



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 AM UTC

PDB ID : 8BVD / pdb_00008bvd
Title : FimH lectin domain in complex with mannose C-linked to quinoline
Authors : Bouckaert, J.; Bridot, C.
Deposited on : 2022-12-03
Resolution : 3.00 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

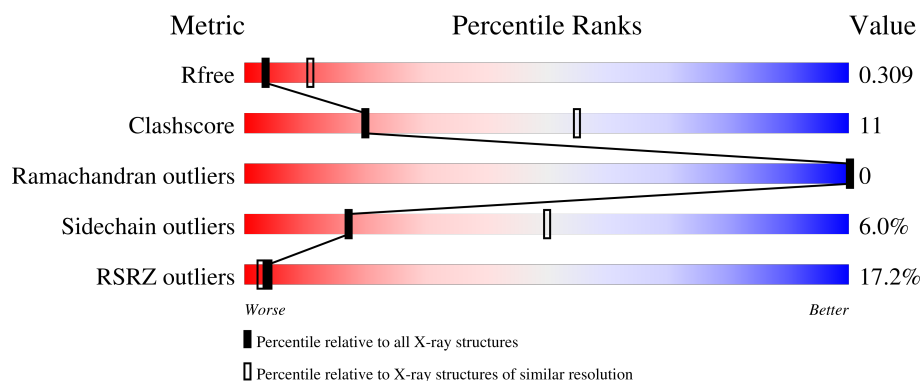
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	158	4% 80% 19% .
1	B	158	44% 62% 34% .
1	C	158	17% 77% 21% .
1	D	158	4% 80% 19% .

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	RLO	B	201	-	X	-	-
2	RLO	C	201	-	X	-	-
2	RLO	D	201	-	X	-	-

2 Entry composition [i](#)

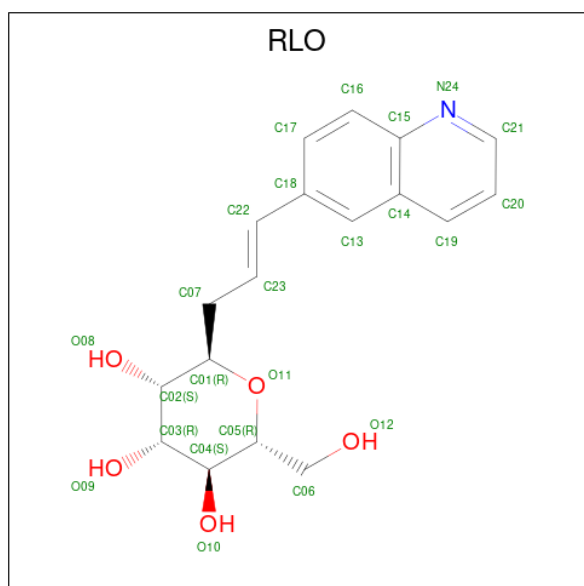
There are 3 unique types of molecules in this entry. The entry contains 5104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Type 1 fimbrin D-mannose specific adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1196	763	197	234	2			
1	B	158	Total	C	N	O	S	0	0	0
			1196	763	197	234	2			
1	C	158	Total	C	N	O	S	0	0	0
			1196	763	197	234	2			
1	D	158	Total	C	N	O	S	0	0	0
			1196	763	197	234	2			

- Molecule 2 is (2R,3S,4R,5S,6R)-2-(hydroxymethyl)-6-[(E)-3-quinolin-6-ylprop-2-enyl]oxane-3,4,5-triol (CCD ID: RLO) (formula: C₁₈H₂₁NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	18	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			24	18	1	5		
2	C	1	Total	C	N	O	0	0
			24	18	1	5		
2	D	1	Total	C	N	O	0	0
			24	18	1	5		

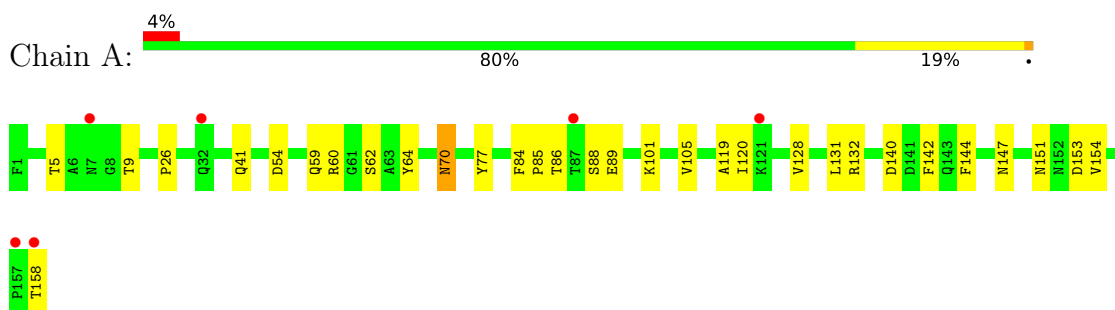
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	101	Total	O	0	0
			101	101		
3	C	36	Total	O	0	0
			36	36		
3	D	45	Total	O	0	0
			45	45		

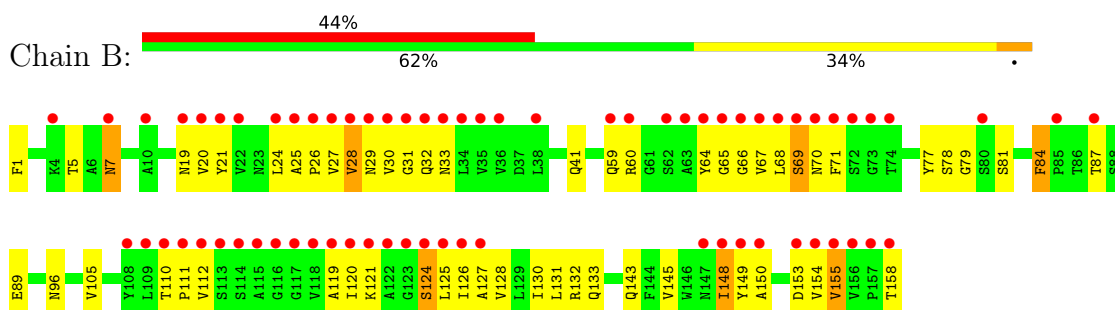
3 Residue-property plots

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.

