



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:31 PM EDT

PDB ID : 7A5Q
Title : Crystal structure of VcSiaP bound to sialic acid
Authors : Schneberger, N.; Peter, M.F.; Hagelueken, G.
Deposited on : 2020-08-21
Resolution : 1.68 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

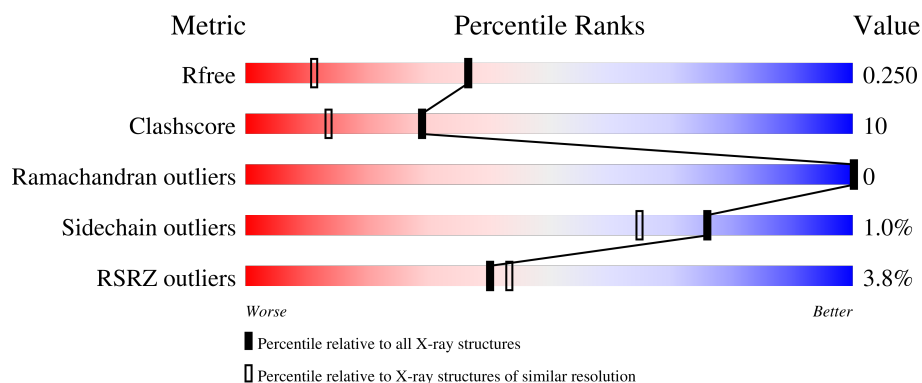
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	299	
1	B	299	

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
3	GOL	A	305	-	-	X	-
3	GOL	A	307	-	-	X	-
3	GOL	B	403	-	-	X	-
3	GOL	B	407	-	X	-	-
3	GOL	B	410	-	-	X	-
5	BGC	B	418	-	-	X	-

2 Entry composition [i](#)

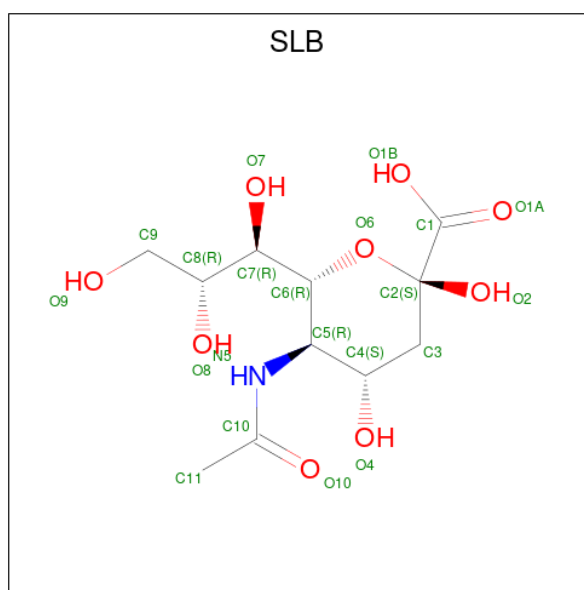
There are 6 unique types of molecules in this entry. The entry contains 5343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DctP family TRAP transporter solute-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	8	0
			2420	1530	405	469	16			
1	B	299	Total	C	N	O	S	0	7	0
			2407	1523	400	468	16			

- Molecule 2 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



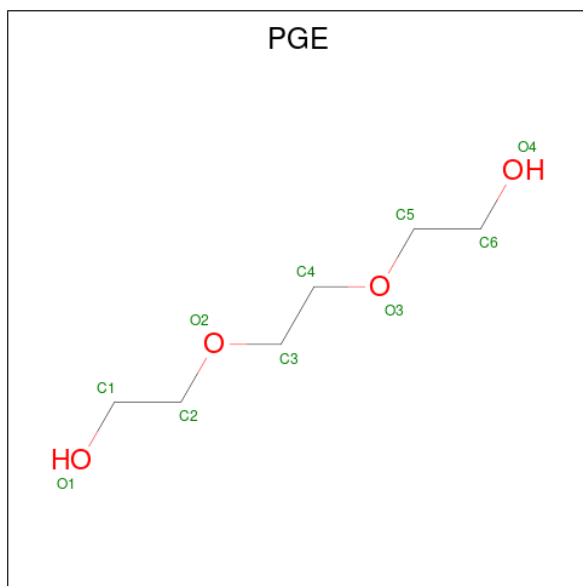
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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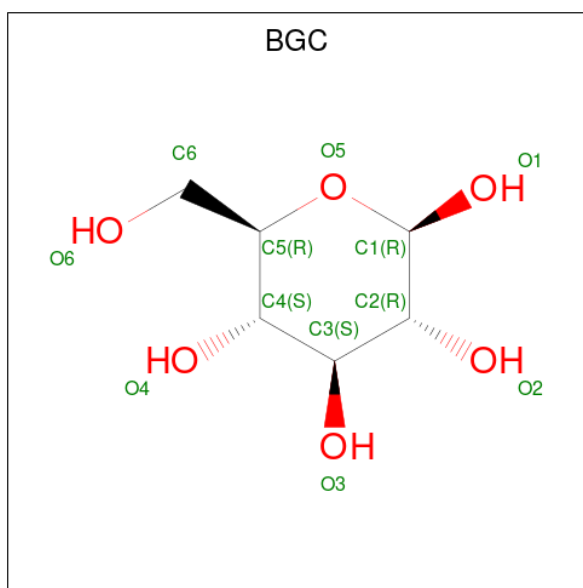
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			12	6	6		

