



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:41 PM UTC

PDB ID : 6SXV / pdb_00006sxv
Title : GH51 a-l-arabinofuranosidase soaked with aziridine inhibitor
Authors : McGregor, N.G.S.; Davies, G.J.
Deposited on : 2019-09-26
Resolution : 1.40 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 ⓘ](#)) 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

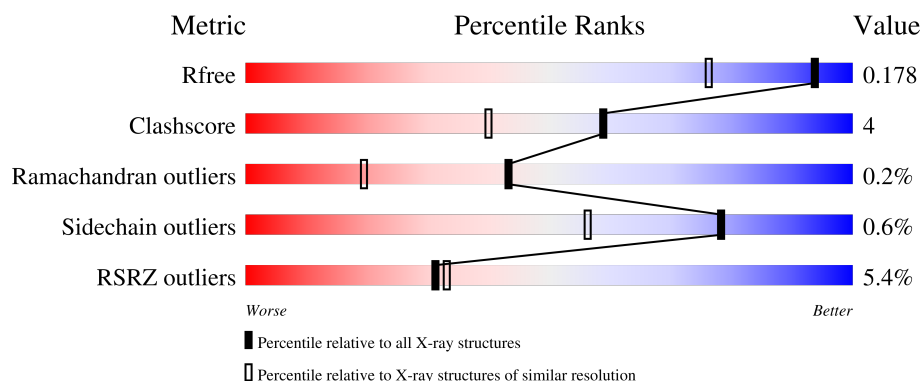
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	502	9% 85% 14% ..
1	B	502	2% 87% 13%

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
6	ETE	B	605	-	-	X	-

2 Entry composition [i](#)

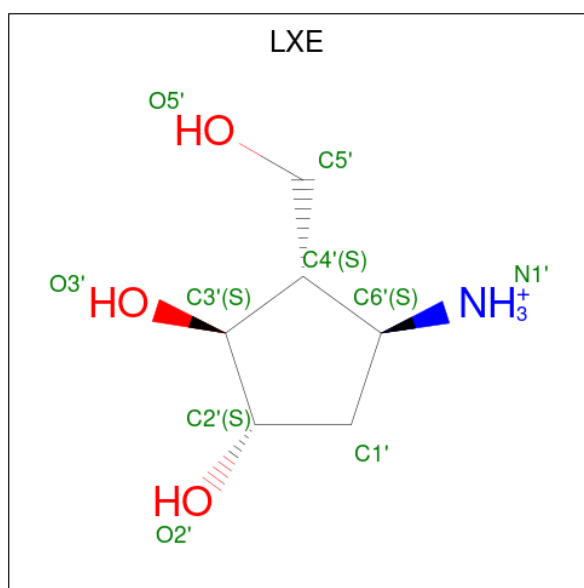
There are 7 unique types of molecules in this entry. The entry contains 16868 atoms, of which 7938 are hydrogens and 0 are deuteriums.

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 GH51 α -l-arabinofuranosidase.

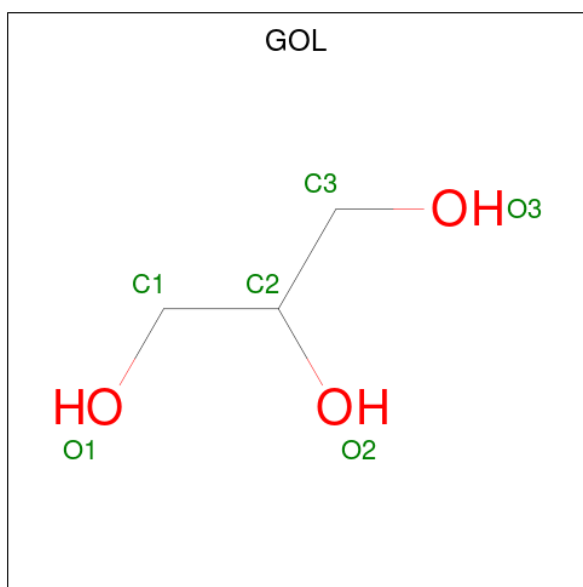
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	499	Total	C	H	N	O	S	222	17	0
			7865	2556	3896	665	722	26			
1	B	500	Total	C	H	N	O	S	220	16	1
			7876	2558	3894	665	734	25			

- Molecule 2 is [(1 {S},2 {S},3 {S},4 {S})-2-(hydroxymethyl)-3,4-bis(oxidanyl)cyclopentyl]azanium (CCD ID: LXE) (formula: $C_6H_{14}NO_3$) (labeled as "Ligand of Interest" by depositor).



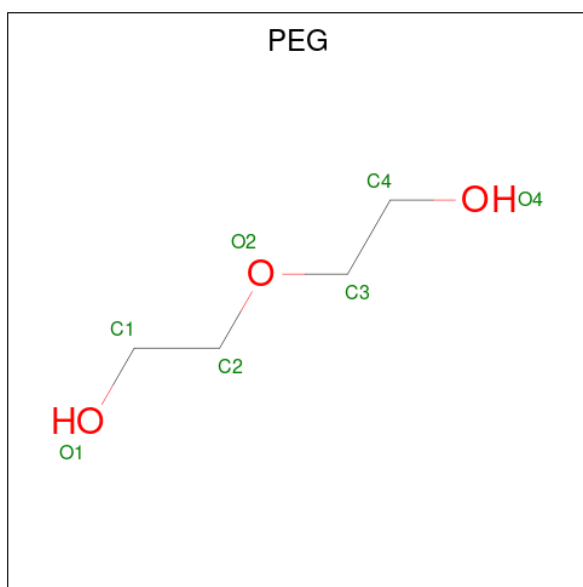
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	2	0
			23	6	13	1	3		
2	B	1	Total	C	H	N	O	2	0
			23	6	13	1	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



