



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:44 AM UTC

PDB ID : 6VC3 / pdb_00006vc3
Title : Peanut lectin complexed with S-beta-D-thiogalactopyranosyl 6-deoxy-6-S-propynyl-beta-D-glucopyranoside (STG)
Authors : Otero, L.H.; Primo, E.D.; Cagnoni, A.J.; Cano, M.E.; Klinke, S.; Goldbaum, F.A.; Uhrig, M.L.
Deposited on : 2019-12-20
Resolution : 1.95 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

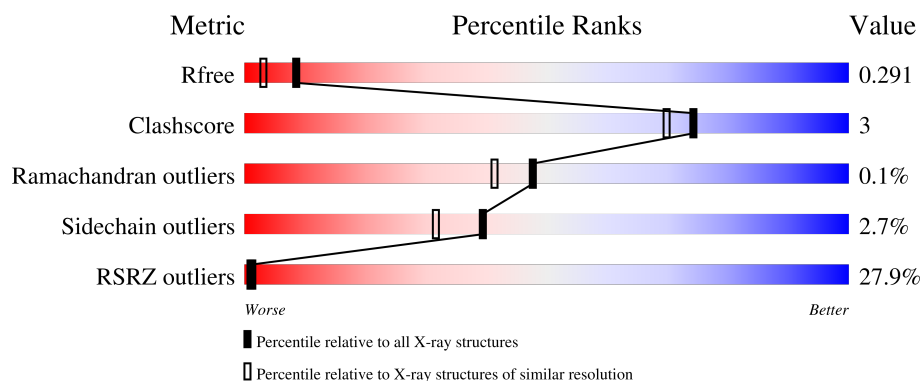
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	236	
1	B	236	
1	C	236	
1	D	236	

2 Entry composition [i](#)

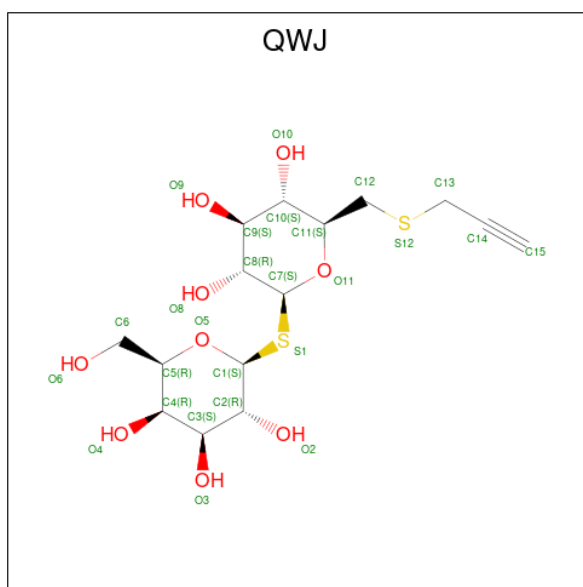
There are 5 unique types of molecules in this entry. The entry contains 7684 atoms, of which 72 are hydrogens and 0 are deuteriums.

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 Galactose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	B	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	C	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	D	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			

- Molecule 2 is 6-S-(prop-2-yn-1-yl)-6-thio-beta-D-glucopyranosyl 1-thio-beta-D-galactopyranoside (CCD ID: QWJ) (formula: C₁₅H₂₄O₉S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	27	0
			50	15	24	9	2		
2	B	1	Total	C	H	O	S	27	0
			50	15	24	9	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	O	S	27	0
			50	15	24	9	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

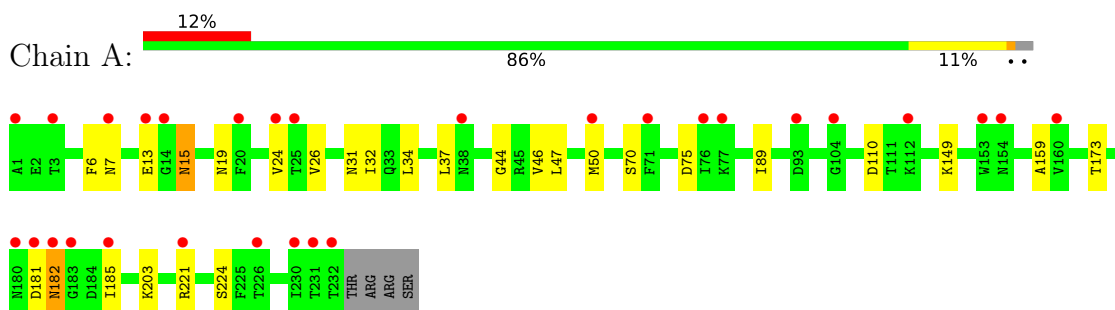
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total	O	0	0
			145	145		
5	B	160	Total	O	0	0
			160	160		
5	C	108	Total	O	0	0
			108	108		
5	D	141	Total	O	0	0
			141	141		

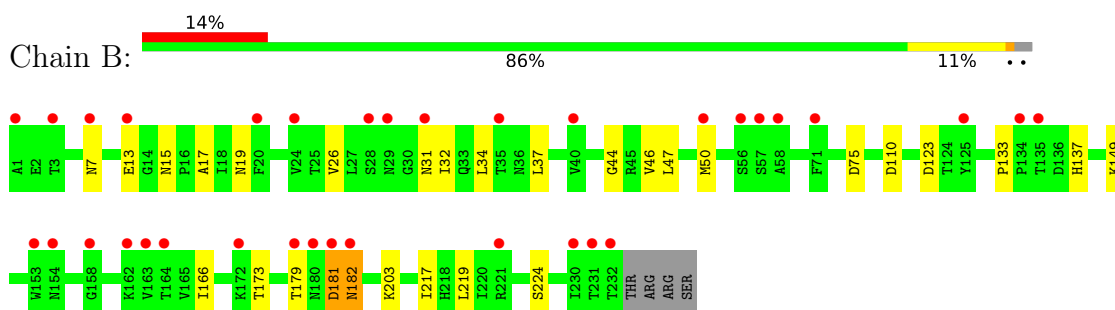
3 Residue-property plots [i](#)

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.

