



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 08:24 AM JST

PDB ID : 6LDB  
Title : Structure of Bifidobacterium dentium beta-glucuronidase complexed with uronic isofagomine  
Authors : Lin, H.-Y.; Hsieh, T.-J.; Lin, C.-H.  
Deposited on : 2019-11-20  
Resolution : 1.65 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

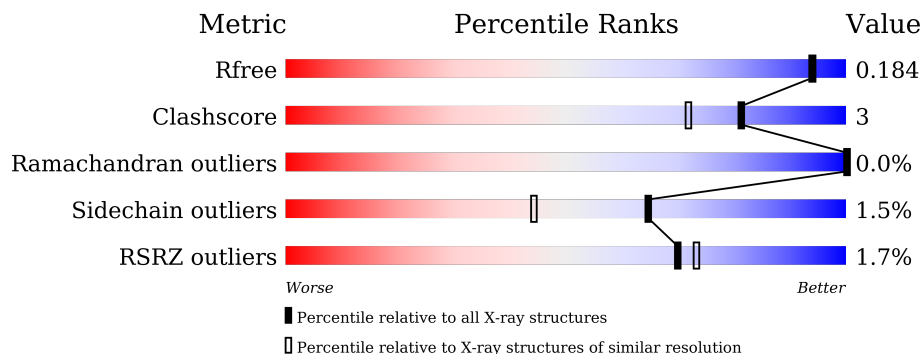
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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  $\geq 3$ , 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	670	 2% 87% 5% 7%
1	B	670	 2% 87% 5% 7%
1	C	670	 2% 86% 7% 7%
1	D	670	 2% 85% 7% 7%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22393 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.

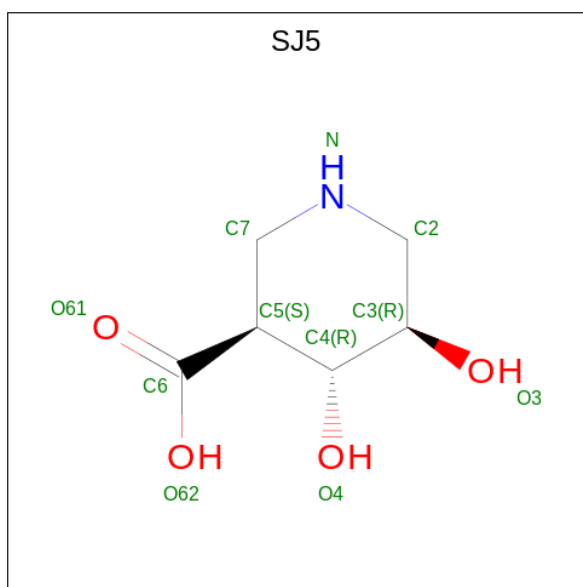
- Molecule 1 is a protein called LacZ1 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	4915	3116	857	922	20	0	1	0
1	B	620	4915	3116	857	922	20	0	1	0
1	C	620	4915	3116	857	922	20	0	1	0
1	D	620	4915	3116	857	922	20	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP D2Q7B1
A	0	GLY	-	expression tag	UNP D2Q7B1
B	-1	ASN	-	expression tag	UNP D2Q7B1
B	0	GLY	-	expression tag	UNP D2Q7B1
C	-1	ASN	-	expression tag	UNP D2Q7B1
C	0	GLY	-	expression tag	UNP D2Q7B1
D	-1	ASN	-	expression tag	UNP D2Q7B1
D	0	GLY	-	expression tag	UNP D2Q7B1

- Molecule 2 is (3S,4R,5R)-4,5-dihydropiperidine-3-carboxylic acid (three-letter code: SJ5) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	6	1	4	0	0
2	B	1	11	6	1	4	0	0
2	C	1	11	6	1	4	0	0
2	D	1	11	6	1	4	0	0