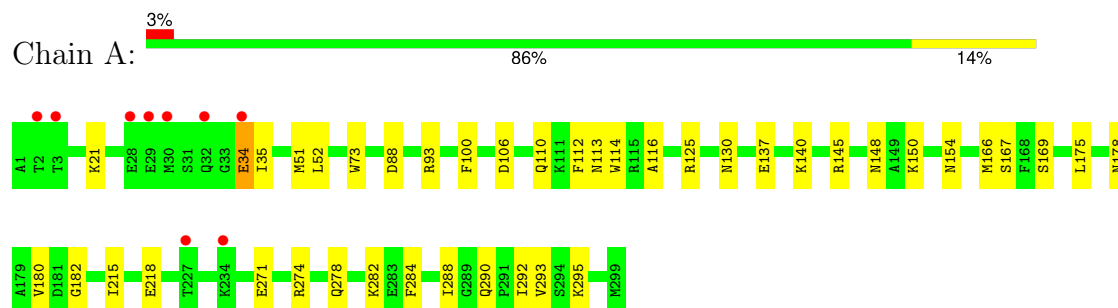
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	137	Total	O	0	0
			137	137		
6	B	167	Total	O	0	0
			167	167		

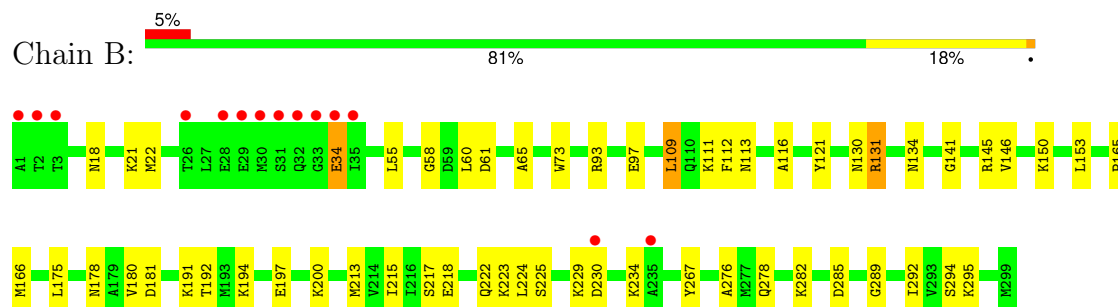
3 Residue-property plots

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: DctP family TRAP transporter solute-binding subunit



- Molecule 1: DctP family TRAP transporter solute-binding subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.35Å 106.74Å 134.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 1.68 45.50 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.50-1.68) 99.5 (45.50-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.247 0.217 , 0.250	Depositor DCC
R_{free} test set	3982 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5343	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7098e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SLB, PGE, GOL, BGC

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	0.77	1/2478 (0.0%)	0.86	3/3348 (0.1%)
1	B	0.85	1/2465 (0.0%)	1.04	4/3332 (0.1%)
All	All	0.81	2/4943 (0.0%)	0.95	7/6680 (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	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	SER	C-N	-6.99	1.18	1.34
1	B	131	ARG	CG-CD	5.11	1.64	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	GLU	OE1-CD-OE2	-28.34	89.30	123.30
1	B	34	GLU	CG-CD-OE1	12.88	144.06	118.30
1	B	34	GLU	CG-CD-OE2	-7.19	103.93	118.30
1	B	292	ILE	CG1-CB-CG2	5.93	124.46	111.40
1	A	125	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	88	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	51	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	109[A]	LEU	Mainchain
1	B	109[B]	LEU	Mainchain
1	B	34	GLU	Sidechain

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	2420	0	2406	35	0
1	B	2407	0	2391	53	0
2	A	21	0	17	0	0
2	B	21	0	17	0	0
3	A	48	0	62	13	0
3	B	90	0	116	18	0
4	A	10	0	14	0	0
4	B	10	0	14	1	0
5	B	12	0	11	6	0
6	A	137	0	0	8	2
6	B	167	0	0	16	2
All	All	5343	0	5048	97	2

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 10.