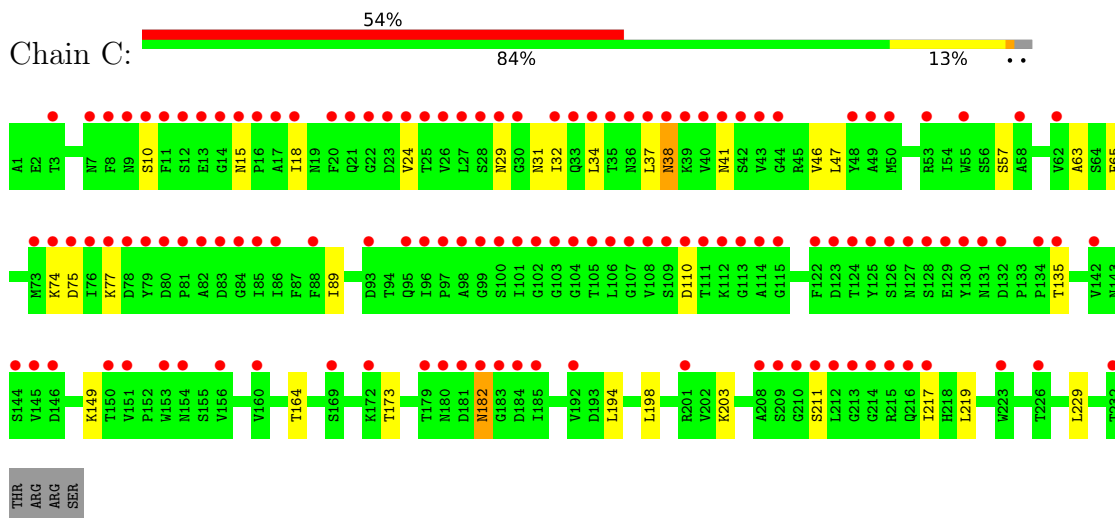
• Molecule 1: Galactose-binding lectin



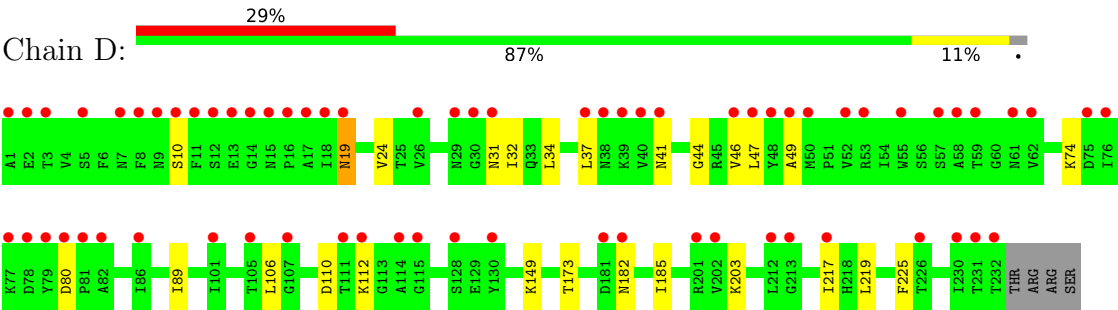
• Molecule 1: Galactose-binding lectin



• Molecule 1: Galactose-binding lectin



● Molecule 1: Galactose-binding lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.19Å 125.42Å 128.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 1.95 49.03 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.03-1.95) 91.8 (49.03-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.267 , 0.283 0.274 , 0.291	Depositor DCC
R_{free} test set	4228 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7684	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: QWJ, CA, MN

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	0.85	0/1779	1.21	7/2426 (0.3%)
1	B	0.88	0/1779	1.22	9/2426 (0.4%)
1	C	0.80	0/1779	1.23	7/2426 (0.3%)
1	D	0.84	0/1779	1.23	7/2426 (0.3%)
All	All	0.84	0/7116	1.22	30/9704 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	PHE	CA-CB-CG	8.21	122.01	113.80
1	C	38	ASN	CA-CB-CG	7.02	119.62	112.60
1	D	225	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	6	PHE	CA-CB-CG	6.29	120.09	113.80
1	C	31	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	15	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	110	ASP	CA-CB-CG	5.75	118.36	112.60
1	C	75	ASP	CA-CB-CG	5.72	118.33	112.60
1	B	75	ASP	CA-CB-CG	5.72	118.32	112.60
1	D	182	ASN	CA-CB-CG	5.67	118.27	112.60
1	B	31	ASN	CA-CB-CG	5.65	118.25	112.60
1	D	19	ASN	CA-CB-CG	5.61	118.21	112.60
1	B	19	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	182	ASN	CA-CB-CG	5.50	118.09	112.60
1	A	182	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	179	THR	CA-C-N	5.47	130.92	120.97
1	B	179	THR	C-N-CA	5.47	130.92	120.97
1	D	31	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	182	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	15	ASN	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	181	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	110	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	31	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	19	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	15	ASN	N-CA-C	5.20	115.58	109.60
1	D	41	ASN	CA-CB-CG	5.18	117.78	112.60
1	D	110	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	75	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	80	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	1743	0	1699	11	0
1	B	1743	0	1699	13	0
1	C	1743	0	1699	18	0
1	D	1743	0	1699	12	0
2	A	26	24	0	0	0
2	B	26	24	0	0	0
2	D	26	24	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	145	0	0	0	0
5	B	160	0	0	0	0
5	C	108	0	0	2	0
5	D	141	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7612	72	6796	43	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 3.

