1 (11%)
6	ACT	B	606	-	3,3,3	1.05	0	3,3,3	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	604	-	-	0/4/4/4	-
2	GOL	B	607	-	-	2/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
2	GOL	A	608	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
5	KDN	A	610	-	-	0/16/34/34	0/1/1/1
2	GOL	A	607	-	-	2/4/4/4	-
2	GOL	A	609	-	-	4/4/4/4	-
2	GOL	B	608	-	-	0/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
4	TRS	A	603	-	-	5/9/9/9	-
5	KDN	B	609	-	-	1/16/34/34	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	KDN	C7-C6	-3.16	1.49	1.52
5	A	610	KDN	C4-C5	2.51	1.56	1.52
5	B	609	KDN	C2-C1	-2.36	1.50	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	609	KDN	O2-C2-C1	-6.46	97.09	110.73
5	B	609	KDN	O1A-C1-C2	-4.37	116.56	123.85
5	A	610	KDN	O2-C2-C1	-4.30	101.64	110.73
5	B	609	KDN	O6-C6-C5	3.68	113.64	108.50
5	A	610	KDN	O7-C7-C6	-3.42	102.05	109.44
5	A	610	KDN	O2-C2-C3	3.17	114.25	109.44
5	B	609	KDN	O7-C7-C8	3.10	115.97	108.93
5	B	609	KDN	C4-C5-C6	-3.05	104.34	110.51
5	B	609	KDN	O5-C5-C6	2.93	117.45	109.94
5	A	610	KDN	O1A-C1-C2	-2.52	119.65	123.85
4	A	603	TRS	C1-C-N	-2.33	102.23	108.17
5	B	609	KDN	C9-C8-C7	-2.08	107.92	112.17
5	A	610	KDN	C9-C8-C7	-2.05	107.99	112.17
5	A	610	KDN	O5-C5-C4	-2.05	105.88	110.05

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	A	605	GOL	O1-C1-C2-C3
2	A	607	GOL	C1-C2-C3-O3
2	A	609	GOL	O1-C1-C2-C3
2	A	609	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-C3
2	B	607	GOL	O1-C1-C2-O2
2	B	607	GOL	O1-C1-C2-C3
4	A	603	TRS	C2-C-C1-O1
4	A	603	TRS	C3-C-C1-O1
4	A	603	TRS	N-C-C1-O1
5	B	609	KDN	O1A-C1-C2-O6
2	A	609	GOL	O2-C2-C3-O3
2	A	608	GOL	O1-C1-C2-C3
2	B	603	GOL	C1-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	A	605	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-O2
2	A	607	GOL	O2-C2-C3-O3
2	A	608	GOL	O1-C1-C2-O2
2	B	603	GOL	O2-C2-C3-O3
2	A	609	GOL	O1-C1-C2-O2