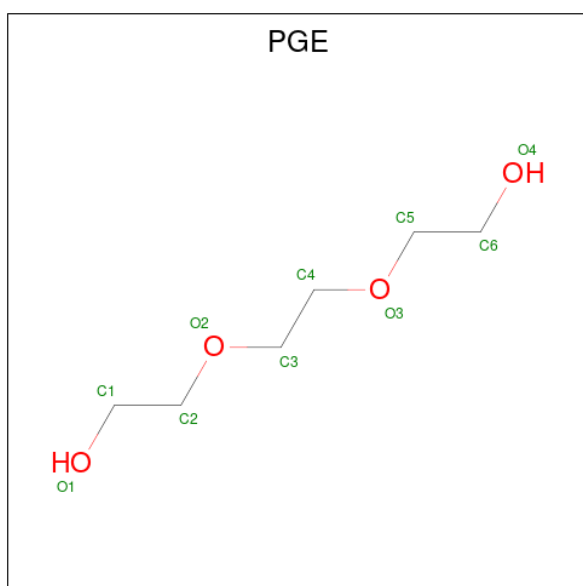
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			17	4	10	3		
4	B	1	Total	C	H	O	1	1
			12	3	7	2		

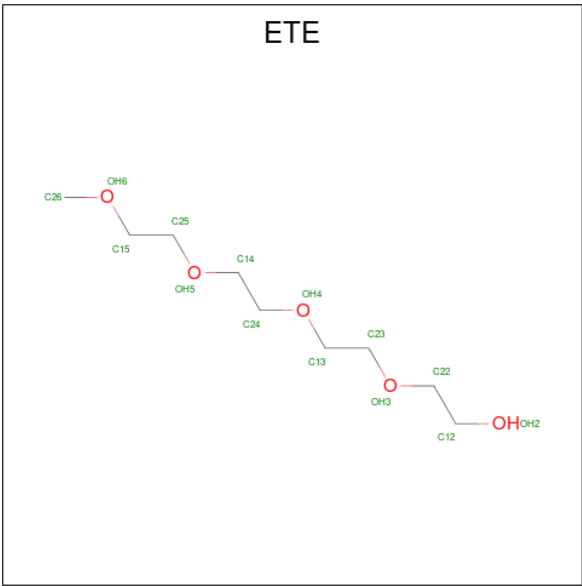
- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 6 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD

ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			33	9	19	5		

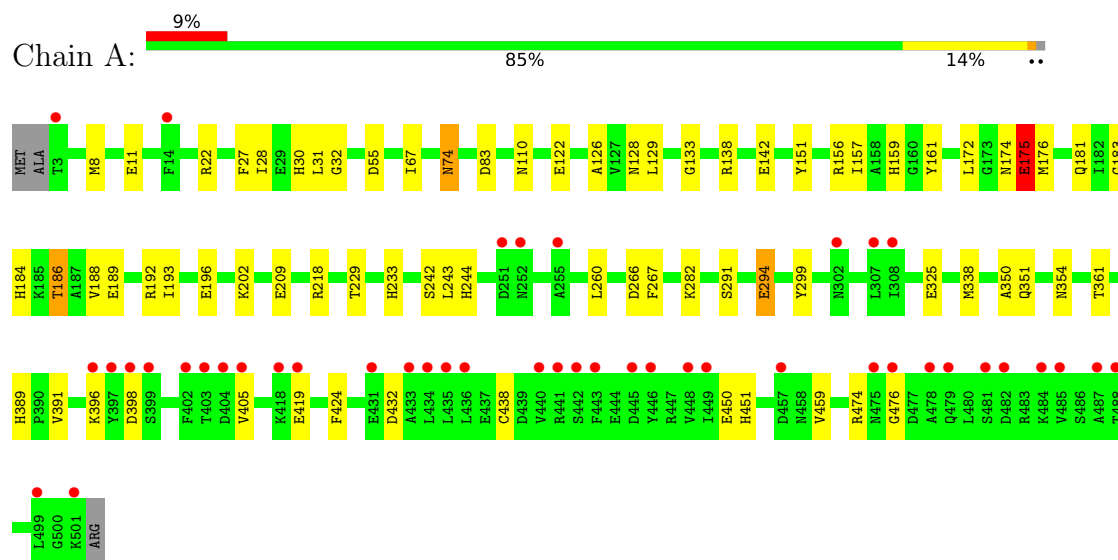
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	427	Total	O	0	5
			432	432		
7	B	432	Total	O	0	5
			437	437		

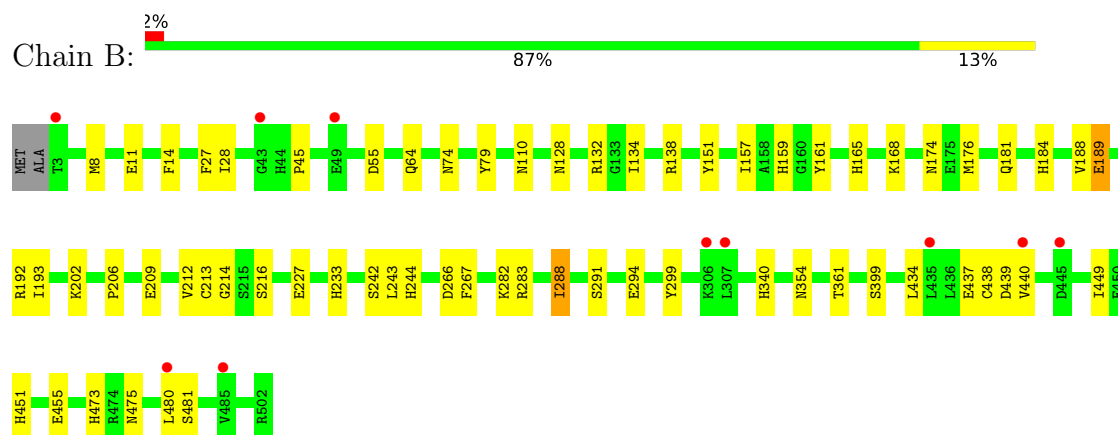
3 Residue-property plots

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: GH51 a-l-arabinofuranosidase