All (43) 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:C:74:LYS:HE2	1:D:10:SER:HB3	1.76	0.67
1:D:32:ILE:HD13	1:D:46:VAL:HG11	1.77	0.67
1:C:29:ASN:HA	1:D:217:ILE:HD13	1.78	0.66
1:A:32:ILE:HD13	1:A:46:VAL:HG11	1.79	0.63
1:B:7:ASN:HD22	1:B:224:SER:HB3	1.65	0.62
1:B:32:ILE:HD13	1:B:46:VAL:HG11	1.82	0.61
1:D:24:VAL:HG23	1:D:34:LEU:HA	1.82	0.60
1:C:29:ASN:O	1:D:74:LYS:HD3	2.03	0.59
1:C:32:ILE:HD13	1:C:46:VAL:HG21	1.89	0.55
1:A:34:LEU:O	1:A:44:GLY:HA3	2.07	0.54
1:A:50:MET:SD	1:B:17:ALA:HA	2.48	0.54
1:B:173:THR:HG21	1:C:173:THR:HG21	1.91	0.52
1:C:194:LEU:HD22	1:C:198:LEU:HD12	1.92	0.52
1:A:173:THR:HG21	1:D:173:THR:HG21	1.92	0.51
1:C:41:ASN:HD22	1:C:211:SER:HA	1.76	0.51
1:C:24:VAL:HG22	1:C:34:LEU:HA	1.94	0.49
1:C:57:SER:HA	5:C:421:HOH:O	2.13	0.48
1:A:24:VAL:HG22	1:A:34:LEU:HA	1.96	0.47
1:A:50:MET:HB2	1:B:50:MET:HE3	1.96	0.47
1:A:13:GLU:HG3	1:A:26:VAL:HB	1.98	0.46
1:B:123:ASP:HB3	1:B:137:HIS:CE1	2.52	0.45
1:A:70:SER:OG	1:A:221:ARG:HB2	2.18	0.44
1:A:7:ASN:HD22	1:A:224:SER:HB3	1.82	0.44
1:C:18:ILE:CG2	1:C:46:VAL:HG22	2.48	0.43
1:B:13:GLU:HG3	1:B:26:VAL:HB	2.00	0.43
1:C:29:ASN:HB3	1:D:219:LEU:HD11	2.01	0.43
1:B:217:ILE:HG22	1:B:219:LEU:HG	2.00	0.43
1:C:63:ALA:HB2	1:C:229:LEU:HB2	2.01	0.43
1:A:47:LEU:HD22	1:A:203:LYS:HB3	2.01	0.42
1:B:133:PRO:HD2	1:B:137:HIS:CE1	2.55	0.42
1:B:34:LEU:O	1:B:44:GLY:HA3	2.18	0.42
1:D:34:LEU:O	1:D:44:GLY:HA3	2.19	0.42
1:C:74:LYS:CE	1:D:10:SER:HB3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:HB1	1:A:181:ASP:HB2	2.03	0.41
1:B:166:ILE:HD11	1:C:164:THR:HG22	2.03	0.41
1:D:47:LEU:HD22	1:D:203:LYS:HB3	2.03	0.41
1:B:47:LEU:HD22	1:B:203:LYS:HB3	2.02	0.40
1:C:135:THR:HB	5:C:434:HOH:O	2.20	0.40
1:D:19:ASN:ND2	1:D:49:ALA:HA	2.35	0.40
1:B:7:ASN:ND2	1:B:224:SER:HB3	2.34	0.40
1:C:10:SER:HB3	1:D:74:LYS:HE2	2.03	0.40
1:C:217:ILE:HG22	1:C:219:LEU:HG	2.03	0.40
1:C:47:LEU:HD22	1:C:203:LYS:HB3	2.03	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	230/236 (98%)	224 (97%)	6 (3%)	0	100	100
1	B	230/236 (98%)	223 (97%)	7 (3%)	0	100	100
1	C	230/236 (98%)	224 (97%)	6 (3%)	0	100	100
1	D	230/236 (98%)	223 (97%)	6 (3%)	1 (0%)	30	21
All	All	920/944 (98%)	894 (97%)	25 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	LEU

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	197/201 (98%)	191 (97%)	6 (3%)	36	27
1	B	197/201 (98%)	193 (98%)	4 (2%)	48	43
1	C	197/201 (98%)	191 (97%)	6 (3%)	36	27
1	D	197/201 (98%)	192 (98%)	5 (2%)	42	34
All	All	788/804 (98%)	767 (97%)	21 (3%)	39	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	37	LEU
1	A	89	ILE
1	A	149	LYS
1	A	182	ASN
1	A	185	ILE
1	B	37	LEU
1	B	149	LYS
1	B	181	ASP
1	B	182	ASN
1	C	37	LEU
1	C	38	ASN
1	C	77	LYS
1	C	89	ILE
1	C	149	LYS
1	C	182	ASN
1	D	37	LEU
1	D	89	ILE
1	D	112	LYS
1	D	149	LYS
1	D	185	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	ASN
1	A	31	ASN
1	A	41	ASN
1	A	95	GLN
1	B	7	ASN
1	B	15	ASN
1	B	61	ASN
1	B	190	GLN
1	C	7	ASN
1	C	41	ASN
1	C	61	ASN
1	C	154	ASN
1	D	9	ASN
1	D	15	ASN
1	D	19	ASN
1	D	36	ASN
1	D	61	ASN
1	D	95	GLN
1	D	154	ASN
1	D	182	ASN
1	D	216	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	QWJ	D	301	-	27,27,27	0.56	1 (3%)	33,38,38	0.51	1 (3%)
2	QWJ	A	301	-	27,27,27	0.90	1 (3%)	33,38,38	0.29	0
2	QWJ	B	301	-	27,27,27	1.52	1 (3%)	33,38,38	0.36	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	QWJ	D	301	-	-	3/10/51/51	0/2/2/2
2	QWJ	A	301	-	-	4/10/51/51	0/2/2/2
2	QWJ	B	301	-	-	4/10/51/51	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	QWJ	C13-C14	-7.86	1.41	1.45
2	A	301	QWJ	C13-C14	-4.59	1.43	1.45
2	D	301	QWJ	C13-C14	-2.81	1.44	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	QWJ	C13-C14-C15	-2.29	176.40	178.42