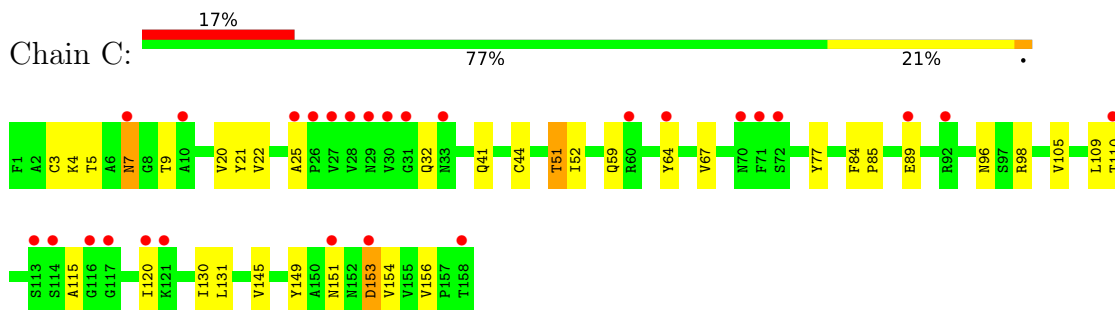
- Molecule 1: Type 1 fimbrin D-mannose specific adhesin



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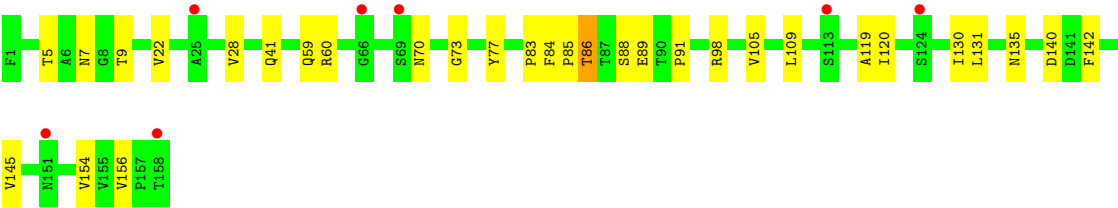


- Molecule 1: Type 1 fimbrin D-mannose specific adhesin



- Molecule 1: Type 1 fimbrin D-mannose specific adhesin





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.78Å 151.78Å 225.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.73 – 3.00 49.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.73-3.00) 91.9 (49.73-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.251 , 0.303 0.256 , 0.309	Depositor DCC
R_{free} test set	1439 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5104	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: RLO

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	0.56	0/1226	0.99	1/1684 (0.1%)
1	B	0.59	0/1226	1.04	1/1684 (0.1%)
1	C	0.53	0/1226	0.96	0/1684
1	D	0.56	0/1226	0.99	1/1684 (0.1%)
All	All	0.56	0/4904	0.99	3/6736 (0.0%)

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	4
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	CA-CB-CG	7.29	119.89	112.60
1	B	84	PHE	O-C-N	-5.35	117.00	121.44
1	D	86	THR	CA-CB-OG1	-5.31	101.63	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	B	111	PRO	Peptide
1	B	132	ARG	Sidechain
1	B	60	ARG	Sidechain
1	B	84	PHE	Peptide
1	D	98	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	1196	0	1166	22	0
1	B	1196	0	1166	51	0
1	C	1196	0	1166	21	0
1	D	1196	0	1166	17	0
2	A	24	0	0	1	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	1	0
3	A	42	0	0	1	0
3	B	101	0	0	6	0
3	C	36	0	0	4	0
3	D	45	0	0	0	0
All	All	5104	0	4664	105	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 11.