All (97) 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)
3:B:403:GOL:H12	6:B:606:HOH:O	1.43	1.18
1:B:130:ASN:HD22	1:B:178:ASN:HD21	1.04	0.98
1:B:131:ARG:HE	5:B:418:BGC:H6C2	1.42	0.84
3:B:404:GOL:O1	6:B:501:HOH:O	1.95	0.84
1:A:180:VAL:HG23	6:A:401:HOH:O	1.79	0.83
1:B:225:SER:HB3	3:B:403:GOL:H32	1.58	0.83
1:A:130:ASN:HD22	1:A:178:ASN:HD21	1.30	0.80
1:B:130:ASN:ND2	1:B:178:ASN:HD21	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:N	6:A:401:HOH:O	2.18	0.77
1:A:175:LEU:HD23	6:A:401:HOH:O	1.85	0.76
1:B:131:ARG:HE	5:B:418:BGC:C6	1.99	0.75
1:A:167[A]:SER:H	3:A:307:GOL:H12	1.56	0.71
1:B:285:ASP:OD2	6:B:502:HOH:O	2.09	0.71
1:B:294:SER:OG	6:B:502:HOH:O	2.10	0.70
1:A:167[B]:SER:H	3:A:307:GOL:H12	1.57	0.69
1:B:21:LYS:NZ	6:B:509:HOH:O	2.26	0.68
1:B:223:LYS:O	3:B:403:GOL:H11	1.93	0.68
1:B:18:ASN:OD1	6:B:501:HOH:O	2.11	0.68
1:B:130:ASN:HD22	1:B:178:ASN:ND2	1.86	0.68
3:B:402:GOL:H2	6:B:556:HOH:O	1.94	0.67
1:A:150:LYS:NZ	3:A:306:GOL:O2	2.24	0.66
1:B:294:SER:OG	6:B:503:HOH:O	2.14	0.66
1:B:131:ARG:NE	5:B:418:BGC:H6C2	2.12	0.64
1:B:181:ASP:OD2	5:B:418:BGC:H6C1	1.98	0.64
1:A:271:GLU:HG3	1:A:274[B]:ARG:NH1	2.14	0.62
1:B:230:ASP:OD2	1:B:234:LYS:HE2	2.01	0.61
1:A:154:ASN:ND2	3:A:306:GOL:O2	2.32	0.61
1:B:93:ARG:NH1	6:B:514:HOH:O	2.35	0.60
1:A:175:LEU:CD2	6:A:401:HOH:O	2.47	0.60
1:A:166:MET:HA	3:A:307:GOL:H11	1.84	0.59
1:A:148[B]:ASN:HD21	3:A:307:GOL:H32	1.67	0.59
1:A:290:GLN:HE21	1:A:292[A]:ILE:HG13	1.67	0.59
1:B:150:LYS:HE2	1:B:153:LEU:HD22	1.84	0.59
1:A:288:ILE:HD12	1:A:290:GLN:HG3	1.85	0.58
1:B:134:ASN:OD1	3:B:407:GOL:O2	2.22	0.57
1:A:113:ASN:OD1	1:A:218:GLU:HB3	2.04	0.57
1:B:113:ASN:OD1	1:B:218:GLU:HB3	2.06	0.56
1:A:100:PHE:CE1	1:A:292[B]:ILE:HD11	2.42	0.54
1:B:58:GLY:HA2	6:B:544:HOH:O	2.07	0.54
1:B:191:LYS:HZ1	3:B:408:GOL:H2	1.72	0.54
1:B:278:GLN:HE21	1:B:282:LYS:HE3	1.74	0.53
1:A:140:LYS:HD2	3:A:305:GOL:H11	1.91	0.52
1:A:290:GLN:HE21	1:A:292[A]:ILE:CG1	2.22	0.52
1:B:175:LEU:HD23	1:B:180:VAL:HG23	1.91	0.52
1:A:116:ALA:HA	1:A:215:ILE:HD13	1.91	0.52
1:B:224:LEU:O	1:B:229:LYS:NZ	2.43	0.52
1:A:278:GLN:OE1	1:A:278:GLN:HA	2.09	0.52
1:B:116:ALA:HA	1:B:215:ILE:HD13	1.91	0.51
1:B:121:TYR:OH	3:B:409:GOL:H12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:ND2	1:A:178:ASN:HD21	2.04	0.50
1:A:145:ARG:HD3	1:A:145:ARG:C	2.32	0.50
3:A:305:GOL:H12	6:A:448:HOH:O	2.13	0.48
1:B:194:LYS:HD3	1:B:197:GLU:OE2	2.13	0.48
1:B:200:LYS:HA	4:B:417:PGE:H5	1.94	0.48
1:B:289:GLY:O	6:B:504:HOH:O	2.20	0.48
1:A:271:GLU:HG2	1:B:267:TYR:HD1	1.79	0.47
1:B:222:GLN:NE2	6:B:526:HOH:O	2.47	0.47
1:B:93:ARG:O	1:B:97:GLU:HG2	2.15	0.47
1:B:191:LYS:HD2	3:B:410:GOL:H12	1.95	0.47
1:A:137[B]:GLU:OE1	6:A:402:HOH:O	2.21	0.46
1:B:146:VAL:O	1:B:165:PRO:HA	2.16	0.46
1:A:73:TRP:HB3	1:A:112:PHE:CZ	2.51	0.46
1:B:61:ASP:OD2	6:B:505:HOH:O	2.21	0.45
1:B:191:LYS:O	3:B:410:GOL:H12	2.17	0.45
3:B:404:GOL:C1	6:B:501:HOH:O	2.55	0.45
1:A:284:PHE:O	1:A:288:ILE:HG12	2.17	0.45
3:A:305:GOL:H31	6:A:425:HOH:O	2.17	0.44
1:B:191:LYS:NZ	3:B:410:GOL:O1	2.49	0.44
1:B:55:LEU:HD12	1:B:60:LEU:HB3	1.99	0.44
3:A:306:GOL:H12	6:A:477:HOH:O	2.18	0.44
1:A:34:GLU:HG3	1:A:35:ILE:HG13	1.99	0.44
3:A:308:GOL:H11	3:A:309:GOL:C1	2.48	0.44
1:A:106:ASP:O	1:A:110:GLN:HG3	2.18	0.43
1:B:276:ALA:HA	3:B:402:GOL:H32	2.00	0.43
1:B:145:ARG:CG	1:B:166:MET:HG2	2.48	0.43
1:B:121:TYR:CZ	3:B:409:GOL:H12	2.52	0.43
1:A:21:LYS:HD2	1:A:21:LYS:HA	1.66	0.43
1:B:181:ASP:CG	5:B:418:BGC:H6C1	2.38	0.43
3:B:404:GOL:H32	6:B:633:HOH:O	2.17	0.43
1:B:295:LYS:HD3	1:B:295:LYS:HA	1.67	0.43
1:B:22:MET:CE	3:B:413:GOL:H32	2.49	0.43
1:A:292[B]:ILE:HG23	1:A:293:VAL:N	2.34	0.42
1:B:111:LYS:HD2	1:B:112:PHE:CZ	2.54	0.42
1:B:65:ALA:O	1:B:213:MET:HG3	2.19	0.42
1:B:73:TRP:HB3	1:B:112:PHE:CZ	2.54	0.42
1:B:145:ARG:HG3	1:B:166:MET:HG2	2.00	0.42
1:A:295:LYS:HA	1:A:295:LYS:HE2	2.01	0.41
1:A:140:LYS:HB2	3:A:305:GOL:H11	2.02	0.41
1:B:230:ASP:O	1:B:234:LYS:HG3	2.19	0.41
1:A:145:ARG:CG	1:A:166:MET:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:THR:HA	3:B:410:GOL:H2	2.03	0.41
1:B:141:GLY:O	5:B:418:BGC:H3	2.21	0.41
1:B:18:ASN:CG	6:B:501:HOH:O	2.54	0.41
1:B:225:SER:CB	3:B:403:GOL:H32	2.42	0.40
1:A:52:LEU:HB3	1:A:114:TRP:CZ2	2.56	0.40
3:A:308:GOL:H32	3:A:309:GOL:H11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:536:HOH:O	6:B:659:HOH:O[4_445]	2.12	0.08
6:A:525:HOH:O	6:B:568:HOH:O[4_455]	2.16	0.04