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	QWJ	C14-C13-S12-C12
2	A	301	QWJ	C4-C5-C6-O6
2	D	301	QWJ	C4-C5-C6-O6
2	B	301	QWJ	C4-C5-C6-O6

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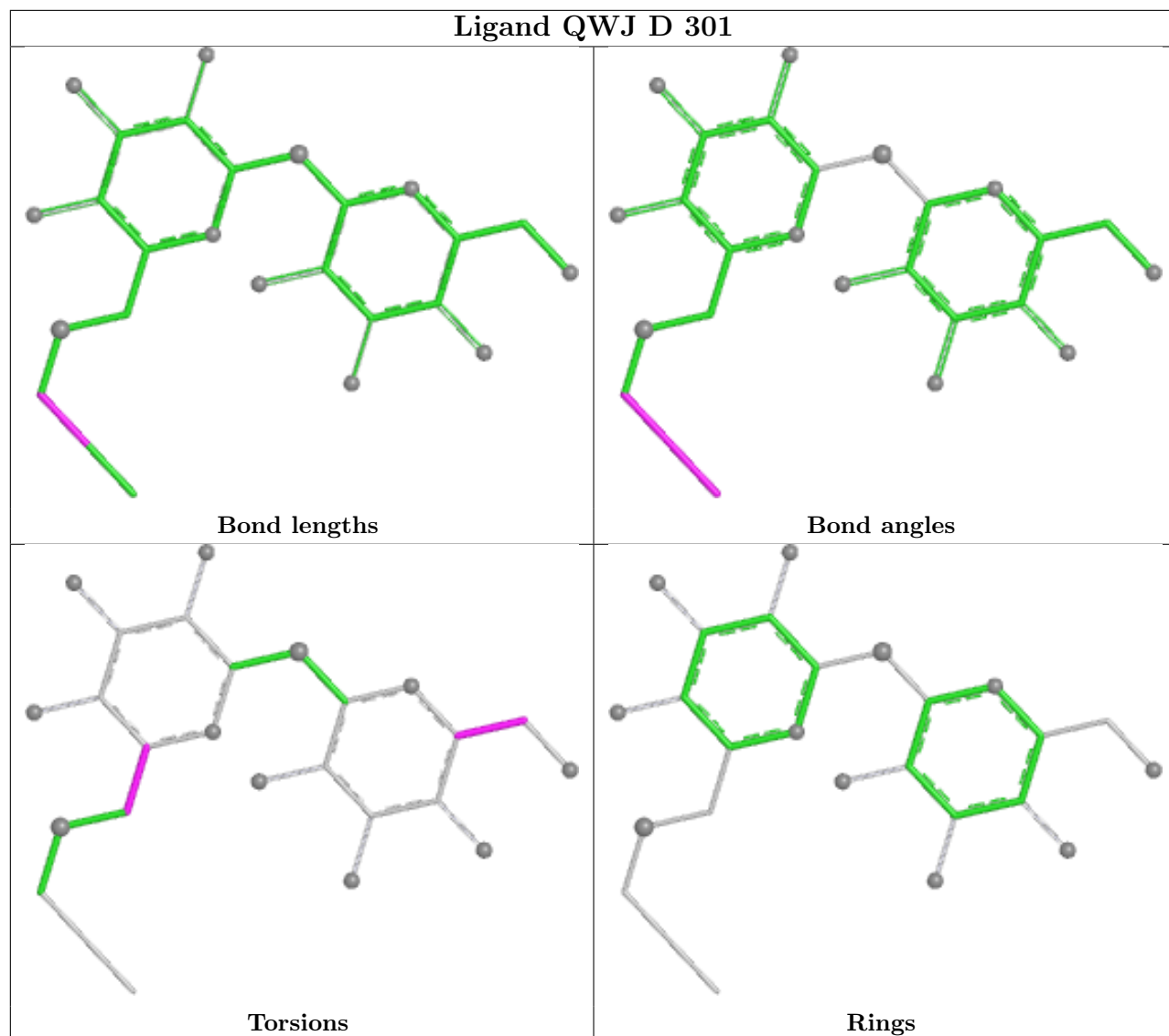
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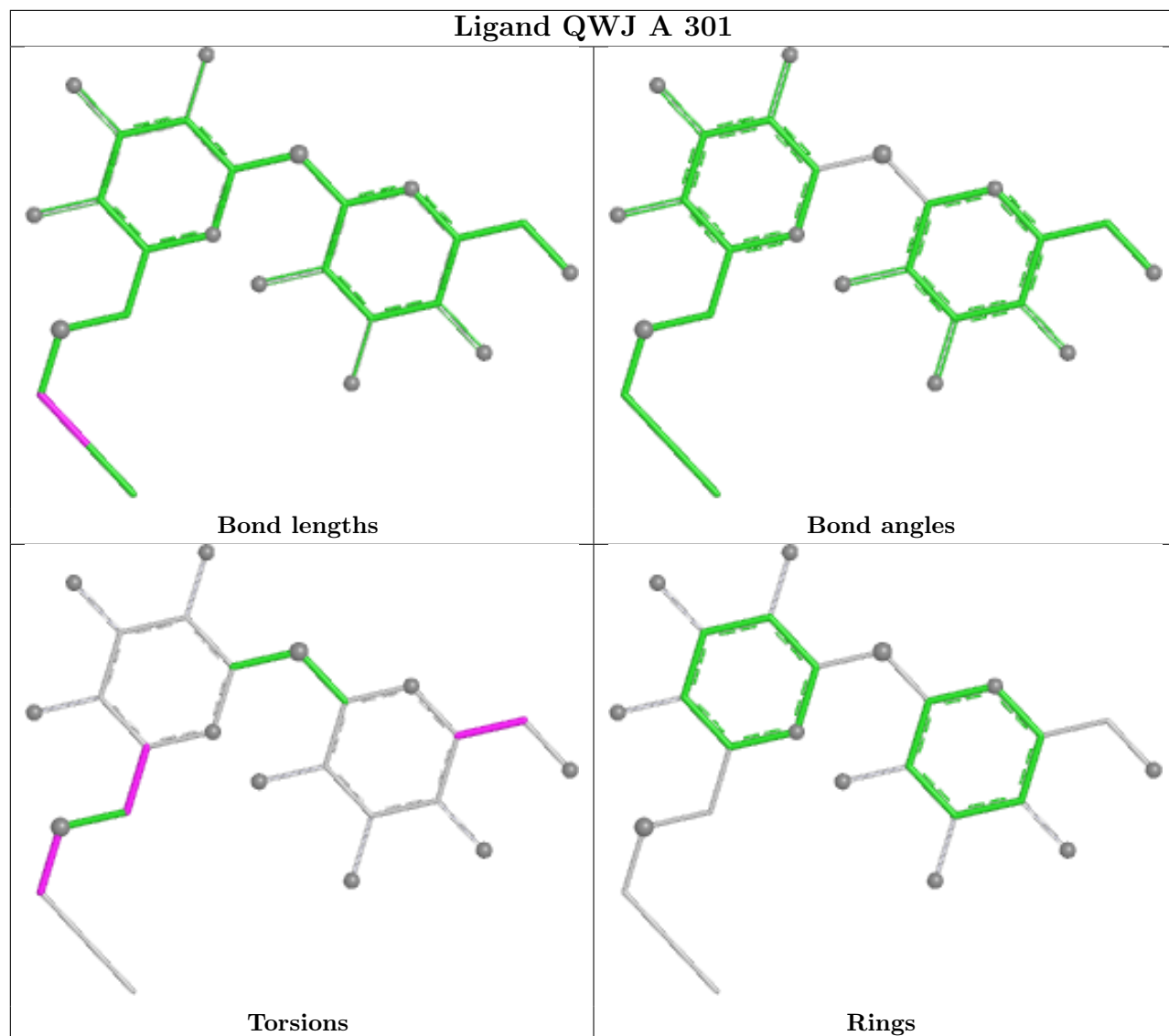
Mol	Chain	Res	Type	Atoms
2	D	301	QWJ	O5-C5-C6-O6
2	A	301	QWJ	O5-C5-C6-O6
2	B	301	QWJ	O5-C5-C6-O6
2	A	301	QWJ	C14-C13-S12-C12
2	A	301	QWJ	O11-C11-C12-S12
2	B	301	QWJ	O11-C11-C12-S12
2	D	301	QWJ	O11-C11-C12-S12