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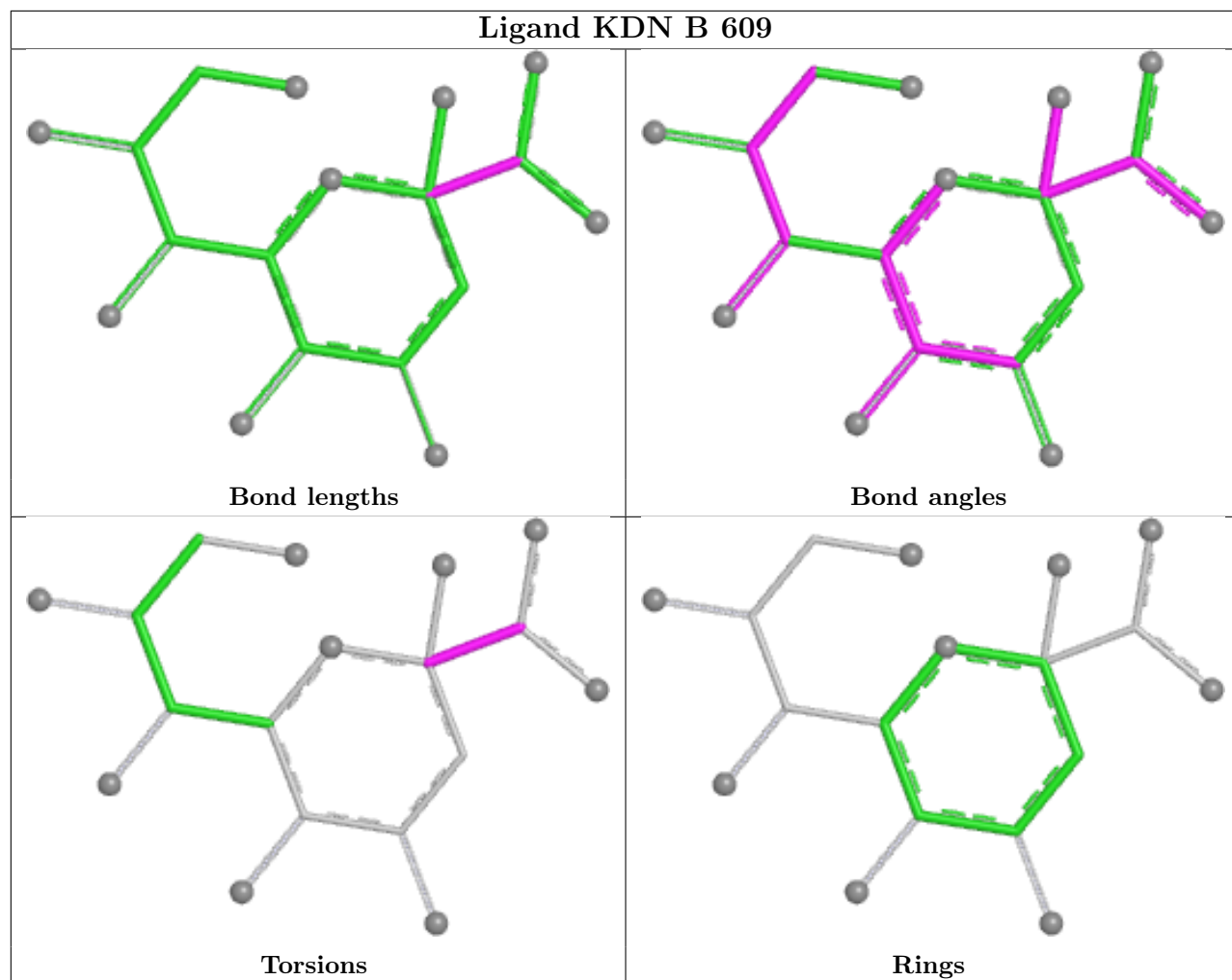
Mol	Chain	Res	Type	Atoms
4	A	603	TRS	C1-C-C2-O2
4	A	603	TRS	N-C-C2-O2