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	305/299 (102%)	301 (99%)	4 (1%)	0	100	100
1	B	304/299 (102%)	295 (97%)	9 (3%)	0	100	100
All	All	609/598 (102%)	596 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	267/259 (103%)	264 (99%)	3 (1%)	73	61
1	B	265/259 (102%)	261 (98%)	4 (2%)	65	48
All	All	532/518 (103%)	525 (99%)	7 (1%)	76	54

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

Mol	Chain	Res	Type
1	A	34	GLU
1	A	93	ARG
1	A	282	LYS
1	B	109[A]	LEU
1	B	109[B]	LEU
1	B	217[A]	SER
1	B	217[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	290	GLN
1	B	134	ASN
1	B	178	ASN
1	B	278	GLN
1	B	290	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

28 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	415	-	5,5,5	1.08	0	5,5,5	1.11	0
3	GOL	B	402	-	5,5,5	1.29	1 (20%)	5,5,5	1.02	0
3	GOL	A	307	-	5,5,5	1.14	0	5,5,5	0.89	0
3	GOL	B	408	-	5,5,5	1.07	0	5,5,5	1.18	0
3	GOL	B	414	-	5,5,5	0.70	0	5,5,5	1.32	1 (20%)
3	GOL	B	413	-	5,5,5	1.30	0	5,5,5	1.02	0
3	GOL	A	306	-	5,5,5	1.47	1 (20%)	5,5,5	1.34	0
3	GOL	A	305	-	5,5,5	0.83	0	5,5,5	1.03	0
3	GOL	B	404	-	5,5,5	0.10	0	5,5,5	0.35	0
3	GOL	B	416	-	5,5,5	1.00	0	5,5,5	1.07	0
3	GOL	A	304	-	5,5,5	1.15	0	5,5,5	1.30	0
4	PGE	A	310	-	9,9,9	0.31	0	8,8,8	0.64	0
3	GOL	B	405	-	5,5,5	1.04	0	5,5,5	1.18	0
2	SLB	A	301	-	21,21,21	2.52	6 (28%)	24,31,31	2.32	9 (37%)
3	GOL	A	303	-	5,5,5	0.97	0	5,5,5	1.30	0
3	GOL	B	407	-	5,5,5	3.58	2 (40%)	5,5,5	1.71	1 (20%)
3	GOL	B	411	-	5,5,5	1.19	0	5,5,5	0.99	0
3	GOL	B	409	-	5,5,5	1.44	1 (20%)	5,5,5	0.81	0
3	GOL	B	406	-	5,5,5	0.94	0	5,5,5	1.13	0
3	GOL	B	412	-	5,5,5	1.10	0	5,5,5	0.91	0
5	BGC	B	418	-	12,12,12	1.52	2 (16%)	17,17,17	2.90	8 (47%)
3	GOL	A	309	-	5,5,5	0.77	0	5,5,5	0.84	0
3	GOL	B	410	-	5,5,5	0.97	0	5,5,5	1.17	1 (20%)
4	PGE	B	417	-	9,9,9	0.30	0	8,8,8	0.63	0
3	GOL	A	302	-	5,5,5	0.09	0	5,5,5	0.34	0
2	SLB	B	401	-	21,21,21	2.37	7 (33%)	24,31,31	2.46	9 (37%)
3	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.33	0
3	GOL	A	308	-	5,5,5	0.68	0	5,5,5	1.08	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	415	-	-	2/4/4/4	-
3	GOL	B	402	-	-	4/4/4/4	-
3	GOL	A	307	-	-	4/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	B	414	-	-	4/4/4/4	-
3	GOL	B	413	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	A	305	-	-	4/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	B	416	-	-	2/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-
4	PGE	A	310	-	-	4/7/7/7	-
3	GOL	B	405	-	-	2/4/4/4	-
2	SLB	A	301	-	-	0/20/38/38	0/1/1/1
3	GOL	A	303	-	-	4/4/4/4	-
3	GOL	B	407	-	-	3/4/4/4	-
3	GOL	B	411	-	-	2/4/4/4	-
3	GOL	B	409	-	-	4/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	B	412	-	-	4/4/4/4	-
5	BGC	B	418	-	-	0/2/22/22	0/1/1/1
3	GOL	A	309	-	-	2/4/4/4	-
3	GOL	B	410	-	-	4/4/4/4	-
4	PGE	B	417	-	-	4/7/7/7	-
3	GOL	A	302	-	-	4/4/4/4	-
2	SLB	B	401	-	-	1/20/38/38	0/1/1/1
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	A	308	-	-	4/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	407	GOL	O2-C2	-7.45	1.21	1.43
2	A	301	SLB	C2-C1	7.35	1.64	1.53
2	B	401	SLB	C2-C1	7.31	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SLB	C4-C5	5.79	1.58	1.53
2	A	301	SLB	O2-C2	-3.65	1.34	1.39
5	B	418	BGC	O5-C1	3.60	1.51	1.42
2	B	401	SLB	C7-C6	3.40	1.57	1.52
2	B	401	SLB	O2-C2	-3.25	1.35	1.39
2	A	301	SLB	C5-N5	2.87	1.50	1.45
2	B	401	SLB	O1A-C1	2.85	1.31	1.22
2	B	401	SLB	C3-C2	-2.66	1.48	1.51
2	A	301	SLB	O6-C6	2.58	1.47	1.44
2	B	401	SLB	C6-C5	2.54	1.57	1.53
3	B	407	GOL	O3-C3	-2.48	1.32	1.42
2	B	401	SLB	O6-C6	2.45	1.47	1.44
3	A	306	GOL	O2-C2	-2.42	1.36	1.43
3	B	409	GOL	C1-C2	2.35	1.60	1.51
3	B	402	GOL	O2-C2	-2.35	1.36	1.43
5	B	418	BGC	O1-C1	-2.30	1.32	1.39
2	A	301	SLB	O6-C2	-2.18	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SLB	O6-C6-C5	-6.71	103.70	109.84
5	B	418	BGC	O6-C6-C5	6.45	133.29	111.33
2	A	301	SLB	C3-C2-C1	-5.27	103.05	112.84
5	B	418	BGC	O5-C5-C6	5.11	119.10	106.44
2	A	301	SLB	O1A-C1-C2	-4.98	115.55	123.85
2	B	401	SLB	C3-C2-C1	-4.78	103.95	112.84
5	B	418	BGC	O5-C1-C2	4.63	118.44	110.30
2	A	301	SLB	O6-C6-C5	-4.42	105.80	109.84
5	B	418	BGC	O5-C5-C4	-3.79	102.87	109.70
3	B	407	GOL	O2-C2-C3	3.76	124.73	109.18
2	A	301	SLB	C8-C7-C6	-3.55	106.39	113.05
2	B	401	SLB	O10-C10-N5	3.46	128.10	121.98
2	B	401	SLB	C8-C7-C6	-3.32	106.81	113.05
2	B	401	SLB	O2-C2-C3	3.27	114.40	109.44
2	A	301	SLB	C6-C5-N5	-3.13	105.91	110.91
5	B	418	BGC	C1-O5-C5	-2.99	107.88	113.65
2	B	401	SLB	O9-C9-C8	-2.84	105.19	111.16
5	B	418	BGC	C4-C3-C2	-2.83	105.86	110.83
2	A	301	SLB	O2-C2-O6	2.83	116.64	109.51
2	B	401	SLB	C3-C4-C5	-2.63	105.66	109.72
5	B	418	BGC	O1-C1-O5	-2.59	102.73	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	414	GOL	C3-C2-C1	-2.57	102.36	111.80
2	B	401	SLB	O2-C2-O6	2.45	115.67	109.51
5	B	418	BGC	O4-C4-C5	2.27	114.91	109.32
3	B	410	GOL	C3-C2-C1	-2.15	103.91	111.80
2	A	301	SLB	O2-C2-C3	2.14	112.68	109.44
2	B	401	SLB	O2-C2-C1	-2.14	106.22	110.73
2	A	301	SLB	C4-C5-N5	-2.06	106.38	110.44
2	A	301	SLB	O2-C2-C1	-2.02	106.45	110.73