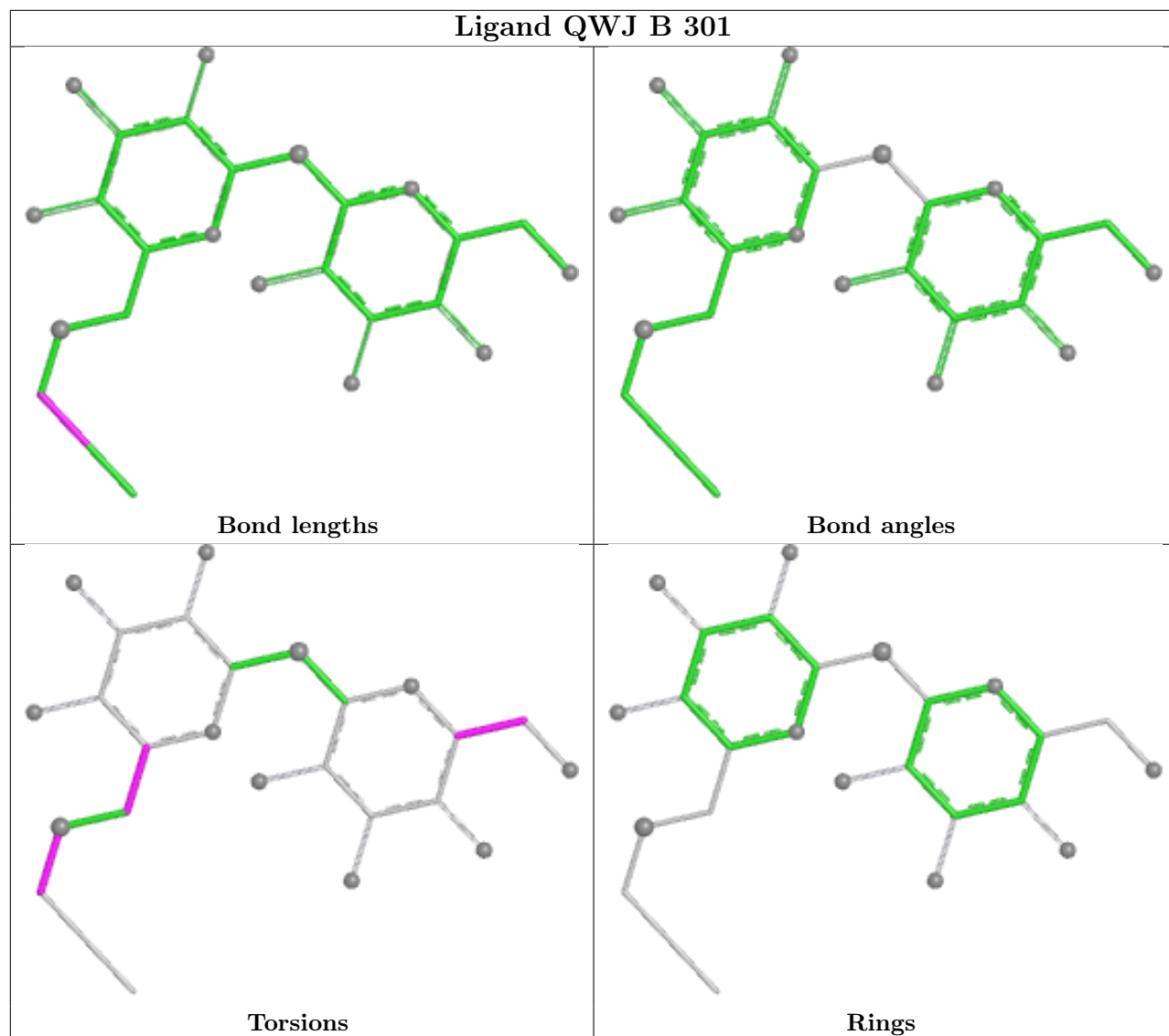
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	232/236 (98%)	1.10	29 (12%) 8 9	17, 28, 47, 128	0
1	B	232/236 (98%)	1.08	34 (14%) 6 6	18, 26, 48, 111	0
1	C	232/236 (98%)	2.91	128 (55%) 0 0	18, 43, 96, 121	0
1	D	232/236 (98%)	1.63	68 (29%) 1 1	18, 30, 68, 113	0
All	All	928/944 (98%)	1.68	259 (27%) 1 1	17, 30, 78, 128	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	ILE	10.6
1	C	108	VAL	10.0
1	C	103	GLY	9.9
1	C	106	LEU	9.9
1	C	37	LEU	9.3
1	C	105	THR	9.2
1	C	107	GLY	8.7
1	C	104	GLY	8.6
1	C	79	TYR	8.5
1	C	82	ALA	7.8
1	C	109	SER	7.8
1	C	40	VAL	7.8
1	C	102	GLY	7.4
1	C	35	THR	7.1
1	C	12	SER	6.9
1	D	11	PHE	6.9
1	C	81	PRO	6.8
1	D	17	ALA	6.7
1	C	232	THR	6.7
1	C	29	ASN	6.7
1	C	100	SER	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	232	THR	6.6
1	C	130	TYR	6.6
1	D	16	PRO	6.6
1	C	14	GLY	6.5
1	C	99	GLY	6.4
1	C	98	ALA	6.3
1	C	41	ASN	6.1
1	C	34	LEU	6.1
1	C	96	ILE	6.0
1	C	36	ASN	5.9
1	C	11	PHE	5.9
1	A	232	THR	5.9
1	C	76	ILE	5.8
1	C	111	THR	5.6
1	C	179	THR	5.6
1	B	3	THR	5.5
1	C	114	ALA	5.5
1	C	77	LYS	5.5
1	C	97	PRO	5.4
1	C	42	SER	5.3
1	D	1	ALA	5.3
1	B	232	THR	5.2
1	C	39	LYS	5.1
1	C	181	ASP	5.1
1	A	50	MET	5.1
1	C	180	ASN	5.0
1	D	15	ASN	5.0
1	C	110	ASP	5.0
1	C	182	ASN	4.9
1	A	181	ASP	4.8
1	C	80	ASP	4.8
1	C	17	ALA	4.8
1	C	126	SER	4.8
1	D	12	SER	4.8
1	C	127	ASN	4.8
1	D	9	ASN	4.7
1	D	18	ILE	4.7
1	C	212	LEU	4.7
1	C	43	VAL	4.7
1	C	7	ASN	4.7
1	C	215	ARG	4.6
1	D	29	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	32	ILE	4.6
1	C	125	TYR	4.6
1	C	214	GLY	4.6
1	A	180	ASN	4.5
1	D	13	GLU	4.5
1	D	79	TYR	4.5
1	C	131	ASN	4.4
1	C	22	GLY	4.4
1	C	78	ASP	4.4
1	C	156	VAL	4.4
1	C	128	SER	4.3
1	C	132	ASP	4.3
1	C	38	ASN	4.3
1	D	10	SER	4.2
1	D	38	ASN	4.2
1	C	85	ILE	4.2
1	C	210	GLY	4.2
1	C	13	GLU	4.2
1	B	230	ILE	4.1
1	A	3	THR	4.1
1	D	231	THR	4.1
1	C	21	GLN	4.0
1	B	179	THR	4.0
1	B	181	ASP	4.0
1	C	15	ASN	4.0
1	A	230	ILE	4.0
1	C	8	PHE	4.0
1	D	217	ILE	4.0
1	C	95	GLN	3.9
1	D	78	ASP	3.9
1	C	83	ASP	3.9
1	D	31	ASN	3.9
1	C	211	SER	3.9
1	D	58	ALA	3.9
1	A	183	GLY	3.9
1	C	124	THR	3.8
1	A	231	THR	3.8
1	C	113	GLY	3.8
1	C	129	GLU	3.8
1	C	49	ALA	3.8
1	C	112	LYS	3.8
1	D	76	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	57	SER	3.7
1	C	3	THR	3.7
1	C	10	SER	3.7
1	C	50	MET	3.7
1	D	230	ILE	3.7
1	C	16	PRO	3.7
1	A	153	TRP	3.7
1	D	39	LYS	3.6
1	C	115	GLY	3.6
1	C	27	LEU	3.6
1	A	13	GLU	3.6
1	D	115	GLY	3.5