All (105) 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:7:ASN:ND2	3:C:301:HOH:O	1.99	0.95
1:B:33:ASN:ND2	1:B:110:THR:HG23	1.92	0.85
1:B:126:ILE:HD11	1:B:150:ALA:HB2	1.61	0.80
1:B:5:THR:HG21	1:B:20:VAL:HG12	1.67	0.76
1:B:67:VAL:HG21	1:B:126:ILE:HG23	1.68	0.74
1:B:67:VAL:CG2	1:B:126:ILE:HG23	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:VAL:HG21	1:B:126:ILE:CG2	2.19	0.72
1:C:59:GLN:HG3	3:C:327:HOH:O	1.91	0.70
1:A:62:SER:HB3	1:B:79:GLY:HA2	1.75	0.68
1:A:70:ASN:ND2	1:A:119:ALA:HB1	2.11	0.66
1:A:62:SER:CB	1:B:79:GLY:HA2	2.26	0.66
1:B:67:VAL:HA	1:B:71:PHE:HD2	1.65	0.62
1:B:32:GLN:O	1:B:110:THR:HG22	1.99	0.61
1:B:127:ALA:HB3	1:B:148:ILE:HG12	1.83	0.60
1:A:77:TYR:HD1	1:A:105:VAL:HG22	1.65	0.60
1:B:77:TYR:HD1	1:B:105:VAL:HG22	1.67	0.60
1:D:77:TYR:HD1	1:D:105:VAL:HG22	1.66	0.59
1:B:33:ASN:HD22	1:B:110:THR:HG23	1.65	0.59
1:A:60:ARG:NH2	1:A:88:SER:HA	2.18	0.59
1:B:33:ASN:ND2	1:B:110:THR:CG2	2.65	0.58
1:C:77:TYR:HD1	1:C:105:VAL:HG22	1.68	0.58
1:B:77:TYR:CD1	1:B:105:VAL:HG22	2.41	0.56
1:C:7:ASN:OD1	1:C:7:ASN:N	2.38	0.56
1:B:25:ALA:O	3:B:301:HOH:O	2.18	0.55
1:A:60:ARG:NH1	1:A:86:THR:O	2.40	0.55
1:B:131:LEU:HD23	1:B:131:LEU:C	2.32	0.55
1:B:31:GLY:HA3	1:C:151:ASN:OD1	2.06	0.55
1:B:64:TYR:CG	1:B:125:LEU:HD23	2.42	0.54
1:C:131:LEU:C	1:C:131:LEU:HD23	2.32	0.54
1:C:77:TYR:CD1	1:C:105:VAL:HG22	2.42	0.54
1:D:131:LEU:C	1:D:131:LEU:HD23	2.33	0.54
1:A:64:TYR:HE2	1:A:128:VAL:HG22	1.73	0.54
1:B:5:THR:CG2	1:B:20:VAL:HG12	2.38	0.53
1:C:22:VAL:HG12	1:C:41:GLN:OE1	2.07	0.53
1:A:77:TYR:CD1	1:A:105:VAL:HG22	2.44	0.53
1:D:60:ARG:NH1	1:D:88:SER:HA	2.23	0.52
1:A:131:LEU:C	1:A:131:LEU:HD23	2.35	0.52
1:B:28:VAL:HG23	3:B:301:HOH:O	2.09	0.52
1:B:66:GLY:HA3	1:B:120:ILE:HD13	1.91	0.51
1:B:26:PRO:O	1:B:155:VAL:HG23	2.11	0.51
1:C:130:ILE:HG12	1:C:145:VAL:HG22	1.93	0.51
1:D:77:TYR:CD1	1:D:105:VAL:HG22	2.45	0.51
1:A:120:ILE:HB	1:A:154:VAL:HB	1.92	0.51
1:B:26:PRO:HB2	1:B:27:VAL:HG23	1.93	0.50
1:D:83:PRO:O	1:D:86:THR:HG22	2.11	0.50
1:B:70:ASN:ND2	1:B:119:ALA:HB1	2.27	0.50
1:C:32:GLN:O	1:C:110:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLN:HA	1:B:89:GLU:HG3	1.94	0.49
1:C:5:THR:HG21	3:C:307:HOH:O	2.11	0.49
1:C:64:TYR:O	1:C:67:VAL:HG12	2.12	0.49
1:D:130:ILE:HG12	1:D:145:VAL:HG22	1.94	0.49
1:A:26:PRO:HD2	1:D:91:PRO:HG2	1.94	0.49
1:B:33:ASN:HA	1:B:110:THR:HG22	1.95	0.49
1:D:140:ASP:HB3	1:D:142:PHE:CE2	2.49	0.48
1:D:156:VAL:O	1:D:156:VAL:HG13	2.13	0.48
1:B:126:ILE:HD11	1:B:150:ALA:CB	2.37	0.48
1:B:67:VAL:CB	1:B:126:ILE:HG23	2.43	0.48
1:B:130:ILE:HG12	1:B:145:VAL:HG22	1.96	0.48
1:B:19:ASN:OD1	1:B:149:TYR:HE2	1.96	0.47
1:B:29:ASN:HB3	3:B:321:HOH:O	2.14	0.47
1:B:148:ILE:O	1:B:148:ILE:HG13	2.13	0.47
1:C:21:TYR:CD1	1:C:149:TYR:HB2	2.49	0.47
1:D:73:GLY:HA3	1:D:109:LEU:HD23	1.96	0.47
1:B:69:SER:HA	3:B:316:HOH:O	2.13	0.47
1:A:140:ASP:HB3	1:A:142:PHE:CE2	2.49	0.47
1:B:126:ILE:CD1	1:B:150:ALA:HB2	2.40	0.47
1:D:135:ASN:ND2	2:D:201:RLO:O10	2.42	0.47
1:B:66:GLY:HA3	1:B:119:ALA:O	2.15	0.46
1:C:51:THR:HG22	1:C:52:ILE:HG13	1.97	0.46
1:A:128:VAL:HG21	1:B:78:SER:C	2.41	0.46
1:C:84:PHE:HA	1:C:85:PRO:C	2.41	0.46
1:A:62:SER:HB2	1:B:79:GLY:HA2	1.97	0.45
1:C:115:ALA:HB1	1:C:156:VAL:HG21	1.98	0.45
1:D:84:PHE:HA	1:D:85:PRO:C	2.40	0.45
1:A:151:ASN:O	3:A:301:HOH:O	2.20	0.45
1:D:120:ILE:HB	1:D:154:VAL:HB	1.99	0.45
1:A:59:GLN:HA	1:A:89:GLU:HG3	2.00	0.44
1:A:60:ARG:NH2	1:A:88:SER:CA	2.81	0.44
1:B:21:TYR:CD1	1:B:149:TYR:HB2	2.52	0.44
1:B:70:ASN:ND2	1:B:119:ALA:O	2.51	0.43
1:C:3:CYS:CB	1:C:44:CYS:HG	2.26	0.43
1:C:59:GLN:HA	1:C:89:GLU:HG3	2.01	0.43
1:B:31:GLY:CA	3:B:311:HOH:O	2.66	0.43
1:D:22:VAL:HG12	1:D:41:GLN:OE1	2.18	0.43
1:B:30:VAL:HG12	3:B:311:HOH:O	2.18	0.43
1:D:5:THR:HA	1:D:41:GLN:O	2.19	0.43
1:B:67:VAL:HB	1:B:126:ILE:HG23	2.01	0.42
1:B:7:ASN:HD22	1:B:7:ASN:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HB	1:B:154:VAL:HB	2.00	0.42
1:A:54:ASP:OD2	2:A:201:RLO:O12	2.37	0.42
1:A:131:LEU:HB3	1:A:144:PHE:HB2	2.02	0.42
1:A:128:VAL:HG12	1:A:147:ASN:OD1	2.20	0.42
1:D:59:GLN:HA	1:D:89:GLU:HG3	2.02	0.42
1:A:5:THR:HA	1:A:41:GLN:O	2.20	0.42
1:B:124:SER:O	1:B:126:ILE:HD12	2.20	0.42
1:A:84:PHE:HA	1:A:85:PRO:C	2.45	0.41
1:B:67:VAL:HA	1:B:71:PHE:CD2	2.50	0.41
1:B:119:ALA:O	1:B:120:ILE:HD13	2.21	0.41
1:D:70:ASN:ND2	1:D:119:ALA:O	2.51	0.41
1:C:25:ALA:O	1:C:154:VAL:HG22	2.20	0.41
1:C:120:ILE:O	1:C:153:ASP:HA	2.21	0.41
1:B:65:GLY:O	1:B:69:SER:OG	2.39	0.41
1:B:120:ILE:O	1:B:153:ASP:HA	2.19	0.40
1:C:4:LYS:NZ	3:C:305:HOH:O	2.51	0.40
1:B:1:PHE:CD1	1:B:133:GLN:HG3	2.57	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	156/158 (99%)	149 (96%)	7 (4%)	0	100	100
1	B	156/158 (99%)	147 (94%)	9 (6%)	0	100	100
1	C	156/158 (99%)	146 (94%)	10 (6%)	0	100	100
1	D	156/158 (99%)	149 (96%)	7 (4%)	0	100	100
All	All	624/632 (99%)	591 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	133/133 (100%)	129 (97%)	4 (3%)	36	69
1	B	133/133 (100%)	116 (87%)	17 (13%)	4	19
1	C	133/133 (100%)	125 (94%)	8 (6%)	17	50
1	D	133/133 (100%)	130 (98%)	3 (2%)	44	74
All	All	532/532 (100%)	500 (94%)	32 (6%)	17	50