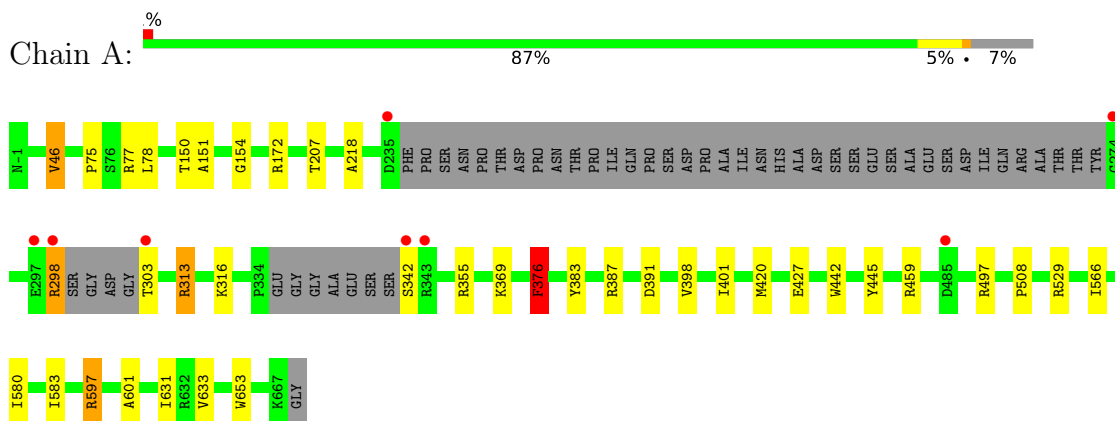
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	774	774	774	0	0
3	B	719	719	719	0	0
3	C	616	616	616	0	0
3	D	580	580	580	0	0

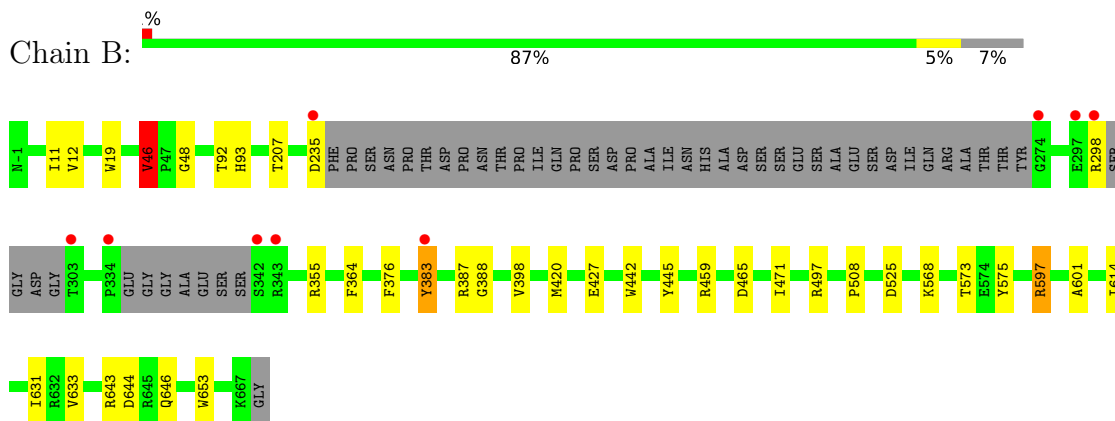
### 3 Residue-property plots [i](#)

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.

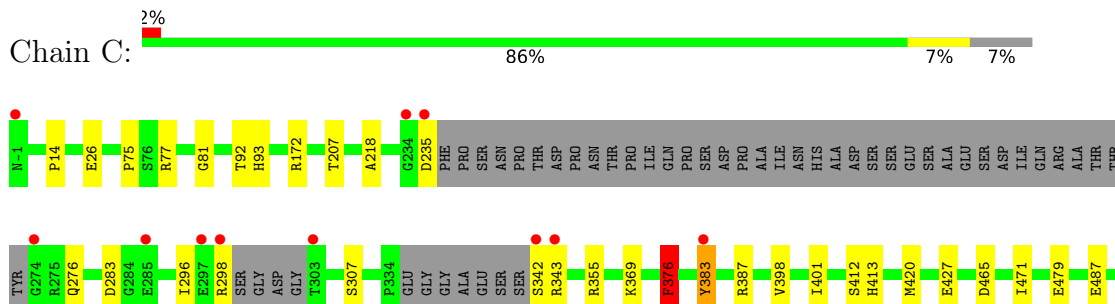
- Molecule 1: LacZ1 Beta-galactosidase



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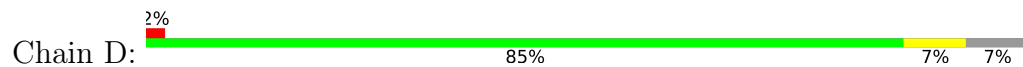