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	A	304	GOL	O1-C1-C2-C3
3	A	307	GOL	C1-C2-C3-O3
3	A	308	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	B	403	GOL	O1-C1-C2-C3
3	B	407	GOL	C1-C2-C3-O3
3	B	409	GOL	C1-C2-C3-O3
3	B	410	GOL	C1-C2-C3-O3
3	B	413	GOL	C1-C2-C3-O3
3	B	414	GOL	C1-C2-C3-O3
3	B	414	GOL	O2-C2-C3-O3
3	B	415	GOL	O1-C1-C2-C3
3	B	416	GOL	C1-C2-C3-O3
4	B	417	PGE	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-C3
3	A	303	GOL	O1-C1-C2-C3
3	A	303	GOL	C1-C2-C3-O3
3	A	305	GOL	O1-C1-C2-C3
3	A	305	GOL	C1-C2-C3-O3
3	A	307	GOL	O1-C1-C2-C3
3	A	308	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	405	GOL	O1-C1-C2-C3
3	B	410	GOL	O1-C1-C2-C3
3	B	411	GOL	O1-C1-C2-C3
3	B	412	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	412	GOL	C1-C2-C3-O3
4	A	310	PGE	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-O2
3	A	304	GOL	O1-C1-C2-O2
3	A	307	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-O2
3	B	405	GOL	O1-C1-C2-O2
3	B	409	GOL	O2-C2-C3-O3
3	B	410	GOL	O2-C2-C3-O3
3	B	413	GOL	O2-C2-C3-O3
3	B	415	GOL	O1-C1-C2-O2
3	B	416	GOL	O2-C2-C3-O3
3	A	305	GOL	O1-C1-C2-O2
3	A	308	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-O2
3	B	407	GOL	O2-C2-C3-O3
3	B	410	GOL	O1-C1-C2-O2
3	B	412	GOL	O1-C1-C2-O2
3	A	303	GOL	O2-C2-C3-O3
3	A	307	GOL	O2-C2-C3-O3
3	A	308	GOL	O2-C2-C3-O3
3	B	412	GOL	O2-C2-C3-O3
3	B	414	GOL	O1-C1-C2-C3
4	A	310	PGE	C1-C2-O2-C3
3	B	409	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-O2
4	B	417	PGE	C6-C5-O3-C4
4	B	417	PGE	C4-C3-O2-C2
4	B	417	PGE	O2-C3-C4-O3
3	A	309	GOL	C1-C2-C3-O3
3	B	409	GOL	O1-C1-C2-C3
3	A	305	GOL	O2-C2-C3-O3
3	B	407	GOL	O1-C1-C2-O2
3	B	411	GOL	O1-C1-C2-O2
3	B	414	GOL	O1-C1-C2-O2
2	B	401	SLB	O1B-C1-C2-C3
4	A	310	PGE	C6-C5-O3-C4
3	A	309	GOL	O2-C2-C3-O3
4	A	310	PGE	O2-C3-C4-O3