1	C	26	VAL	3.5
1	D	8	PHE	3.5
1	C	18	ILE	3.5
1	C	9	ASN	3.5
1	B	180	ASN	3.5
1	D	19	ASN	3.4
1	C	86	ILE	3.4
1	C	25	THR	3.4
1	B	221	ARG	3.4
1	C	24	VAL	3.4
1	C	145	VAL	3.4
1	D	40	VAL	3.4
1	D	212	LEU	3.4
1	C	75	ASP	3.3
1	C	217	ILE	3.3
1	B	20	PHE	3.3
1	A	20	PHE	3.3
1	C	58	ALA	3.2
1	C	33	GLN	3.2
1	D	112	LYS	3.2
1	C	134	PRO	3.2
1	B	50	MET	3.2
1	C	30	GLY	3.1
1	D	30	GLY	3.1
1	D	181	ASP	3.1
1	A	182	ASN	3.1
1	D	50	MET	3.1
1	C	213	GLY	3.1
1	D	14	GLY	3.1
1	B	182	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	53	ARG	3.0
1	C	201	ARG	3.0
1	A	25	THR	3.0
1	D	105	THR	3.0
1	D	202	VAL	3.0
1	C	153	TRP	3.0
1	C	151	VAL	2.9
1	D	77	LYS	2.9
1	D	7	ASN	2.9
1	A	221	ARG	2.9
1	A	112	LYS	2.9
1	C	146	ASP	2.9
1	C	20	PHE	2.8
1	C	93	ASP	2.8
1	A	226	THR	2.8
1	B	231	THR	2.8
1	C	169	SER	2.8
1	C	216	GLN	2.8
1	D	101	ILE	2.8
1	C	123	ASP	2.8
1	D	53	ARG	2.8
1	C	226	THR	2.8
1	D	3	THR	2.8
1	C	160	VAL	2.7
1	D	26	VAL	2.7
1	D	82	ALA	2.7
1	D	111	THR	2.7
1	B	153	TRP	2.7
1	C	208	ALA	2.7
1	C	183	GLY	2.7
1	D	37	LEU	2.7
1	C	74	LYS	2.6
1	B	24	VAL	2.6
1	C	84	GLY	2.6
1	C	142	VAL	2.6
1	D	62	VAL	2.6
1	D	49	ALA	2.6
1	D	48	TYR	2.6
1	D	128	SER	2.6
1	D	201	ARG	2.6
1	D	41	ASN	2.6
1	D	61	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	93	ASP	2.5
1	B	154	ASN	2.5
1	B	13	GLU	2.5
1	C	48	TYR	2.5
1	C	28	SER	2.5
1	D	5	SER	2.5
1	C	73	MET	2.5
1	B	125	TYR	2.5
1	D	130	TYR	2.5
1	C	88	PHE	2.5
1	A	38	ASN	2.5
1	B	29	ASN	2.5
1	C	209	SER	2.5
1	C	135	THR	2.5
1	D	59	THR	2.5
1	C	23	ASP	2.5
1	C	62	VAL	2.5
1	D	81	PRO	2.5
1	A	104	GLY	2.4
1	A	1	ALA	2.4
1	C	150	THR	2.4
1	D	55	TRP	2.4
1	C	154	ASN	2.4
1	C	184	ASP	2.4
1	B	134	PRO	2.4
1	C	223	TRP	2.4
1	D	114	ALA	2.3
1	A	7	ASN	2.3
1	B	57	SER	2.3
1	D	52	VAL	2.3
1	B	58	ALA	2.3
1	C	172	LYS	2.3
1	C	185	ILE	2.3
1	C	144	SER	2.3
1	B	163	VAL	2.3
1	B	7	ASN	2.3
1	B	172	LYS	2.3
1	D	2	GLU	2.2
1	B	31	ASN	2.2
1	A	77	LYS	2.2
1	A	76	ILE	2.2
1	A	160	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	2.2
1	D	213	GLY	2.2
1	A	185	ILE	2.2
1	B	162	LYS	2.2
1	C	192	VAL	2.2
1	B	35	THR	2.2
1	A	14	GLY	2.2
1	D	47	LEU	2.2
1	B	71	PHE	2.1
1	B	40	VAL	2.1
1	B	56	SER	2.1
1	D	107	GLY	2.1
1	B	1	ALA	2.1
1	A	71	PHE	2.1
1	A	24	VAL	2.1
1	C	122	PHE	2.1
1	D	80	ASP	2.1
1	B	28	SER	2.1
1	A	154	ASN	2.1
1	D	182	ASN	2.1
1	D	75	ASP	2.1
1	B	135	THR	2.0
1	B	164	THR	2.0
1	C	55	TRP	2.0
1	D	86	ILE	2.0
1	C	44	GLY	2.0
1	D	226	THR	2.0
1	D	46	VAL	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.