- Molecule 1: LacZ1 Beta-galactosidase





● Molecule 1: LacZ1 Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.69Å 104.64Å 160.50Å 90.00° 91.29° 90.00°	Depositor
Resolution (Å)	24.85 – 1.65 24.85 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.2 (24.85-1.65) 91.1 (24.85-1.65)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 1.65Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.156 , 0.183 0.156 , 0.184	Depositor DCC
$R_{free}$ test set	1999 reflections (0.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SJ5

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	0.73	4/5046 (0.1%)	0.85	11/6865 (0.2%)
1	B	0.68	0/5046	0.82	5/6865 (0.1%)
1	C	0.64	1/5046 (0.0%)	0.81	9/6865 (0.1%)
1	D	0.63	0/5046	0.78	6/6865 (0.1%)
All	All	0.67	5/20184 (0.0%)	0.82	31/27460 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	ARG	NE-CZ	-11.90	1.17	1.33
1	A	313	ARG	CZ-NH1	-11.13	1.18	1.33
1	A	376	PHE	CD1-CE1	-7.61	1.24	1.39
1	A	313	ARG	CZ-NH2	-6.70	1.24	1.33
1	C	376	PHE	CD2-CE2	5.10	1.49	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	376	PHE	CB-CG-CD1	-10.12	113.72	120.80
1	C	376	PHE	CB-CG-CD1	-10.04	113.77	120.80
1	C	387	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	B	387	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	C	511	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	376	PHE	CB-CG-CD2	8.56	126.79	120.80
1	D	387	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	376	PHE	CB-CG-CD2	8.01	126.41	120.80
1	D	387	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	387	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	313	ARG	NE-CZ-NH1	-7.39	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	VAL	CG1-CB-CG2	7.23	122.46	110.90
1	C	283	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	376	PHE	CG-CD2-CE2	-6.41	113.75	120.80
1	D	108	PHE	CA-C-N	6.21	128.63	116.20
1	D	108	PHE	O-C-N	-6.20	112.65	123.20
1	A	46	VAL	CG1-CB-CG2	6.17	120.78	110.90
1	A	387	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	D	426	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	383	TYR	CA-CB-CG	-5.83	102.31	113.40
1	C	387	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	376	PHE	CG-CD2-CE2	-5.62	114.62	120.80
1	A	529	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	525	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	597	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	387	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	597	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	410	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	459	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	525	ASP	CB-CG-OD1	5.05	122.85	118.30

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	4915	0	4663	23	0
1	B	4915	0	4663	19	0
1	C	4915	0	4663	31	0
1	D	4915	0	4663	34	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	11	0	0	1	0
3	A	774	0	0	8	1
3	B	719	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	616	0	0	6	0
3	D	580	0	0	8	0
All	All	22393	0	18652	100	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 3.