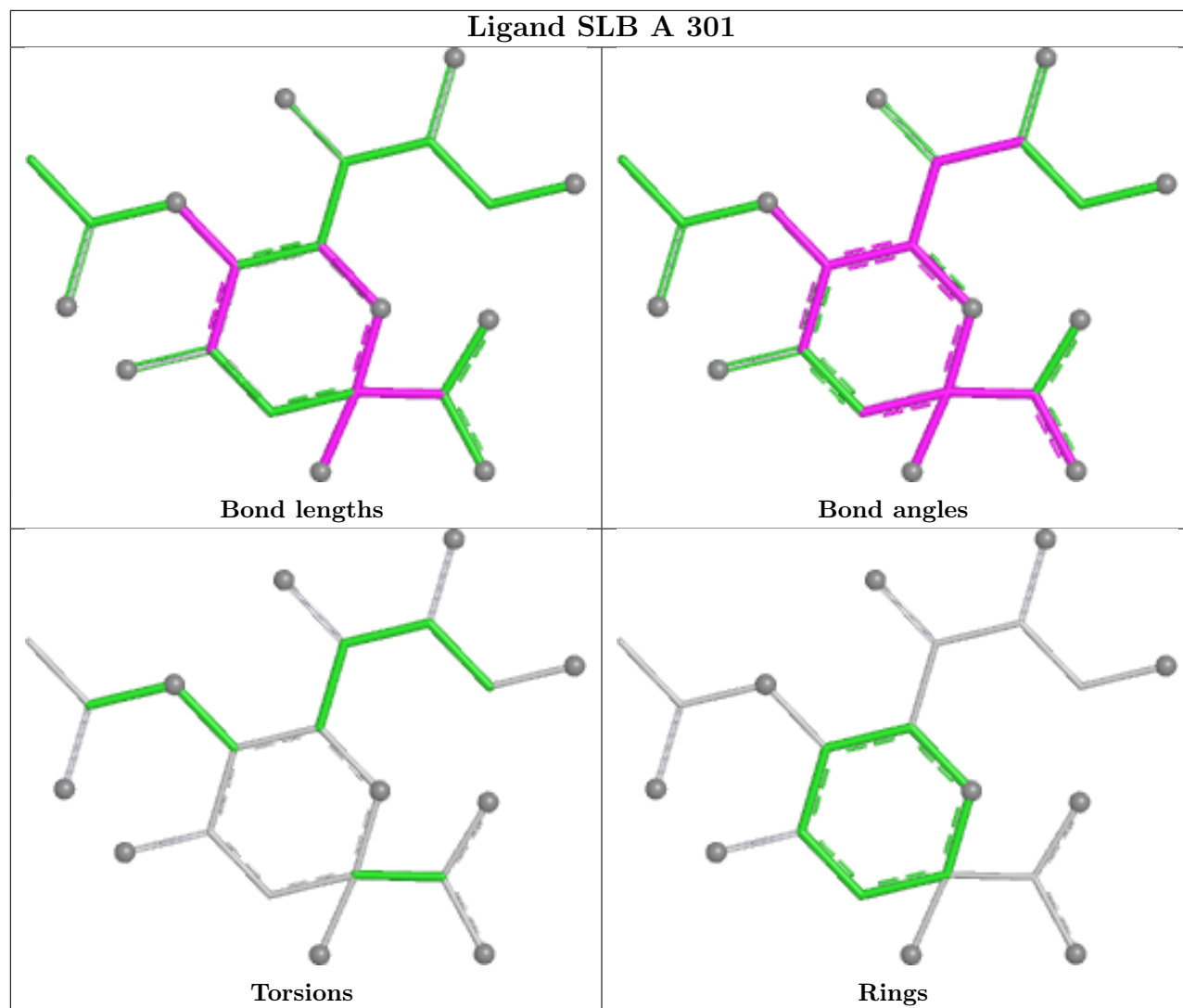
There are no ring outliers.