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	70	ASN
1	A	101	LYS
1	A	158	THR
1	B	7	ASN
1	B	24	LEU
1	B	28	VAL
1	B	41	GLN
1	B	68	LEU
1	B	69	SER
1	B	81	SER
1	B	87	THR
1	B	96	ASN
1	B	112	VAL
1	B	121	LYS
1	B	124	SER
1	B	128	VAL
1	B	143	GLN
1	B	148	ILE
1	B	155	VAL
1	B	158	THR
1	C	7	ASN
1	C	9	THR
1	C	20	VAL

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Mol	Chain	Res	Type
1	C	51	THR
1	C	96	ASN
1	C	98	ARG
1	C	109	LEU
1	C	153	ASP
1	D	7	ASN
1	D	9	THR
1	D	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	33	ASN
1	B	143	GLN
1	C	23	ASN
1	C	32	GLN
1	C	70	ASN
1	D	7	ASN
1	D	70	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](#)

4 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	RLO	B	201	-	26,26,26	3.38	19 (73%)	36,36,36	3.23	18 (50%)
2	RLO	A	201	-	26,26,26	3.60	19 (73%)	36,36,36	3.24	12 (33%)
2	RLO	D	201	-	26,26,26	3.54	19 (73%)	36,36,36	3.39	15 (41%)
2	RLO	C	201	-	26,26,26	3.39	20 (76%)	36,36,36	3.42	14 (38%)