All (100) 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:D:173:GLN:NE2	3:D:801:HOH:O	1.86	1.06
1:A:172:ARG:NH2	3:A:801:HOH:O	2.00	0.93
1:D:219:CYS:SG	3:D:1309:HOH:O	2.28	0.90
1:B:597:ARG:NH2	3:B:801:HOH:O	2.07	0.88
1:D:342:SER:OG	1:D:343:ARG:NH1	2.07	0.87
1:A:77:ARG:NH1	3:A:802:HOH:O	2.08	0.85
1:B:497:ARG:NH1	3:B:803:HOH:O	2.13	0.82
1:A:298:ARG:CZ	1:A:303:THR:N	2.45	0.79
1:C:342:SER:HB2	1:C:343:ARG:HH11	1.49	0.78
1:B:631:ILE:HG22	1:C:631:ILE:HG22	1.65	0.78
1:C:235:ASP:OD2	3:C:801:HOH:O	2.02	0.77
1:A:631:ILE:HG22	1:D:631:ILE:HG22	1.71	0.72
1:D:497:ARG:NH1	3:D:802:HOH:O	2.09	0.72
1:B:646:GLN:OE1	3:B:802:HOH:O	2.08	0.72
1:A:391:ASP:OD1	3:A:803:HOH:O	2.08	0.71
1:A:497:ARG:NH1	3:A:804:HOH:O	2.11	0.70
1:A:150:THR:HG22	1:A:151:ALA:O	1.92	0.69
1:C:81:GLY:O	3:C:802:HOH:O	2.10	0.69
1:C:26:GLU:OE1	1:C:172:ARG:NH2	2.30	0.65
1:C:383:TYR:O	3:C:803:HOH:O	2.14	0.64
1:C:77:ARG:O	1:D:77:ARG:NH1	2.31	0.64
1:C:518[A]:CYS:SG	3:C:1338:HOH:O	2.56	0.62
1:D:27:ASP:OD1	3:D:803:HOH:O	2.16	0.61
1:A:566:ILE:HB	3:A:1202:HOH:O	2.00	0.61
1:D:93:HIS:O	1:D:108:PHE:O	2.19	0.60
1:D:218:ALA:HB2	1:D:369:LYS:HE2	1.83	0.59
1:C:376:PHE:HZ	1:C:401:ILE:HG12	1.68	0.58
1:B:207:THR:HG21	1:B:508:PRO:HB2	1.86	0.58
1:C:509:GLN:HB3	1:C:511:ARG:HD2	1.86	0.58
1:C:26:GLU:OE1	1:C:172:ARG:NE	2.37	0.57
1:C:14:PRO:HG2	1:D:14:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:VAL:HG11	1:D:427:GLU:HG3	1.87	0.56
1:A:298:ARG:NH1	1:A:303:THR:N	2.54	0.55
1:A:376:PHE:HZ	1:A:401:ILE:HG12	1.72	0.55
1:C:507:ASP:OD2	1:C:511:ARG:HD3	2.08	0.53
1:C:580:ILE:HB	1:C:583:ILE:HD12	1.90	0.53
1:A:580:ILE:HB	1:A:583:ILE:HD12	1.89	0.53
1:A:75:PRO:HD2	1:A:78:LEU:HD23	1.91	0.53
1:D:342:SER:OG	1:D:343:ARG:CZ	2.57	0.53
1:A:398:VAL:HG11	1:A:427:GLU:HG3	1.90	0.53
1:C:398:VAL:HG11	1:C:427:GLU:HG3	1.90	0.53
1:C:26:GLU:OE1	1:C:172:ARG:CZ	2.57	0.53
1:C:276:GLN:NE2	3:C:809:HOH:O	2.29	0.52
1:D:507:ASP:OD2	1:D:511:ARG:HD2	2.09	0.51
1:D:490:ARG:HD2	3:D:838:HOH:O	2.11	0.51
1:A:316:LYS:NZ	3:A:805:HOH:O	2.20	0.51
1:D:207:THR:HG21	1:D:508:PRO:HB2	1.92	0.50
1:C:296:ILE:O	1:C:298:ARG:NH1	2.45	0.50
1:A:75:PRO:HD2	1:A:78:LEU:CD2	2.42	0.49
1:D:152:PHE:CE1	1:D:153:MET:HG3	2.47	0.49
1:C:487:GLU:OE2	3:C:805:HOH:O	2.19	0.49