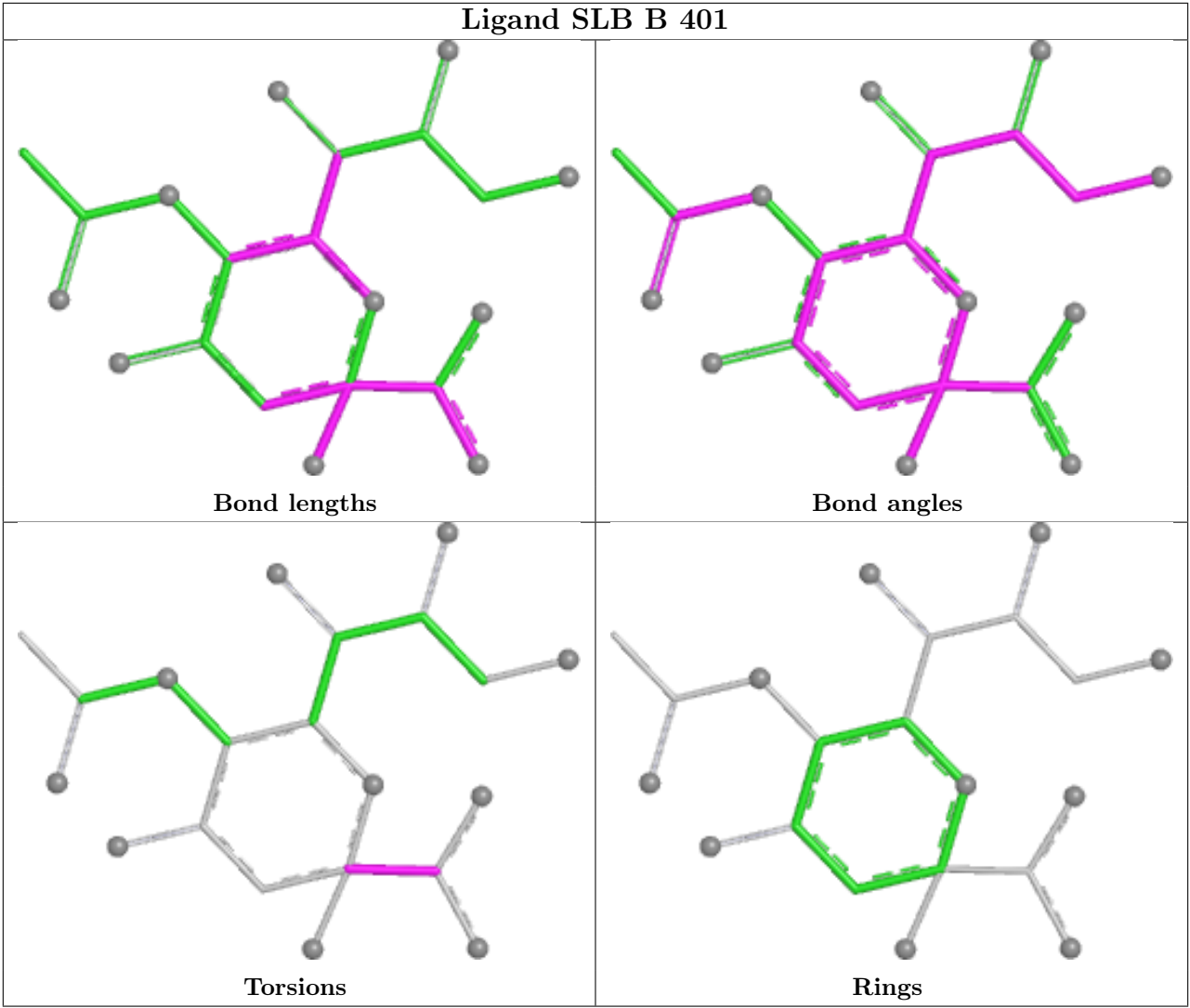
15 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	2	0
3	A	307	GOL	4	0
3	B	408	GOL	1	0
3	B	413	GOL	1	0
3	A	306	GOL	3	0
3	A	305	GOL	4	0
3	B	404	GOL	3	0
3	B	407	GOL	1	0
3	B	409	GOL	2	0
5	B	418	BGC	6	0
3	A	309	GOL	2	0
3	B	410	GOL	4	0
4	B	417	PGE	1	0
3	B	403	GOL	4	0
3	A	308	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.

Ligand SLB A 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	169:SER	C	170:GLU	N	1.18

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	299/299 (100%)	0.18	9 (3%)	50	53	17, 28, 54, 68	0
1	B	299/299 (100%)	0.31	14 (4%)	31	33	17, 27, 50, 80	0
All	All	598/598 (100%)	0.24	23 (3%)	40	43	17, 27, 51, 80	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	GLU	6.8
1	B	2	THR	5.2
1	A	34	GLU	5.2
1	B	32	GLN	5.0
1	A	28	GLU	4.6
1	A	32	GLN	4.4
1	B	35	ILE	4.3
1	B	33	GLY	4.1
1	A	2	THR	3.7
1	B	1	ALA	3.4
1	A	30	MET	3.3
1	B	30	MET	3.3
1	B	28	GLU	3.2
1	A	3	THR	2.9
1	A	29	GLU	2.9
1	B	3	THR	2.7
1	B	235	ALA	2.7
1	B	26	THR	2.6
1	B	31	SER	2.5
1	B	29	GLU	2.5
1	A	227	THR	2.2
1	A	234	LYS	2.2
1	B	230	ASP	2.2

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 monosaccharides 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(\AA^2)	Q<0.9
3	GOL	B	416	6/6	0.54	0.33	85,87,96,99	0
3	GOL	B	411	6/6	0.55	0.28	59,67,79,80	0
3	GOL	B	414	6/6	0.57	0.23	53,58,64,68	0
3	GOL	B	404	6/6	0.57	0.20	76,85,97,98	0
3	GOL	A	302	6/6	0.61	0.16	56,89,101,109	0
3	GOL	A	306	6/6	0.63	0.24	35,51,55,55	0
3	GOL	A	309	6/6	0.63	0.28	38,58,66,71	0
3	GOL	A	308	6/6	0.68	0.14	50,54,62,66	0
3	GOL	A	307	6/6	0.69	0.15	40,47,58,58	0
3	GOL	B	415	6/6	0.74	0.17	40,53,53,54	0
3	GOL	B	405	6/6	0.79	0.17	54,58,74,76	0
3	GOL	B	412	6/6	0.80	0.27	59,70,79,80	0
3	GOL	B	408	6/6	0.81	0.13	44,53,58,64	0
3	GOL	A	305	6/6	0.83	0.27	21,47,60,62	0
3	GOL	B	403	6/6	0.83	0.18	69,75,80,82	0
3	GOL	B	409	6/6	0.83	0.16	25,46,50,53	0
3	GOL	A	304	6/6	0.83	0.27	35,49,60,64	0
5	BGC	B	418	12/12	0.83	0.21	22,37,49,52	0
4	PGE	A	310	10/10	0.84	0.13	41,46,60,62	0
3	GOL	B	410	6/6	0.85	0.16	49,51,63,63	0
3	GOL	A	303	6/6	0.85	0.12	48,53,56,61	0
3	GOL	B	406	6/6	0.86	0.28	73,82,88,107	0
4	PGE	B	417	10/10	0.87	0.15	30,44,56,57	0
3	GOL	B	407	6/6	0.90	0.22	25,41,46,51	0
3	GOL	B	413	6/6	0.90	0.14	26,45,48,53	0
2	SLB	B	401	21/21	0.92	0.09	14,18,21,22	0
3	GOL	B	402	6/6	0.93	0.18	49,59,77,82	0

Continued on next page...