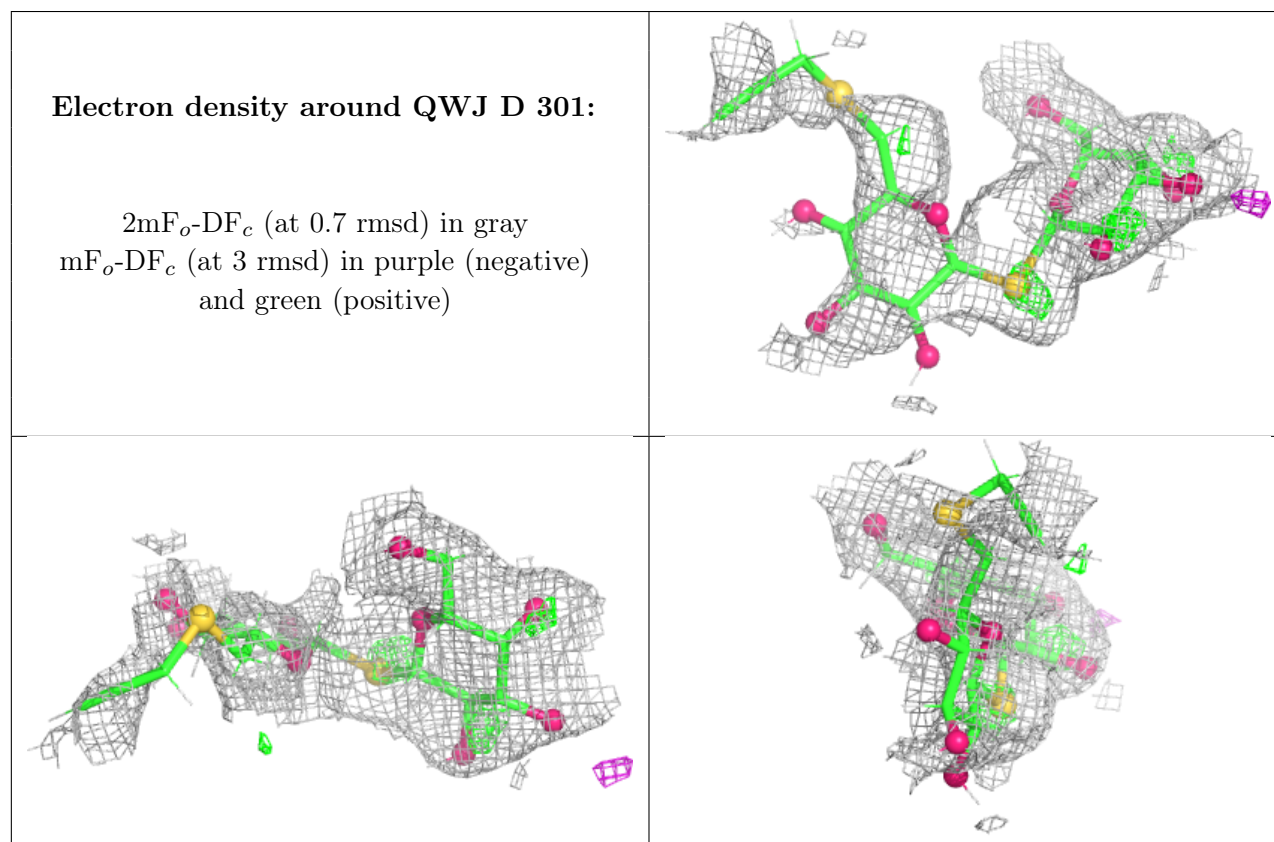
6.4 Ligands [i](#)