• Molecule 1: GH51 a-l-arabinofuranosidase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	178.99Å 178.99Å 100.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 1.40 29.85 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.85-1.40) 99.6 (29.85-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.170 , 0.178 0.170 , 0.178	Depositor DCC
R_{free} test set	12425 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16868	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: LXE, ETE, PEG, GOL, PGE

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	1.39	16/4126 (0.4%)	1.41	30/5622 (0.5%)
1	B	1.36	19/4123 (0.5%)	1.35	19/5616 (0.3%)
All	All	1.37	35/8249 (0.4%)	1.38	49/11238 (0.4%)

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
1	B	0	1
All	All	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	HIS	CE1-NE2	12.64	1.45	1.32
1	B	159	HIS	CE1-NE2	8.87	1.41	1.32
1	B	437	GLU	C-O	-8.52	1.14	1.24
1	A	175	GLU	CD-OE1	8.44	1.41	1.25
1	B	288	ILE	CG1-CD1	-7.48	1.22	1.51
1	B	451	HIS	CE1-NE2	7.16	1.39	1.32
1	A	133	GLY	C-O	6.94	1.30	1.24
1	B	193	ILE	N-CA	6.74	1.55	1.46
1	A	129	LEU	C-O	6.68	1.33	1.24
1	A	193	ILE	N-CA	6.66	1.55	1.46
1	A	189	GLU	N-CA	6.55	1.54	1.46
1	B	439	ASP	CG-OD2	-5.97	1.14	1.25
1	A	126	ALA	C-O	5.87	1.30	1.23
1	A	157	ILE	N-CA	5.84	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ARG	CA-C	5.83	1.60	1.52
1	A	432	ASP	C-O	5.78	1.31	1.24
1	B	282	LYS	CG-CD	-5.74	1.35	1.52
1	B	244	HIS	CD2-NE2	5.72	1.44	1.37
1	B	266	ASP	CG-OD1	-5.67	1.14	1.25
1	A	157	ILE	C-O	5.57	1.30	1.24
1	B	216	SER	CA-CB	-5.57	1.43	1.53
1	A	83	ASP	C-O	5.50	1.31	1.24
1	B	244	HIS	CG-ND1	5.43	1.44	1.38
1	B	244	HIS	CE1-NE2	5.40	1.38	1.32
1	B	294	GLU	CD-OE2	5.36	1.35	1.25
1	A	282	LYS	CG-CD	-5.34	1.36	1.52
1	B	79	TYR	N-CA	5.28	1.52	1.46
1	B	434	LEU	C-O	5.27	1.30	1.24
1	B	157	ILE	C-O	5.25	1.30	1.24
1	A	196	GLU	CA-C	5.21	1.59	1.52
1	A	184	HIS	ND1-CE1	5.14	1.37	1.32
1	B	189	GLU	C-O	5.13	1.29	1.24
1	B	45	PRO	C-O	-5.12	1.17	1.24
1	B	340	HIS	CE1-NE2	5.07	1.37	1.32
1	A	294	GLU	CD-OE2	5.01	1.34	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ASP	CB-CA-C	9.04	127.14	109.33
1	B	449	ILE	N-CA-C	-8.18	103.84	111.45
1	B	192	ARG	O-C-N	7.36	129.65	122.07
1	A	229	THR	O-C-N	7.15	129.43	122.07
1	A	128	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	192	ARG	O-C-N	6.42	128.68	122.07
1	B	27[A]	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	27[B]	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	159	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	A	11[A]	GLU	CB-CG-CD	6.33	123.36	112.60
1	A	11[B]	GLU	CB-CG-CD	6.33	123.36	112.60
1	A	55	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	267	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	172	LEU	O-C-N	-5.93	114.56	122.38
1	A	159	HIS	CG-CD2-NE2	5.92	113.12	107.20
1	B	188	VAL	O-C-N	5.90	128.03	121.90
1	B	267	PHE	CA-CB-CG	5.88	119.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASN	CB-CG-ND2	5.76	125.03	116.40
1	A	398	ASP	N-CA-C	-5.75	100.51	109.72
1	B	151	TYR	O-C-N	-5.75	115.93	122.08
1	A	138	ARG	O-C-N	5.74	128.21	122.12
1	B	159	HIS	CG-CD2-NE2	5.72	112.92	107.20
1	A	27[A]	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	27[B]	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	55	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	233	HIS	CA-C-O	-5.58	112.74	119.27
1	A	183	GLY	O-C-N	5.51	127.59	122.57
1	A	142	GLU	O-C-N	5.50	127.73	122.07
1	B	159	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
1	A	186	THR	O-C-N	-5.44	116.26	122.68
1	A	151	TYR	O-C-N	-5.42	116.28	122.08
1	A	233	HIS	CA-C-O	-5.42	112.92	119.27
1	B	192	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	142	GLU	CA-C-O	-5.41	115.14	120.82
1	A	196	GLU	CA-C-O	-5.39	113.77	119.97
1	A	175	GLU	CA-C-O	-5.36	116.06	122.27
1	A	419	GLU	CB-CA-C	5.35	119.03	111.86
1	B	128	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	288	ILE	CB-CG1-CD1	5.23	124.78	113.80
1	B	227	GLU	CA-C-O	5.14	126.40	120.90
1	A	30	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
1	A	188	VAL	O-C-N	5.13	127.23	121.90
1	B	138	ARG	O-C-N	5.12	127.55	122.12
1	A	192	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	A	74	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	B	134	ILE	CA-C-O	-5.05	115.50	120.85
1	A	156	ARG	O-C-N	5.04	127.46	122.12
1	B	399	SER	CA-C-N	5.01	127.24	120.38
1	B	399	SER	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Mainchain
1	B	132	ARG	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	3969	3896	3814	33	0
1	B	3982	3894	3806	29	0
2	A	10	13	0	0	0
2	B	10	13	0	0	0
3	A	30	40	40	3	0
3	B	24	32	32	0	0
4	A	7	10	10	0	0
4	B	5	7	0	0	0
5	A	10	14	14	2	0
6	B	14	19	20	9	0
7	A	432	0	0	9	0
7	B	437	0	0	10	0
All	All	8930	7938	7736	70	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 4.