1:D:459:ARG:NH1	3:D:812:HOH:O	2.42	0.48
1:C:479:GLU:HB3	1:C:518[A]:CYS:HB3	1.94	0.48
1:D:303:THR:O	1:D:305:LYS:HG3	2.15	0.47
1:D:334:PRO:HB3	1:D:345:ILE:HD11	1.95	0.47
1:A:597:ARG:HD2	3:A:1433:HOH:O	2.14	0.47
1:B:644:ASP:HB2	3:B:802:HOH:O	2.14	0.47
1:C:342:SER:HB2	1:C:343:ARG:NH1	2.23	0.47
1:D:580:ILE:HB	1:D:583:ILE:HD12	1.97	0.46
1:D:342:SER:HG	1:D:343:ARG:NH1	2.10	0.46
1:D:231:THR:OG1	1:D:305:LYS:NZ	2.48	0.46
1:A:633:VAL:HG21	1:D:633:VAL:HG21	1.99	0.45
1:A:442:TRP:HA	1:A:445:TYR:CD2	2.52	0.45
1:C:75:PRO:HA	1:D:8:ASP:HA	1.99	0.44
1:C:343:ARG:N	1:C:343:ARG:HD3	2.32	0.44
1:B:398:VAL:HG11	1:B:427:GLU:HG3	2.00	0.44
1:A:601:ALA:HA	1:A:653:TRP:CH2	2.53	0.43
1:C:218:ALA:HB2	1:C:369:LYS:HE2	2.00	0.43
1:A:218:ALA:HB2	1:A:369:LYS:HE2	2.00	0.43
1:D:314:ASP:OD1	3:D:804:HOH:O	2.21	0.43
1:D:92:THR:HA	1:D:93:HIS:HA	1.86	0.43
1:D:412:SER:HA	1:D:413:HIS:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:ALA:HA	1:C:653:TRP:CH2	2.53	0.43
1:C:207:THR:HG21	1:C:508:PRO:HB2	2.01	0.43
1:C:412:SER:HA	1:C:413:HIS:HA	1.80	0.43
1:C:465:ASP:HB3	1:C:471:ILE:CD1	2.49	0.42
1:D:172:ARG:HA	1:D:172:ARG:HD2	1.68	0.42
1:B:643:ARG:NH1	3:B:829:HOH:O	2.51	0.42
1:B:92:THR:HA	1:B:93:HIS:HA	1.88	0.42
1:C:92:THR:HA	1:C:93:HIS:HA	1.86	0.42
1:D:165:GLU:HG2	3:D:1281:HOH:O	2.20	0.42
1:A:207:THR:HG21	1:A:508:PRO:HB2	2.02	0.41
1:B:601:ALA:HA	1:B:653:TRP:CH2	2.54	0.41
1:C:479:GLU:CB	1:C:518[A]:CYS:HB3	2.49	0.41
1:D:429:ILE:O	1:D:470:CYS:HB2	2.19	0.41
1:B:465:ASP:HB3	1:B:471:ILE:CD1	2.49	0.41
1:D:574:GLU:OE1	2:D:701:SJ5:N	2.53	0.41
1:B:235:ASP:OD2	3:B:804:HOH:O	2.22	0.41
1:B:459:ARG:NH1	3:B:814:HOH:O	2.40	0.41
1:A:150:THR:CG2	1:A:154:GLY:HA3	2.51	0.41
1:B:633:VAL:HG21	1:C:633:VAL:HG21	2.02	0.41
1:B:11:ILE:HD12	1:B:12:VAL:H	1.86	0.41
1:D:152:PHE:CE1	1:D:179:ASP:HB2	2.56	0.41
1:A:342:SER:N	3:A:837:HOH:O	2.54	0.41
1:B:48:GLY:HA2	1:B:388:GLY:HA3	2.02	0.40
1:B:442:TRP:HA	1:B:445:TYR:CD2	2.55	0.40
1:B:364:PHE:HB2	1:B:614:ILE:HD13	2.03	0.40
1:D:655:ARG:HH11	1:D:655:ARG:HD3	1.71	0.40
1:B:19:TRP:CD1	1:B:46:VAL:HG13	2.56	0.40
1:D:497:ARG:HD2	1:D:497:ARG:HA	1.78	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)
3:B:1371:HOH:O	3:B:1400:HOH:O[2_544]	2.13	0.07
3:A:875:HOH:O	3:A:1337:HOH:O[2_444]	2.19	0.01