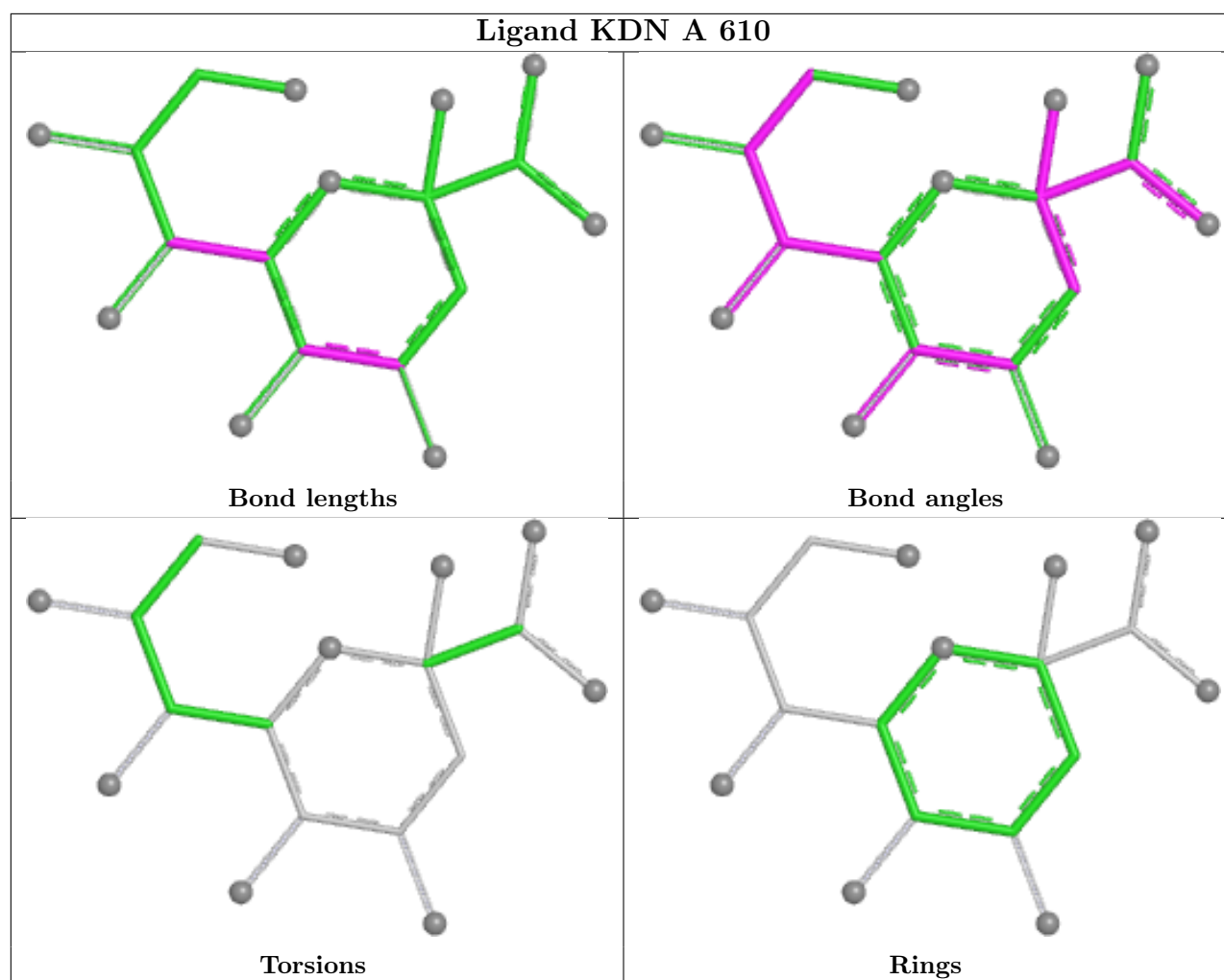
There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	607	GOL	1	0
6	B	605	ACT	2	0
2	A	605	GOL	1	0
2	B	601	GOL	1	0
2	B	607	GOL	1	0
2	B	608	GOL	2	0
2	B	603	GOL	2	0
6	B	602	ACT	1	0
2	A	608	GOL	2	0
2	A	609	GOL	4	0
4	A	603	TRS	5	0
6	B	606	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/511 (97%)	0.59	18 (3%) 46 45	12, 21, 35, 46	4 (0%)
1	B	496/511 (97%)	0.62	16 (3%) 50 49	12, 22, 34, 48	5 (1%)
All	All	993/1022 (97%)	0.60	34 (3%) 48 47	12, 21, 34, 48	9 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ILE	4.0
1	B	26	ARG	4.0
1	A	433	VAL	3.8
1	B	419	GLU	3.3
1	B	25	ARG	3.0
1	A	434	ALA	2.9
1	A	435	ILE	2.9
1	A	421	GLY	2.9
1	A	501	ARG	2.9
1	A	77	ASP	2.8
1	A	401	THR	2.8
1	B	77	ASP	2.7
1	B	432	GLY	2.7
1	B	135	TYR	2.7
1	A	26	ARG	2.7
1	A	87	GLU	2.6
1	B	420	PRO	2.4
1	A	25	ARG	2.3
1	A	30	GLU	2.3
1	B	500	ILE	2.3
1	B	296	GLU	2.3
1	A	315	ASP	2.3
1	A	432	GLY	2.3
1	A	236	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	435	ILE	2.2
1	B	473	LEU	2.2
1	A	300	VAL	2.1
1	B	115	ARG	2.1
1	B	355	GLU	2.1
1	B	27	LEU	2.1
1	A	85	PRO	2.1
1	B	319	PHE	2.1
1	A	158	PRO	2.0
1	A	135	TYR	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SCN	A	602	3/3	0.73	0.19	33,33,36,42	0
2	GOL	A	601	6/6	0.74	0.22	39,40,41,42	0
6	ACT	B	605	4/4	0.75	0.25	44,45,46,46	0
6	ACT	B	606	4/4	0.77	0.14	31,32,32,34	0
3	SCN	A	606	3/3	0.78	0.21	60,60,62,71	0
6	ACT	B	602	4/4	0.79	0.17	38,39,39,39	0
3	SCN	B	604	3/3	0.81	0.18	53,53,56,64	0
2	GOL	B	607	6/6	0.81	0.14	46,46,47,48	0
2	GOL	A	609	6/6	0.82	0.13	34,36,36,37	0
2	GOL	B	601	6/6	0.83	0.15	39,40,41,44	0
2	GOL	A	607	6/6	0.84	0.15	36,37,38,42	0
2	GOL	A	605	6/6	0.85	0.16	29,31,32,38	0
2	GOL	B	608	6/6	0.85	0.17	37,38,40,41	0