All (70) 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)
6:B:605:ETE:H262	7:B:1054:HOH:O	1.48	1.14
1:B:202[A]:LYS:HD2	7:B:776:HOH:O	1.68	0.92
1:A:202:LYS:HD2	7:A:866:HOH:O	1.69	0.91
1:B:213[C]:CYS:CA	1:B:214:GLY:N	2.36	0.88
1:B:473:HIS:HD2	1:B:475:ASN:H	1.22	0.86
1:B:212:VAL:C	1:B:213[C]:CYS:CA	2.48	0.86
1:B:202[B]:LYS:HE3	7:B:787:HOH:O	1.80	0.81
1:A:354:ASN:HD21	1:A:361:THR:H	1.29	0.79
1:B:354:ASN:HD21	1:B:361:THR:H	1.29	0.78
1:A:260:LEU:HD11	3:A:607:GOL:H11	1.67	0.76
6:B:605:ETE:H122	7:B:1067:HOH:O	1.87	0.74
1:A:266:ASP:OD2	7:A:703:HOH:O	2.13	0.66
3:A:602:GOL:O2	7:A:702:HOH:O	2.08	0.66
1:A:28:ILE:HD13	7:A:939:HOH:O	1.97	0.64
1:A:260:LEU:HD11	3:A:607:GOL:C1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:GLU:OE2	1:B:473:HIS:HE1	1.83	0.60
1:B:202[B]:LYS:CE	7:B:787:HOH:O	2.44	0.57
1:A:218[B]:ARG:NE	7:A:703:HOH:O	2.21	0.56
6:B:605:ETE:C26	7:B:966:HOH:O	2.55	0.55
6:B:605:ETE:H121	7:B:1011:HOH:O	2.05	0.55
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.56	0.54
1:B:174:ASN:HD22	1:B:181:GLN:HE22	1.55	0.53
1:A:218[B]:ARG:HH11	1:A:218[B]:ARG:HG3	1.74	0.52
1:B:28:ILE:HD13	7:B:986:HOH:O	2.09	0.52
5:A:604:PGE:H62	7:A:768:HOH:O	2.09	0.52
6:B:605:ETE:H142	7:B:814:HOH:O	2.12	0.49
1:B:189:GLU:OE2	6:B:605:ETE:H252	2.12	0.49
1:B:11[A]:GLU:HG2	1:B:14:PHE:HD2	1.79	0.48
1:A:451:HIS:CG	1:A:476:GLY:HA3	2.49	0.47
1:A:186:THR:HG22	5:A:604:PGE:H1	1.96	0.47
6:B:605:ETE:C23	6:B:605:ETE:OH2	2.63	0.47
1:A:450:GLU:OE1	1:A:474:ARG:NE	2.44	0.47
1:B:242:SER:HA	1:B:291:SER:O	2.14	0.47
1:B:202[B]:LYS:HD2	1:B:206:PRO:HA	1.97	0.47
1:B:110:ASN:HB3	1:B:161:TYR:CZ	2.50	0.47
1:B:8:MET:O	1:B:438:CYS:HA	2.15	0.47
1:A:338[B]:MET:HE1	1:A:424:PHE:CE2	2.50	0.46
1:A:244[B]:HIS:CE1	7:A:781:HOH:O	2.68	0.46
1:A:243:LEU:HD12	1:A:243:LEU:N	2.31	0.46
1:A:354:ASN:HD21	1:A:361:THR:N	2.05	0.46
1:B:168:LYS:HE3	1:B:209[B]:GLU:HG3	1.98	0.45
1:A:389:HIS:HE1	7:A:1076:HOH:O	1.99	0.45
1:A:74:ASN:HA	1:A:181:GLN:HE22	1.81	0.45
1:B:184:HIS:NE2	6:B:605:ETE:C22	2.80	0.44
1:A:391:VAL:HG23	1:B:14:PHE:CE1	2.53	0.44
1:B:11[A]:GLU:CG	1:B:14:PHE:HD2	2.30	0.44
1:A:174:ASN:HD22	1:A:181:GLN:NE2	2.16	0.44
1:B:354:ASN:ND2	1:B:361:THR:H	2.05	0.44
1:B:480:LEU:C	1:B:480:LEU:HD23	2.43	0.44
1:A:325:GLU:HB3	1:A:459:VAL:HB	2.00	0.43
7:A:1005:HOH:O	1:B:283:ARG:CD	2.66	0.43
1:A:396:LYS:HA	1:A:405:VAL:O	2.19	0.43
1:A:110:ASN:HB3	1:A:161:TYR:CZ	2.54	0.43
1:A:174:ASN:O	1:A:175:GLU:C	2.61	0.43
1:A:8:MET:O	1:A:438:CYS:HA	2.19	0.42
1:A:244[A]:HIS:CG	1:A:294:GLU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:605:ETE:H251	7:B:814:HOH:O	2.19	0.42
1:B:440:VAL:HG21	1:B:480:LEU:HD11	2.00	0.42
1:A:22:ARG:NH1	1:A:209[B]:GLU:OE2	2.49	0.42
1:B:11[A]:GLU:HG2	1:B:14:PHE:CD2	2.54	0.42
1:A:31:LEU:HD23	1:A:32:GLY:N	2.35	0.42
1:A:242:SER:HA	1:A:291:SER:O	2.20	0.41
1:B:243:LEU:N	1:B:243:LEU:HD12	2.36	0.41
1:A:67:ILE:HG13	1:A:122:GLU:HG3	2.02	0.41
1:A:350:ALA:HA	1:A:351:GLN:HA	1.89	0.41
1:B:74:ASN:HA	1:B:181:GLN:HE22	1.85	0.41
1:B:174:ASN:HD22	1:B:181:GLN:NE2	2.16	0.41
1:A:244[B]:HIS:HB3	1:A:294:GLU:HB3	2.03	0.41
1:B:110:ASN:ND2	1:B:165:HIS:NE2	2.69	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/502 (103%)	496 (96%)	18 (4%)	1 (0%)	43	19
1	B	515/502 (103%)	494 (96%)	20 (4%)	1 (0%)	43	19
All	All	1030/1004 (103%)	990 (96%)	38 (4%)	2 (0%)	43	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	TYR
1	A	299	TYR