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	RLO	B	201	-	-	2/8/28/28	0/3/3/3
2	RLO	A	201	-	-	2/8/28/28	0/3/3/3
2	RLO	D	201	-	-	4/8/28/28	0/3/3/3
2	RLO	C	201	-	-	5/8/28/28	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	RLO	C22-C23	9.52	1.60	1.31
2	C	201	RLO	C22-C23	9.31	1.60	1.31
2	D	201	RLO	C22-C23	9.12	1.59	1.31
2	B	201	RLO	C22-C23	8.88	1.58	1.31
2	D	201	RLO	C14-C15	5.32	1.50	1.42
2	A	201	RLO	C14-C15	5.08	1.49	1.42
2	A	201	RLO	C21-N24	4.77	1.41	1.32
2	A	201	RLO	C18-C22	4.72	1.60	1.47
2	B	201	RLO	C14-C15	4.61	1.49	1.42
2	D	201	RLO	C21-N24	4.59	1.41	1.32
2	C	201	RLO	C14-C15	4.45	1.48	1.42
2	C	201	RLO	C18-C22	4.44	1.60	1.47
2	D	201	RLO	C18-C22	4.36	1.59	1.47
2	B	201	RLO	C21-N24	4.34	1.40	1.32
2	A	201	RLO	C16-C17	4.27	1.45	1.36
2	C	201	RLO	C21-N24	4.23	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	RLO	C18-C22	4.14	1.59	1.47
2	A	201	RLO	C07-C01	3.96	1.61	1.52
2	C	201	RLO	C16-C17	3.94	1.45	1.36
2	B	201	RLO	C16-C17	3.94	1.45	1.36
2	D	201	RLO	C07-C01	3.92	1.61	1.52
2	D	201	RLO	C16-C17	3.90	1.45	1.36
2	C	201	RLO	C07-C01	3.87	1.61	1.52
2	D	201	RLO	C02-C01	3.86	1.61	1.53
2	A	201	RLO	C02-C01	3.86	1.61	1.53
2	A	201	RLO	C07-C23	3.81	1.61	1.50
2	B	201	RLO	C02-C01	3.69	1.60	1.53
2	C	201	RLO	C07-C23	3.67	1.60	1.50
2	C	201	RLO	C02-C01	3.66	1.60	1.53
2	D	201	RLO	C04-C05	3.62	1.60	1.53
2	B	201	RLO	C04-C05	3.59	1.60	1.53
2	B	201	RLO	C03-C02	3.52	1.61	1.52
2	B	201	RLO	C07-C01	3.50	1.60	1.52
2	D	201	RLO	C07-C23	3.45	1.60	1.50
2	D	201	RLO	C03-C02	3.42	1.61	1.52
2	B	201	RLO	C07-C23	3.39	1.59	1.50
2	D	201	RLO	C04-C03	3.33	1.61	1.52
2	A	201	RLO	C13-C18	3.29	1.44	1.38
2	A	201	RLO	C04-C05	3.26	1.60	1.53
2	D	201	RLO	C13-C18	3.25	1.44	1.38
2	A	201	RLO	C20-C19	3.25	1.43	1.36
2	C	201	RLO	C04-C05	3.24	1.59	1.53
2	A	201	RLO	C03-C02	3.22	1.60	1.52
2	C	201	RLO	C13-C18	3.14	1.44	1.38
2	B	201	RLO	C20-C19	3.14	1.43	1.36
2	D	201	RLO	C20-C19	3.11	1.43	1.36
2	C	201	RLO	C20-C19	3.10	1.43	1.36
2	C	201	RLO	C03-C02	3.07	1.60	1.52
2	A	201	RLO	C16-C15	3.06	1.47	1.41
2	B	201	RLO	C13-C18	3.03	1.44	1.38
2	D	201	RLO	C16-C15	3.02	1.46	1.41
2	A	201	RLO	C17-C18	2.96	1.45	1.39
2	B	201	RLO	C16-C15	2.95	1.46	1.41
2	A	201	RLO	C04-C03	2.93	1.59	1.52
2	A	201	RLO	C15-N24	2.91	1.42	1.37
2	D	201	RLO	C15-N24	2.86	1.42	1.37
2	D	201	RLO	C20-C21	2.85	1.45	1.37
2	B	201	RLO	C04-C03	2.84	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	RLO	C15-N24	2.78	1.42	1.37
2	C	201	RLO	C04-C03	2.77	1.59	1.52
2	C	201	RLO	C15-N24	2.73	1.42	1.37
2	A	201	RLO	C20-C21	2.66	1.45	1.37
2	C	201	RLO	C20-C21	2.61	1.45	1.37
2	B	201	RLO	C06-C05	2.59	1.60	1.51
2	C	201	RLO	C06-C05	2.55	1.60	1.51
2	D	201	RLO	C06-C05	2.52	1.60	1.51
2	D	201	RLO	C17-C18	2.50	1.44	1.39
2	B	201	RLO	C20-C21	2.49	1.44	1.37
2	C	201	RLO	C16-C15	2.49	1.46	1.41
2	A	201	RLO	C06-C05	2.42	1.59	1.51
2	B	201	RLO	C17-C18	2.28	1.44	1.39
2	D	201	RLO	O10-C04	2.15	1.48	1.43
2	C	201	RLO	C13-C14	2.10	1.46	1.42
2	C	201	RLO	C17-C18	2.08	1.43	1.39
2	B	201	RLO	C13-C14	2.06	1.46	1.42
2	A	201	RLO	C13-C14	2.04	1.46	1.42
2	C	201	RLO	O09-C03	2.04	1.48	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	RLO	C07-C23-C22	12.72	140.72	124.31
2	C	201	RLO	C07-C23-C22	11.70	139.41	124.31
2	B	201	RLO	C07-C23-C22	10.94	138.43	124.31
2	C	201	RLO	C18-C22-C23	10.49	152.67	126.99
2	D	201	RLO	C07-C01-C02	-9.76	102.12	114.16
2	D	201	RLO	C07-C23-C22	8.95	135.86	124.31
2	A	201	RLO	C18-C22-C23	7.72	145.89	126.99
2	D	201	RLO	C18-C22-C23	7.50	145.35	126.99
2	B	201	RLO	C18-C22-C23	7.44	145.22	126.99
2	C	201	RLO	C13-C14-C15	5.30	125.10	118.31
2	D	201	RLO	C18-C13-C14	-5.19	114.87	121.69
2	A	201	RLO	C07-C01-C02	-5.01	107.97	114.16
2	B	201	RLO	C18-C13-C14	-4.93	115.21	121.69
2	B	201	RLO	C13-C14-C15	4.80	124.45	118.31
2	C	201	RLO	C19-C20-C21	4.43	124.46	118.92
2	B	201	RLO	C01-C07-C23	-4.42	101.75	113.23
2	A	201	RLO	C13-C14-C15	4.34	123.87	118.31
2	A	201	RLO	C17-C16-C15	-4.26	115.71	120.80
2	D	201	RLO	C19-C20-C21	4.25	124.23	118.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	RLO	C18-C13-C14	-4.19	116.18	121.69
2	C	201	RLO	C16-C15-C14	-4.03	115.00	119.04
2	D	201	RLO	C17-C18-C13	4.00	123.43	118.58
2	B	201	RLO	O11-C05-C04	3.99	116.88	109.70
2	D	201	RLO	C20-C19-C14	-3.85	115.13	120.48
2	B	201	RLO	C07-C01-C02	-3.81	109.46	114.16
2	C	201	RLO	C14-C15-N24	3.77	127.22	122.03
2	D	201	RLO	C13-C14-C15	3.70	123.05	118.31
2	D	201	RLO	O11-C05-C04	3.67	116.31	109.70
2	C	201	RLO	C20-C21-N24	-3.59	118.70	123.97
2	B	201	RLO	C20-C21-N24	-3.57	118.73	123.97
2	A	201	RLO	C16-C17-C18	3.49	125.26	120.90
2	C	201	RLO	C04-C03-C02	-3.44	104.79	110.83
2	C	201	RLO	C13-C18-C22	3.41	127.39	119.64
2	C	201	RLO	C18-C13-C14	-3.34	117.30	121.69
2	D	201	RLO	C17-C16-C15	-3.33	116.81	120.80
2	C	201	RLO	C19-C14-C15	-3.27	114.03	118.43
2	A	201	RLO	C20-C21-N24	-3.24	119.21	123.97
2	D	201	RLO	C01-C07-C23	-3.21	104.89	113.23
2	D	201	RLO	O11-C01-C02	3.03	115.16	109.70
2	B	201	RLO	O11-C01-C02	3.02	115.14	109.70
2	B	201	RLO	C06-C05-C04	-2.97	105.74	113.02
2	D	201	RLO	C19-C14-C13	-2.94	116.95	122.00
2	A	201	RLO	C06-C05-C04	-2.93	105.82	113.02
2	B	201	RLO	C17-C16-C15	-2.93	117.30	120.80
2	C	201	RLO	C16-C17-C18	2.87	124.48	120.90
2	B	201	RLO	C19-C20-C21	2.85	122.48	118.92
2	A	201	RLO	C21-N24-C15	2.82	121.20	116.93
2	B	201	RLO	C17-C18-C13	2.59	121.72	118.58
2	D	201	RLO	C06-C05-C04	-2.44	107.02	113.02
2	A	201	RLO	C03-C04-C05	-2.38	105.92	110.23
2	B	201	RLO	O08-C02-C03	2.37	115.97	110.38
2	D	201	RLO	O12-C06-C05	-2.29	103.54	111.33
2	B	201	RLO	O08-C02-C01	-2.25	103.78	109.32
2	C	201	RLO	C07-C01-C02	-2.22	111.42	114.16
2	B	201	RLO	C03-C04-C05	-2.21	106.22	110.23
2	B	201	RLO	C16-C17-C18	2.18	123.62	120.90
2	A	201	RLO	C19-C14-C13	-2.08	118.43	122.00
2	B	201	RLO	C19-C14-C15	-2.06	115.66	118.43
2	C	201	RLO	C17-C18-C22	-2.03	114.01	121.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	RLO	C18-C22-C23-C07
2	C	201	RLO	C17-C18-C22-C23
2	D	201	RLO	C13-C18-C22-C23
2	C	201	RLO	C13-C18-C22-C23
2	D	201	RLO	C17-C18-C22-C23
2	D	201	RLO	C04-C05-C06-O12
2	A	201	RLO	C18-C22-C23-C07
2	B	201	RLO	C13-C18-C22-C23
2	B	201	RLO	C17-C18-C22-C23
2	C	201	RLO	O11-C05-C06-O12
2	D	201	RLO	O11-C05-C06-O12
2	C	201	RLO	C04-C05-C06-O12
2	A	201	RLO	O11-C01-C07-C23