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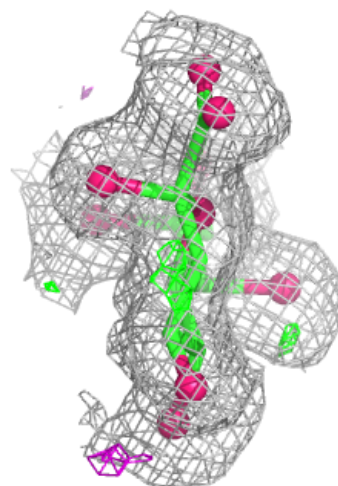
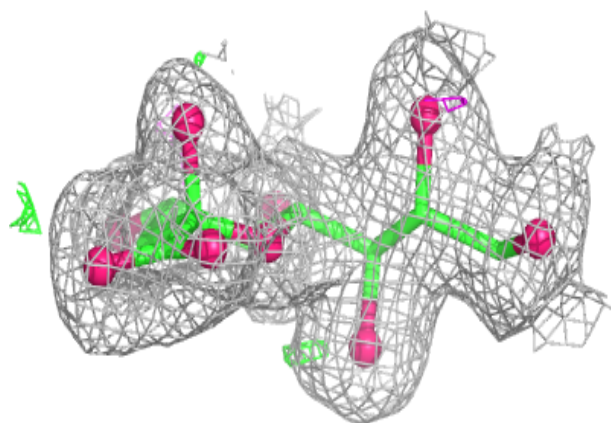
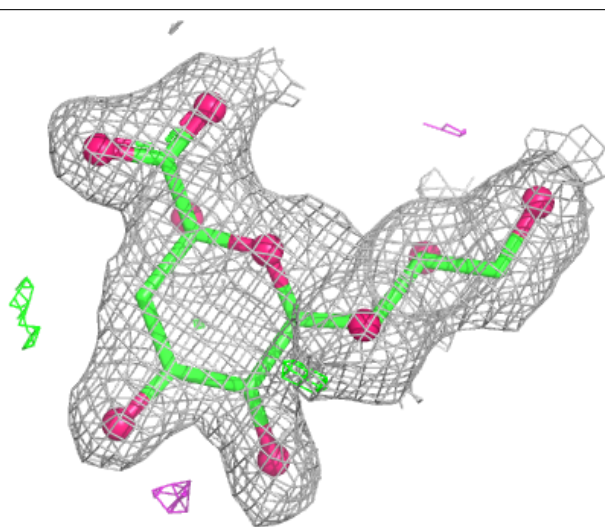
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	608	6/6	0.86	0.14	27,31,32,33	0
2	GOL	A	604	6/6	0.86	0.12	22,24,24,28	0
4	TRS	A	603	8/8	0.86	0.13	27,27,28,28	0
2	GOL	B	603	6/6	0.89	0.10	22,22,24,28	0
5	KDN	B	609	18/18	0.92	0.08	15,19,20,21	0
5	KDN	A	610	18/18	0.92	0.08	15,17,18,19	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.

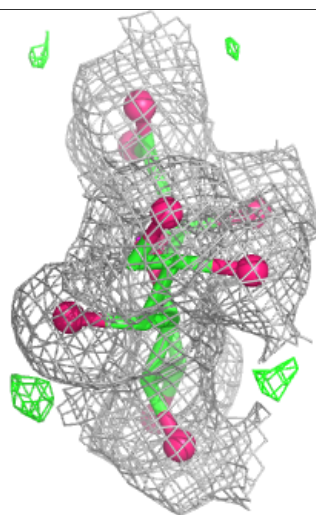
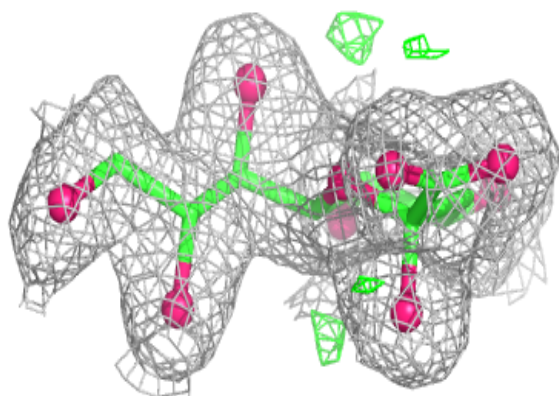
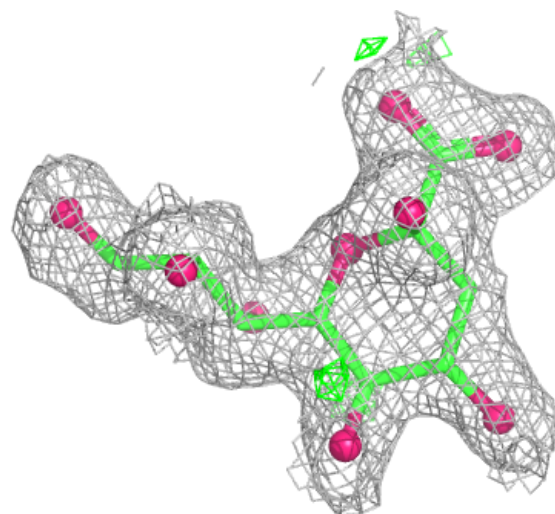
Electron density around KDN B 609:

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 KDN A 610:

$2mF_o-DF_c$ (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.