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	409/434 (94%)	407 (100%)	2 (0%)	81	61
1	B	411/434 (95%)	405 (98%)	6 (2%)	57	26
All	All	820/868 (94%)	812 (99%)	8 (1%)	78	40

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176[A]	MET
1	A	176[B]	MET
1	B	64[A]	GLN
1	B	64[B]	GLN
1	B	176[A]	MET
1	B	176[B]	MET
1	B	288	ILE
1	B	481	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	110	ASN
1	A	181	GLN
1	A	354	ASN
1	A	389	HIS
1	B	110	ASN
1	B	181	GLN
1	B	219	ASN
1	B	354	ASN
1	B	364	ASN
1	B	473	HIS
1	B	475	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	607	-	5,5,5	0.88	0	5,5,5	1.01	0
5	PGE	A	604	-	9,9,9	0.63	0	8,8,8	0.64	0
3	GOL	A	602	-	5,5,5	0.65	0	5,5,5	1.12	0
3	GOL	B	602	-	5,5,5	0.74	0	5,5,5	1.45	1 (20%)
4	PEG	A	603	-	6,6,6	0.87	0	5,5,5	0.47	0
3	GOL	A	608	-	5,5,5	0.79	0	5,5,5	1.05	0
2	LXE	B	601	1	10,10,10	1.02	0	7,14,14	2.28	2 (28%)
3	GOL	A	606	-	5,5,5	0.43	0	5,5,5	0.54	0
3	GOL	B	604	-	5,5,5	0.17	0	5,5,5	0.34	0
3	GOL	A	605	-	5,5,5	0.46	0	5,5,5	0.58	0
6	ETE	B	605	-	13,13,13	0.80	0	12,12,12	1.03	1 (8%)
2	LXE	A	601	1	10,10,10	1.83	2 (20%)	7,14,14	1.96	2 (28%)
3	GOL	A	607	-	5,5,5	0.18	0	5,5,5	0.91	0
3	GOL	B	606	-	5,5,5	0.35	0	5,5,5	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	607	-	-	3/4/4/4	-
5	PGE	A	604	-	-	4/7/7/7	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
4	PEG	A	603	-	-	2/4/4/4	-
3	GOL	A	608	-	-	1/4/4/4	-
2	LXE	B	601	1	-	0/2/18/18	0/1/1/1
3	GOL	A	606	-	-	2/4/4/4	-
3	GOL	B	604	-	-	1/4/4/4	-
3	GOL	A	605	-	-	3/4/4/4	-
6	ETE	B	605	-	-	6/11/11/11	-
2	LXE	A	601	1	-	0/2/18/18	0/1/1/1
3	GOL	A	607	-	-	2/4/4/4	-
3	GOL	B	606	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	LXE	C5'-C4'	3.92	1.58	1.52
2	A	601	LXE	O2'-C2'	2.94	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LXE	C1'-C6'-C4'	4.70	107.60	103.09
2	A	601	LXE	C1'-C6'-C4'	3.54	106.49	103.09
2	A	601	LXE	O2'-C2'-C3'	3.51	118.33	111.43
2	B	601	LXE	O2'-C2'-C3'	2.99	117.32	111.43
3	B	602	GOL	O2-C2-C3	2.04	117.61	109.18
6	B	605	ETE	OH4-C13-C23	2.03	119.60	110.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	607	GOL	C1-C2-C3-O3
3	A	607	GOL	O2-C2-C3-O3
3	B	607	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	605	ETE	C12-C22-OH3-C23
6	B	605	ETE	OH4-C13-C23-OH3
5	A	604	PGE	O2-C3-C4-O3
3	B	607	GOL	O2-C2-C3-O3
4	A	603	PEG	O1-C1-C2-O2
6	B	605	ETE	OH2-C12-C22-OH3
3	A	605	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	B	607	GOL	O1-C1-C2-O2
3	A	605	GOL	O2-C2-C3-O3
5	A	604	PGE	C1-C2-O2-C3
4	A	603	PEG	C1-C2-O2-C3
5	A	604	PGE	O1-C1-C2-O2
6	B	605	ETE	C24-C14-OH5-C25
6	B	605	ETE	C23-C13-OH4-C24
6	B	605	ETE	OH5-C14-C24-OH4
3	A	608	GOL	O2-C2-C3-O3
3	B	604	GOL	O2-C2-C3-O3
5	A	604	PGE	C6-C5-O3-C4