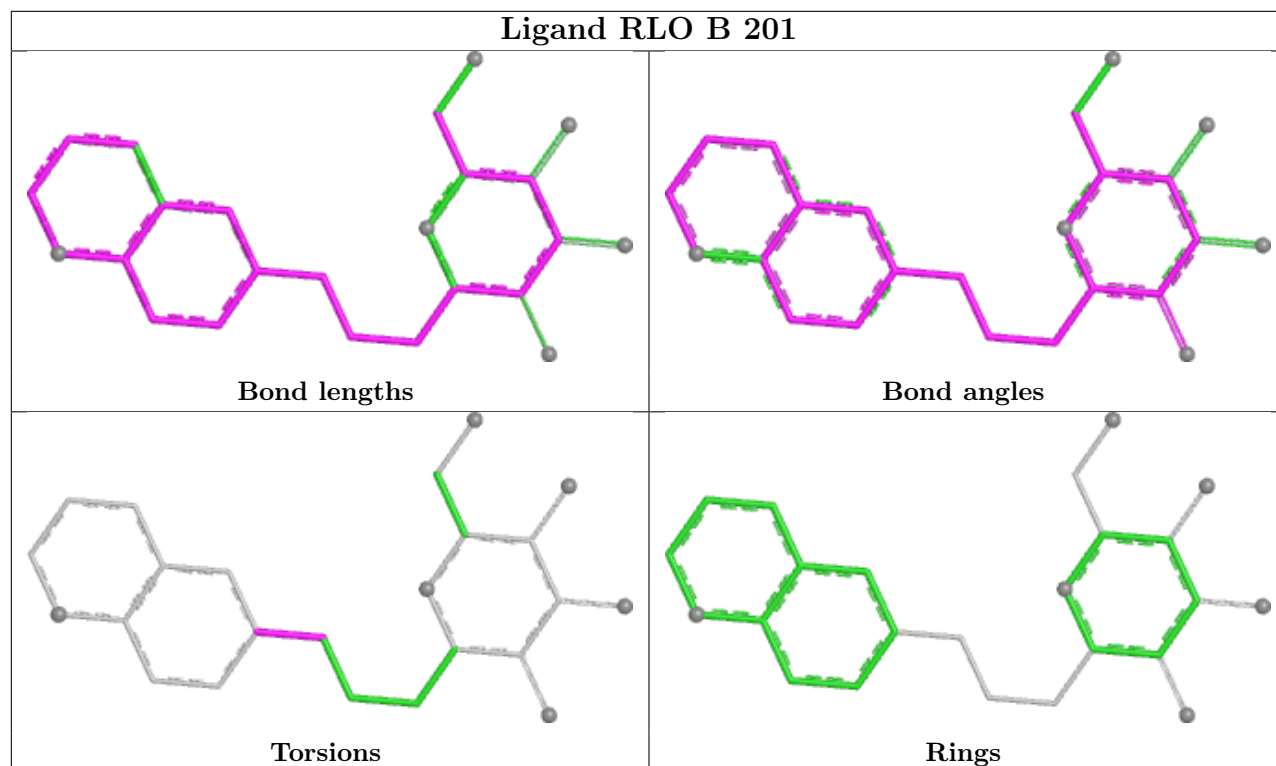
There are no ring outliers.

2 monomers are involved in 2 short contacts:

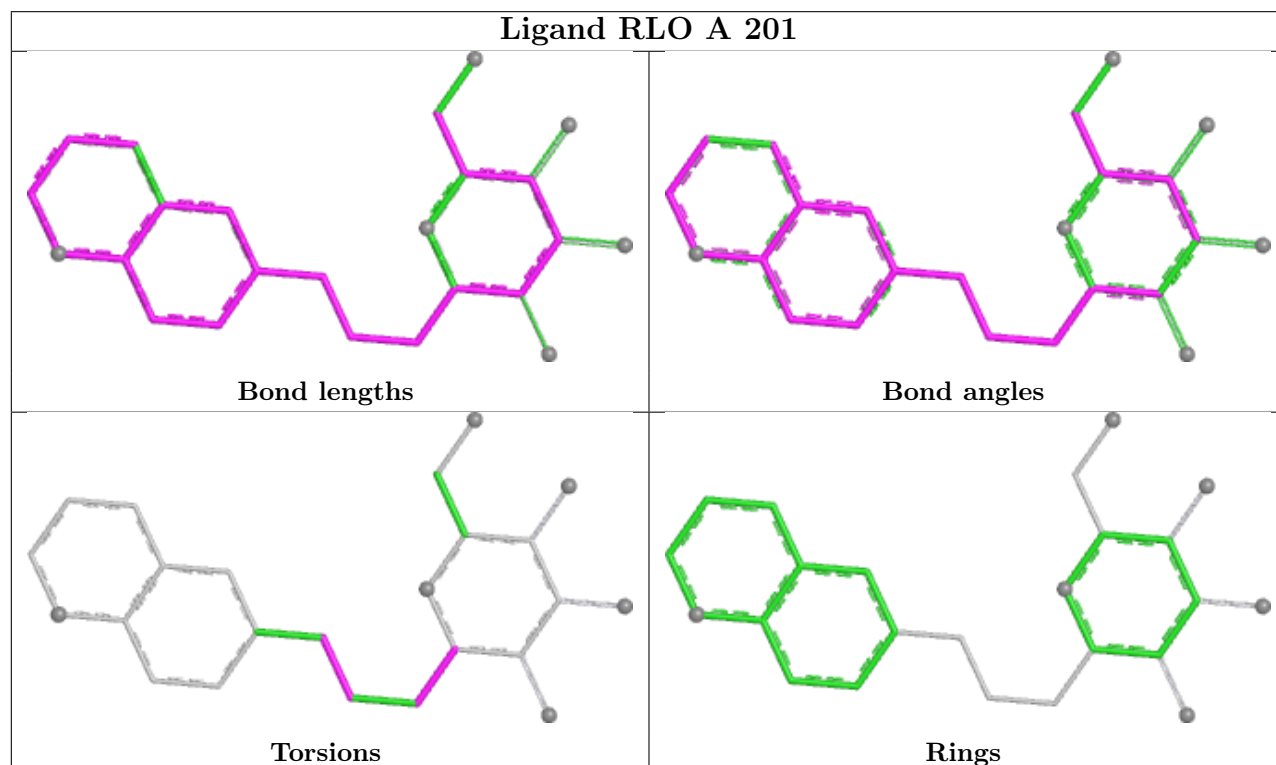
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	RLO	1	0
2	D	201	RLO	1	0