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.

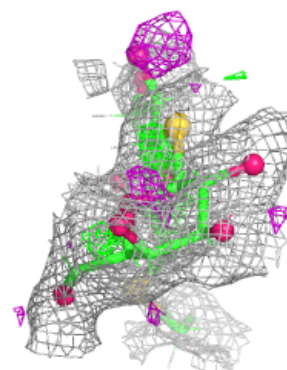
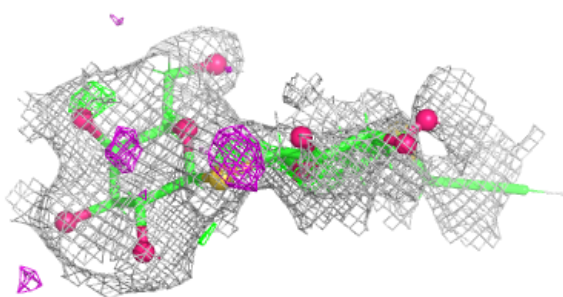
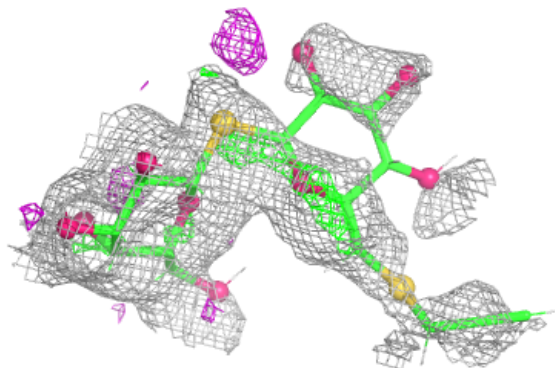
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	QWJ	D	301	26/26	0.79	0.23	105,121,130,131	27
2	QWJ	A	301	26/26	0.83	0.21	53,89,111,113	27
2	QWJ	B	301	26/26	0.85	0.23	75,103,119,121	27
3	MN	C	301	1/1	0.92	0.11	47,47,47,47	0
4	CA	C	302	1/1	0.92	0.07	35,35,35,35	0
4	CA	D	303	1/1	0.94	0.06	30,30,30,30	0
3	MN	D	302	1/1	0.95	0.10	46,46,46,46	0
3	MN	B	302	1/1	0.96	0.06	37,37,37,37	0
4	CA	B	303	1/1	0.98	0.05	25,25,25,25	0
3	MN	A	302	1/1	0.98	0.05	39,39,39,39	0
4	CA	A	303	1/1	0.98	0.03	26,26,26,26	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.

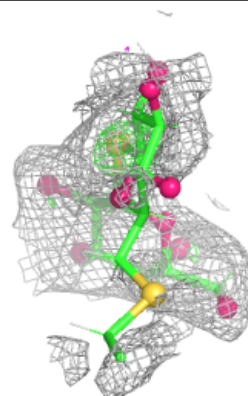
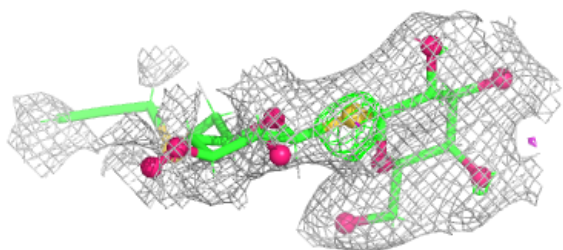
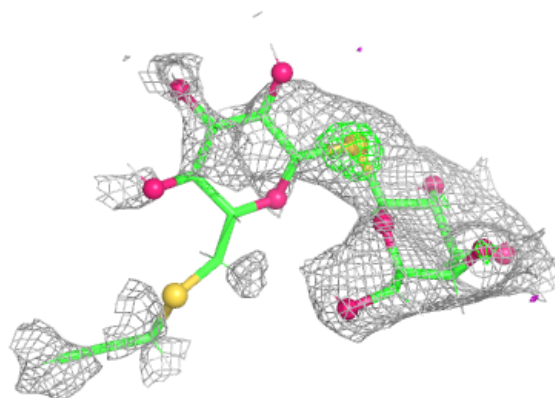


Electron density around QWJ A 301:

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

**Electron density around QWJ B 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.