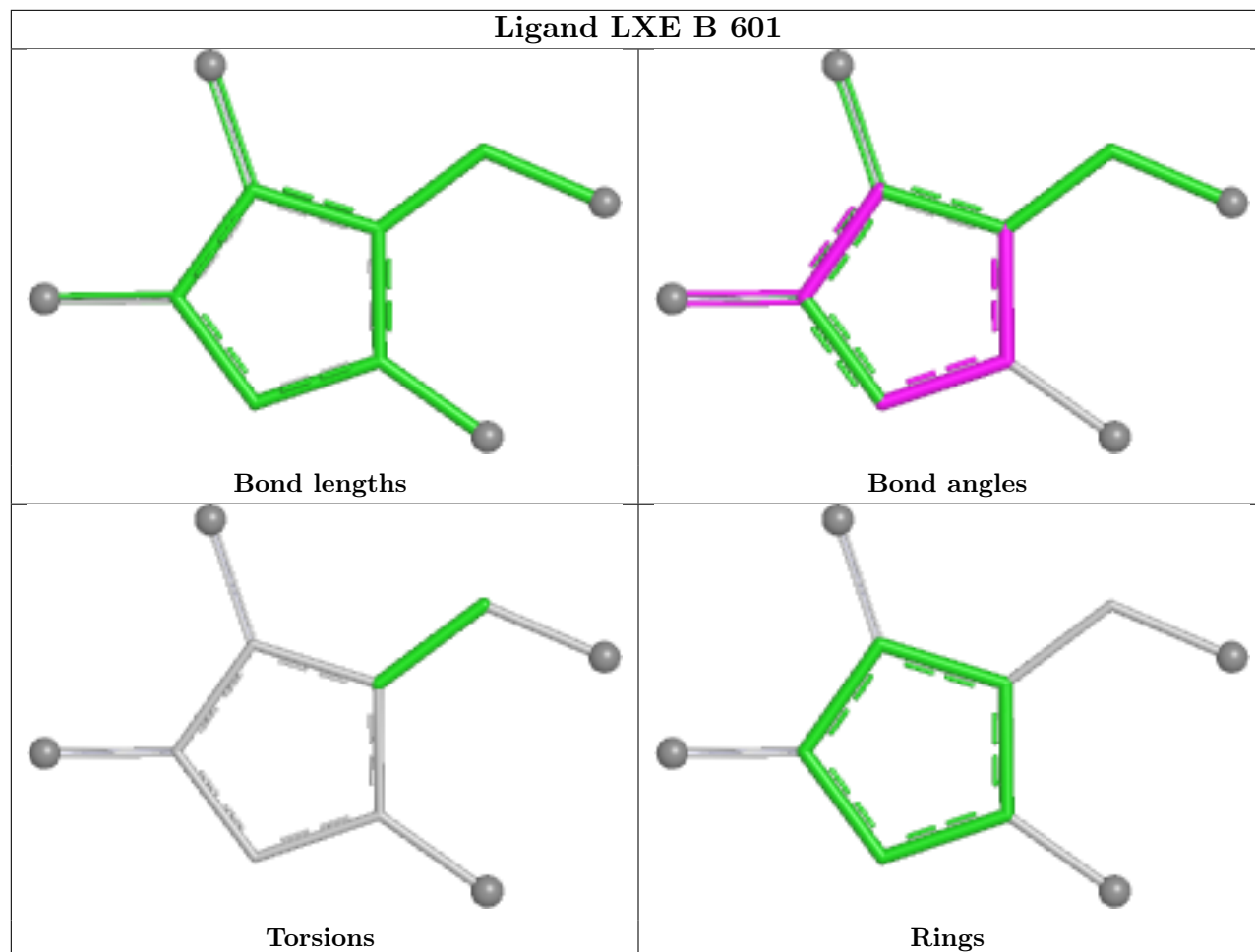
There are no ring outliers.