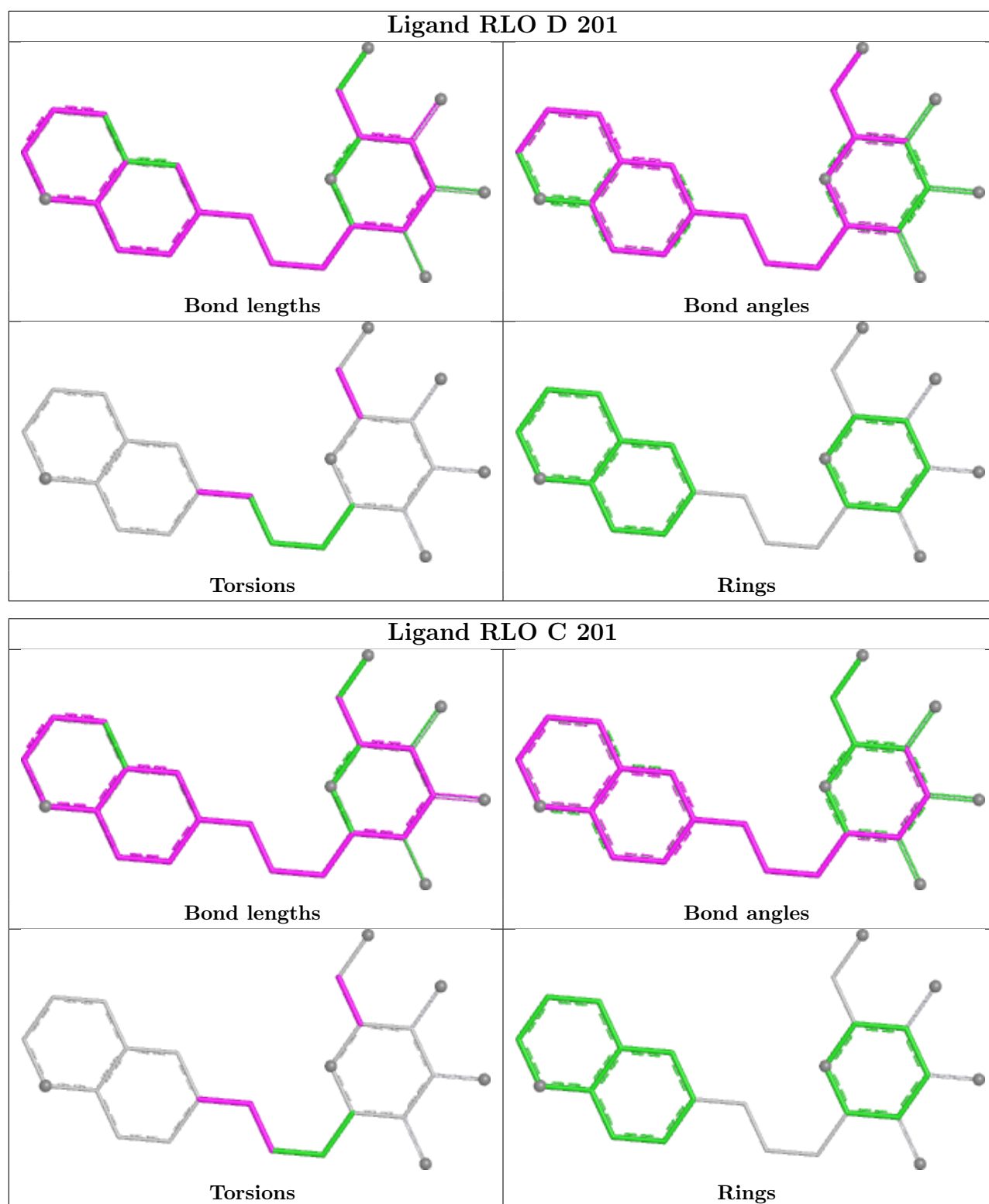
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand RLO B 201



Ligand RLO A 201





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	158/158 (100%)	0.37	6 (3%) 44 24	30, 47, 69, 92	0
1	B	158/158 (100%)	1.73	69 (43%) 0 1	37, 68, 103, 122	0
1	C	158/158 (100%)	1.14	27 (17%) 4 3	40, 60, 92, 144	0
1	D	158/158 (100%)	0.52	7 (4%) 39 21	30, 51, 82, 97	0
All	All	632/632 (100%)	0.94	109 (17%) 4 3	30, 56, 91, 144	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	VAL	7.7
1	B	117	GLY	6.6
1	B	112	VAL	6.1
1	B	64	TYR	5.8
1	C	31	GLY	5.7
1	B	68	LEU	4.9
1	B	150	ALA	4.8
1	B	34	LEU	4.7
1	C	7	ASN	4.4
1	B	119	ALA	4.3
1	B	149	TYR	4.2
1	B	21	TYR	4.1
1	B	85	PRO	4.1
1	C	113	SER	4.0
1	A	158	THR	4.0
1	B	67	VAL	4.0
1	B	156	VAL	4.0
1	B	157	PRO	3.9
1	B	26	PRO	3.9
1	B	115	ALA	3.9
1	B	30	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	62	SER	3.8
1	B	71	PHE	3.6
1	C	29	ASN	3.5
1	D	151	ASN	3.5
1	B	113	SER	3.5
1	B	148	ILE	3.4
1	B	118	VAL	3.4
1	B	158	THR	3.4
1	B	154	VAL	3.4
1	C	28	VAL	3.4
1	C	114	SER	3.4
1	B	121	LYS	3.3
1	B	63	ALA	3.3
1	B	31	GLY	3.3
1	B	74	THR	3.2
1	B	110	THR	3.2
1	B	22	VAL	3.2
1	B	28	VAL	3.2
1	B	123	GLY	3.2
1	B	35	VAL	3.1
1	C	27	VAL	3.1
1	A	87	THR	3.1
1	C	158	THR	3.1
1	D	158	THR	3.1
1	B	25	ALA	3.0
1	B	29	ASN	3.0
1	B	66	GLY	3.0
1	B	126	ILE	3.0
1	B	70	ASN	3.0
1	C	64	TYR	2.9
1	B	33	ASN	2.9
1	B	87	THR	2.9
1	B	111	PRO	2.8
1	B	36	VAL	2.8
1	C	10	ALA	2.8
1	B	114	SER	2.8
1	B	124	SER	2.8
1	C	60	ARG	2.8
1	B	80	SER	2.8
1	B	27	VAL	2.8
1	B	127	ALA	2.8
1	C	121	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	2.7
1	B	32	GLN	2.7
1	B	108	TYR	2.7
1	B	116	GLY	2.7
1	B	120	ILE	2.7
1	B	24	LEU	2.7
1	A	7	ASN	2.7
1	B	19	ASN	2.7
1	C	33	ASN	2.7
1	D	66	GLY	2.7
1	C	89	GLU	2.6
1	B	20	VAL	2.5
1	B	125	LEU	2.5
1	A	157	PRO	2.5
1	B	4	LYS	2.5
1	C	72	SER	2.5
1	D	124	SER	2.5
1	D	25	ALA	2.4
1	B	72	SER	2.4
1	C	25	ALA	2.4
1	B	147	ASN	2.4
1	B	60	ARG	2.4
1	C	153	ASP	2.4
1	C	110	THR	2.3
1	B	73	GLY	2.3
1	D	69	SER	2.3
1	D	113	SER	2.3
1	C	151	ASN	2.2
1	B	59	GLN	2.2
1	B	65	GLY	2.2
1	C	120	ILE	2.2
1	C	92	ARG	2.2
1	C	70	ASN	2.2
1	C	26	PRO	2.2
1	B	155	VAL	2.1
1	C	117	GLY	2.1
1	A	32	GLN	2.1
1	C	116	GLY	2.1
1	B	122	ALA	2.1
1	B	38	LEU	2.1
1	A	121	LYS	2.1
1	B	7	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	153	ASP	2.0
1	B	69	SER	2.0
1	C	71	PHE	2.0
1	B	10	ALA	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](#)