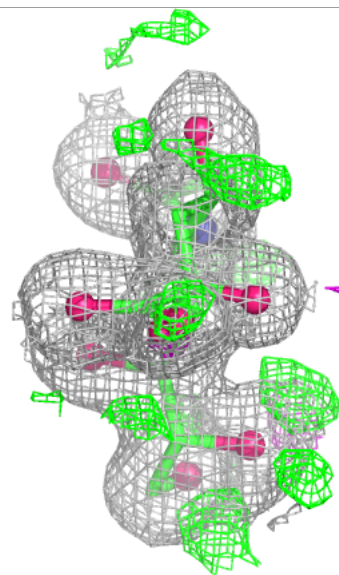
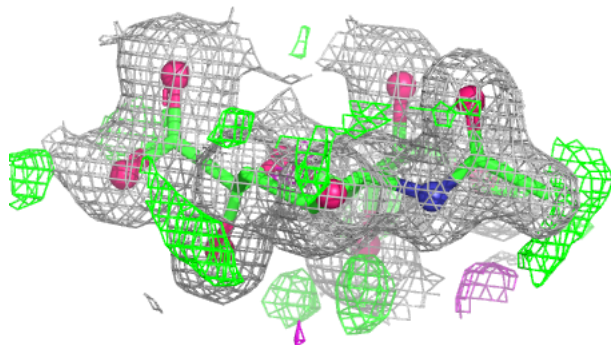
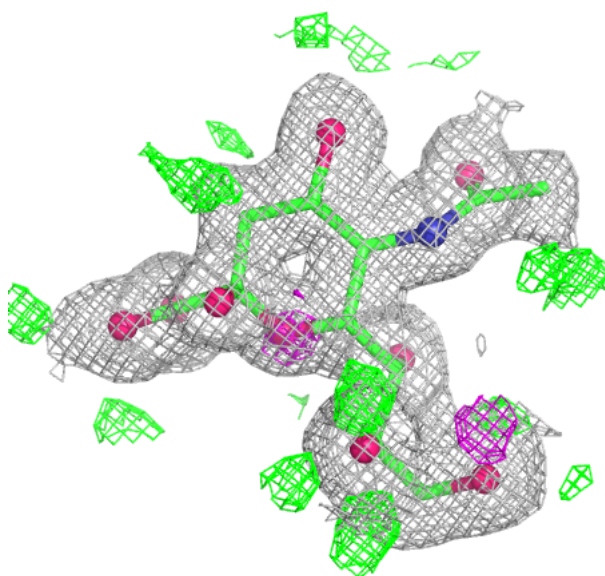
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SLB	A	301	21/21	0.95	0.08	14,18,21,21	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.

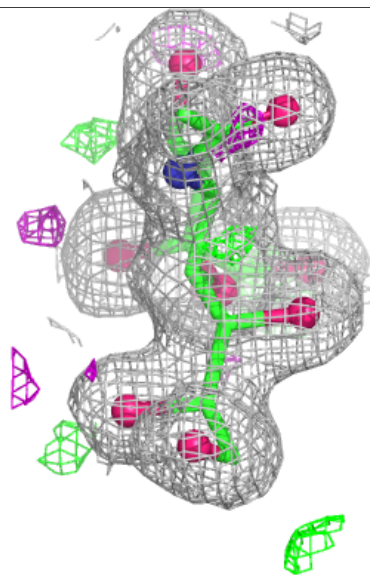
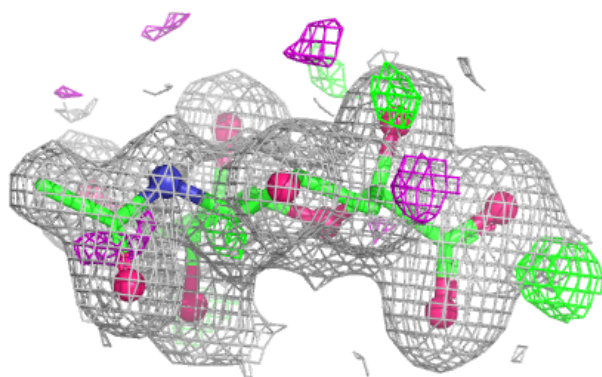
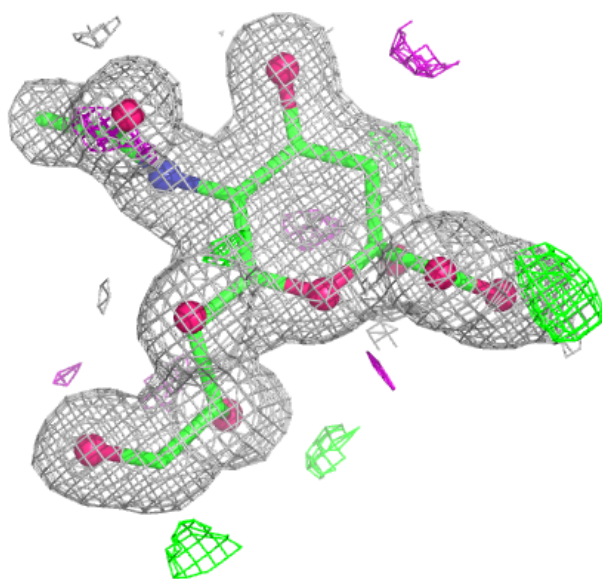
Electron density around SLB B 401:

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 SLB A 301:

$2mF_o-DF_c$ (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.