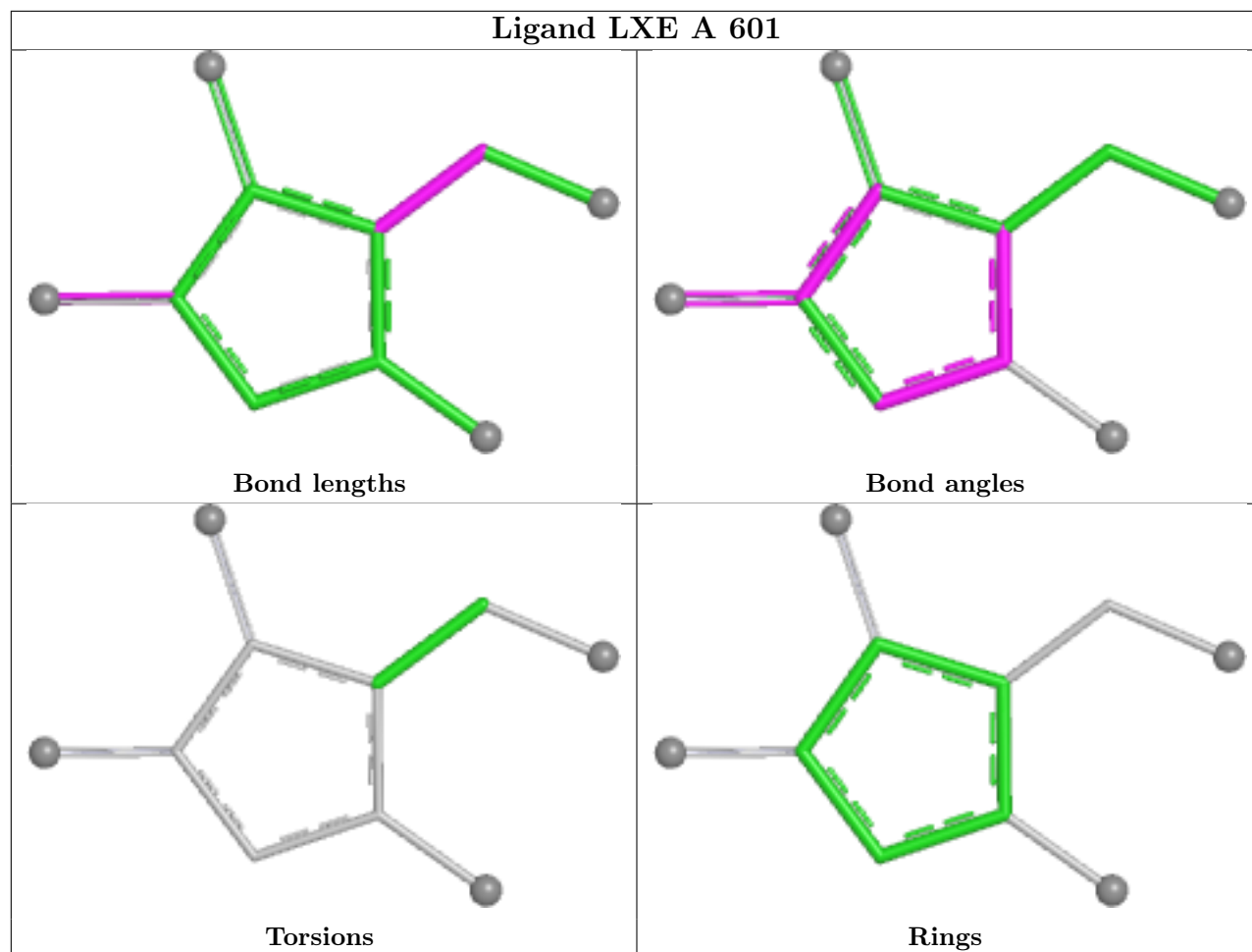
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	PGE	2	0
3	A	602	GOL	1	0
6	B	605	ETE	9	0
3	A	607	GOL	2	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	499/502 (99%)	0.14	44 (8%)	15 15	5, 18, 40, 56	17 (3%)
1	B	500/502 (99%)	-0.15	10 (2%)	65 68	5, 17, 34, 52	16 (3%)
All	All	999/1004 (99%)	-0.01	54 (5%)	31 33	5, 18, 37, 56	33 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LYS	4.9
1	A	398	ASP	4.1
1	A	445	ASP	3.4
1	A	434	LEU	3.2
1	B	480	LEU	3.2
1	A	433	ALA	3.0
1	A	481	SER	3.0
1	A	403	THR	3.0
1	A	308	ILE	2.9
1	B	3	THR	2.9
1	A	482	ASP	2.9
1	A	252	ASN	2.9
1	A	435	LEU	2.9
1	A	485	VAL	2.8
1	A	448	VAL	2.7
1	A	449	ILE	2.7
1	A	446	TYR	2.7
1	A	478	ALA	2.7
1	A	441	ARG	2.7
1	A	307	LEU	2.7
1	B	43	GLY	2.6
1	A	436	LEU	2.6
1	B	485	VAL	2.6
1	A	405	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	479	GLN	2.5
1	B	307	LEU	2.5
1	A	404	ASP	2.5
1	A	442	SER	2.4
1	A	418	LYS	2.4
1	A	3	THR	2.4
1	A	399	SER	2.4
1	A	487	ALA	2.4
1	A	484	LYS	2.4
1	A	443	PHE	2.4
1	A	419	GLU	2.3
1	A	475	ASN	2.3
1	A	255	ALA	2.3
1	A	488	THR	2.3
1	A	14	PHE	2.2
1	B	49	GLU	2.2
1	A	396	LYS	2.2
1	A	457	ASP	2.2
1	A	431	GLU	2.2
1	A	476	GLY	2.2
1	B	445	ASP	2.2
1	A	402	PHE	2.1
1	A	440	VAL	2.1
1	A	251[A]	ASP	2.1
1	B	435	LEU	2.1
1	B	306	LYS	2.1
1	A	302	ASN	2.1
1	B	440	VAL	2.0
1	A	499	LEU	2.0
1	A	397	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