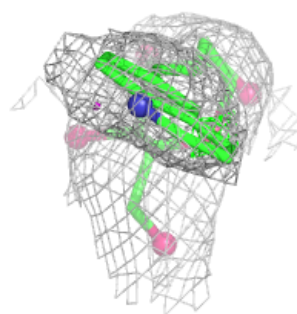
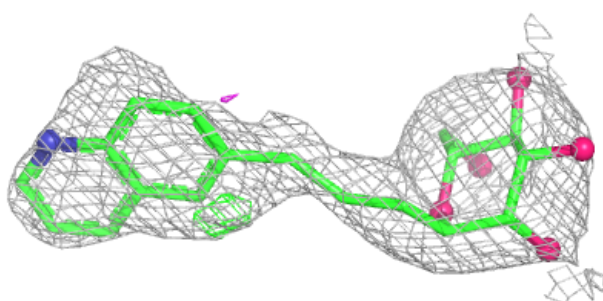
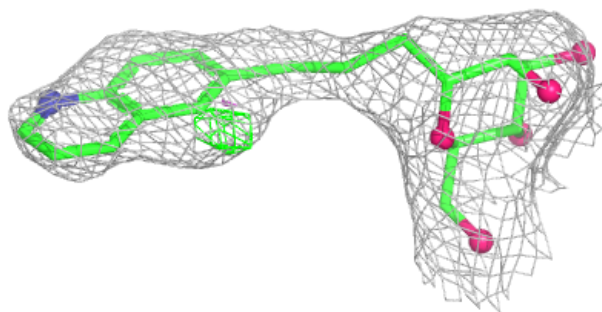
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RLO	A	201	24/24	0.89	0.18	37,56,69,72	0
2	RLO	D	201	24/24	0.93	0.12	34,40,54,61	0
2	RLO	C	201	24/24	0.94	0.14	34,44,65,72	0
2	RLO	B	201	24/24	0.94	0.11	30,34,62,67	0

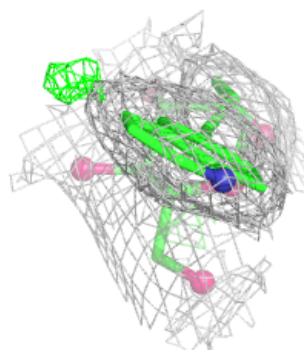
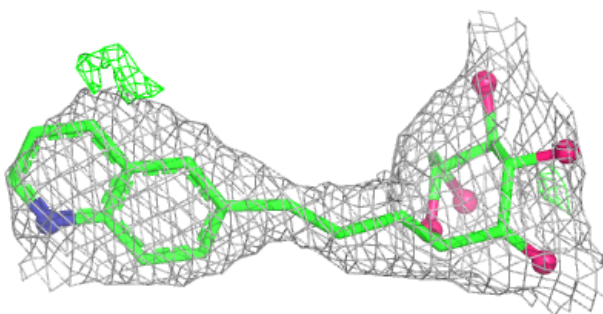
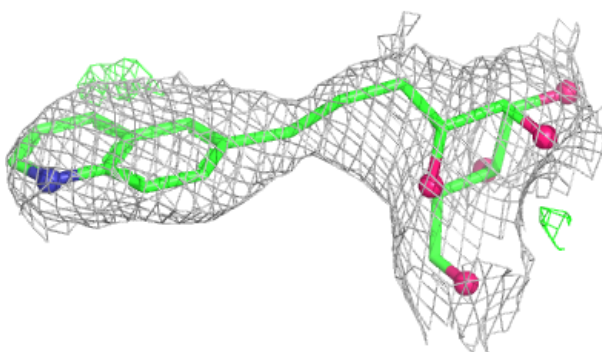
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RLO A 201:

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

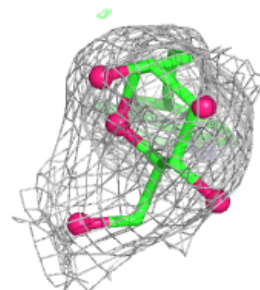
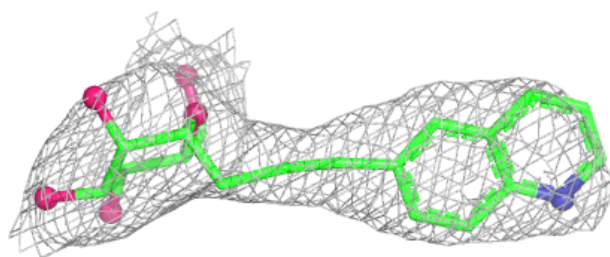
**Electron density around RLO D 201:**

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

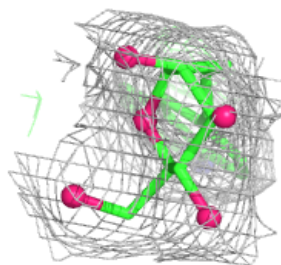
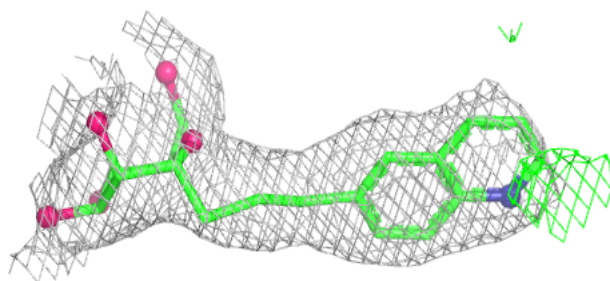
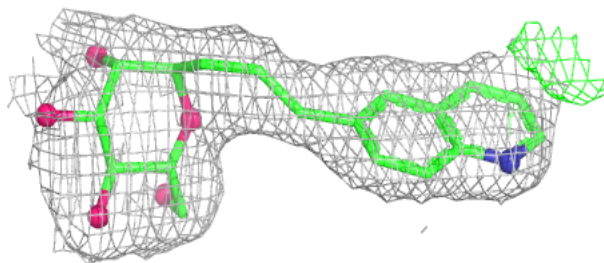


Electron density around RLO C 201:

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

**Electron density around RLO B 201:**

$2mF_o-DF_c$ (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.