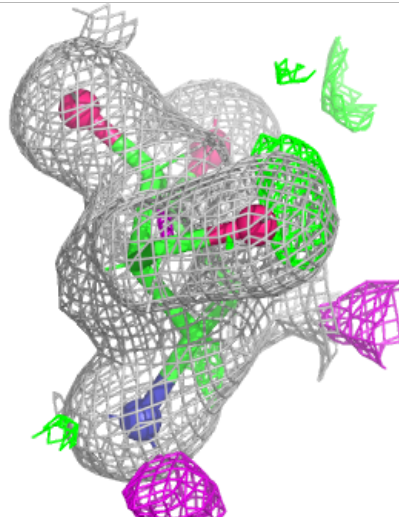
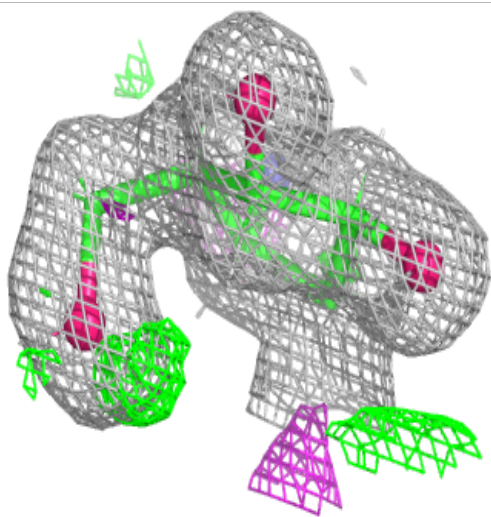
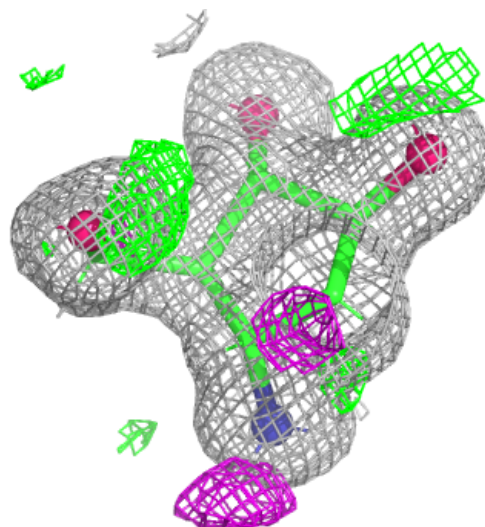
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	607	6/6	0.72	0.24	17,27,32,32	14
3	GOL	A	608	6/6	0.75	0.17	17,25,34,34	14
3	GOL	A	606	6/6	0.75	0.22	51,64,67,67	2
3	GOL	B	602	6/6	0.76	0.19	24,35,45,45	2
3	GOL	A	607	6/6	0.78	0.20	31,42,53,53	14
4	PEG	B	603[A]	5/7	0.79	0.15	25,40,53,53	1
4	PEG	B	603[B]	5/7	0.79	0.15	25,40,53,53	0
6	ETE	B	605	14/14	0.80	0.23	24,29,42,42	33
5	PGE	A	604	10/10	0.83	0.30	16,23,28,35	24
3	GOL	A	605	6/6	0.86	0.17	25,40,53,53	2
3	GOL	A	602	6/6	0.86	0.13	22,28,37,37	2
3	GOL	B	606	6/6	0.88	0.12	30,39,56,56	2
4	PEG	A	603	7/7	0.88	0.13	29,44,51,55	1
3	GOL	B	604	6/6	0.90	0.13	29,36,55,55	2
2	LXE	A	601	10/10	0.96	0.06	13,16,18,22	2
2	LXE	B	601	10/10	0.97	0.05	13,17,18,19	2

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.

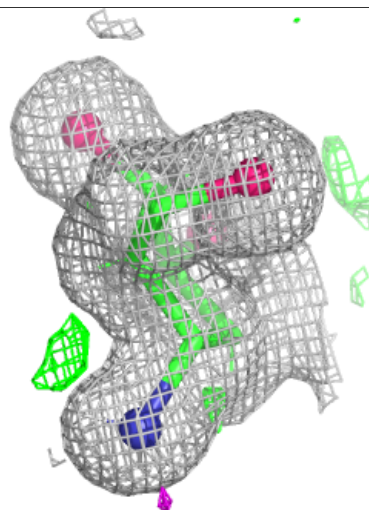
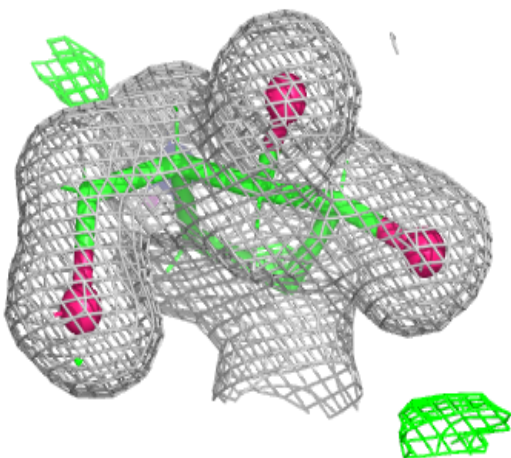
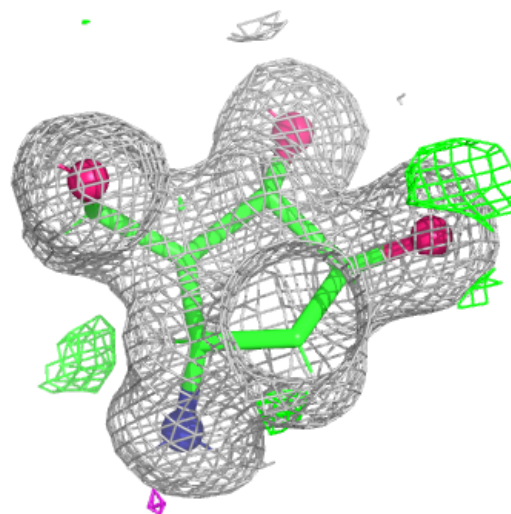
Electron density around LXE A 601:

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



Electron density around LXE B 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.