## 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	613/670 (92%)	598 (98%)	15 (2%)	0	100	100
1	B	613/670 (92%)	595 (97%)	18 (3%)	0	100	100
1	C	613/670 (92%)	597 (97%)	15 (2%)	1 (0%)	47	28
1	D	613/670 (92%)	598 (98%)	15 (2%)	0	100	100
All	All	2452/2680 (92%)	2388 (97%)	63 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	TYR

### 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	504/543 (93%)	497 (99%)	7 (1%)	67	46
1	B	504/543 (93%)	494 (98%)	10 (2%)	55	32
1	C	504/543 (93%)	497 (99%)	7 (1%)	67	46
1	D	504/543 (93%)	497 (99%)	7 (1%)	67	46
All	All	2016/2172 (93%)	1985 (98%)	31 (2%)	65	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	298	ARG
1	A	313	ARG
1	A	355	ARG
1	A	376	PHE
1	A	383	TYR
1	A	420	MET
1	B	46	VAL
1	B	298	ARG
1	B	355	ARG
1	B	376	PHE
1	B	383	TYR
1	B	420	MET
1	B	568	LYS
1	B	573	THR
1	B	575	TYR
1	B	597	ARG
1	C	307	SER
1	C	355	ARG
1	C	376	PHE
1	C	420	MET
1	C	511	ARG
1	C	575	TYR
1	C	597	ARG
1	D	343	ARG
1	D	355	ARG
1	D	376	PHE
1	D	383	TYR
1	D	420	MET
1	D	485	ASP
1	D	575	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	565	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 monosaccharides 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	SJ5	C	701	-	11,11,11	1.45	2 (18%)	11,15,15	1.62	3 (27%)
2	SJ5	D	701	-	11,11,11	0.94	0	11,15,15	1.63	4 (36%)
2	SJ5	A	701	-	11,11,11	1.15	2 (18%)	11,15,15	1.55	3 (27%)
2	SJ5	B	701	-	11,11,11	1.35	2 (18%)	11,15,15	1.40	4 (36%)

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	SJ5	C	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	D	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	A	701	-	-	2/4/18/18	0/1/1/1
2	SJ5	B	701	-	-	2/4/18/18	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	SJ5	O61-C6	3.35	1.32	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	SJ5	O62-C6	-2.75	1.21	1.30
2	A	701	SJ5	O62-C6	-2.39	1.22	1.30
2	B	701	SJ5	O61-C6	2.26	1.29	1.22
2	C	701	SJ5	O62-C6	-2.18	1.23	1.30
2	A	701	SJ5	O61-C6	2.06	1.28	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	SJ5	C7-N-C2	3.20	115.22	111.70
2	A	701	SJ5	O61-C6-C5	-3.08	115.22	122.95
2	C	701	SJ5	O61-C6-C5	-2.96	115.52	122.95
2	C	701	SJ5	C7-N-C2	2.75	114.72	111.70
2	C	701	SJ5	O62-C6-C5	2.51	120.93	114.03
2	B	701	SJ5	O61-C6-C5	-2.30	117.19	122.95
2	B	701	SJ5	C7-C5-C6	-2.28	106.89	111.19
2	D	701	SJ5	O4-C4-C5	2.27	114.74	110.57
2	B	701	SJ5	C7-N-C2	2.20	114.12	111.70
2	D	701	SJ5	C7-C5-C6	-2.19	107.06	111.19
2	A	701	SJ5	O62-C6-C5	2.15	119.94	114.03
2	D	701	SJ5	C2-C3-C4	-2.14	107.82	110.33
2	A	701	SJ5	C7-C5-C6	-2.04	107.35	111.19
2	B	701	SJ5	O62-C6-C5	2.01	119.57	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	SJ5	C4-C5-C6-O62
2	B	701	SJ5	C4-C5-C6-O62
2	B	701	SJ5	C4-C5-C6-O61
2	C	701	SJ5	C4-C5-C6-O61
2	D	701	SJ5	C4-C5-C6-O62
2	D	701	SJ5	C4-C5-C6-O61
2	A	701	SJ5	C4-C5-C6-O61
2	C	701	SJ5	C4-C5-C6-O62

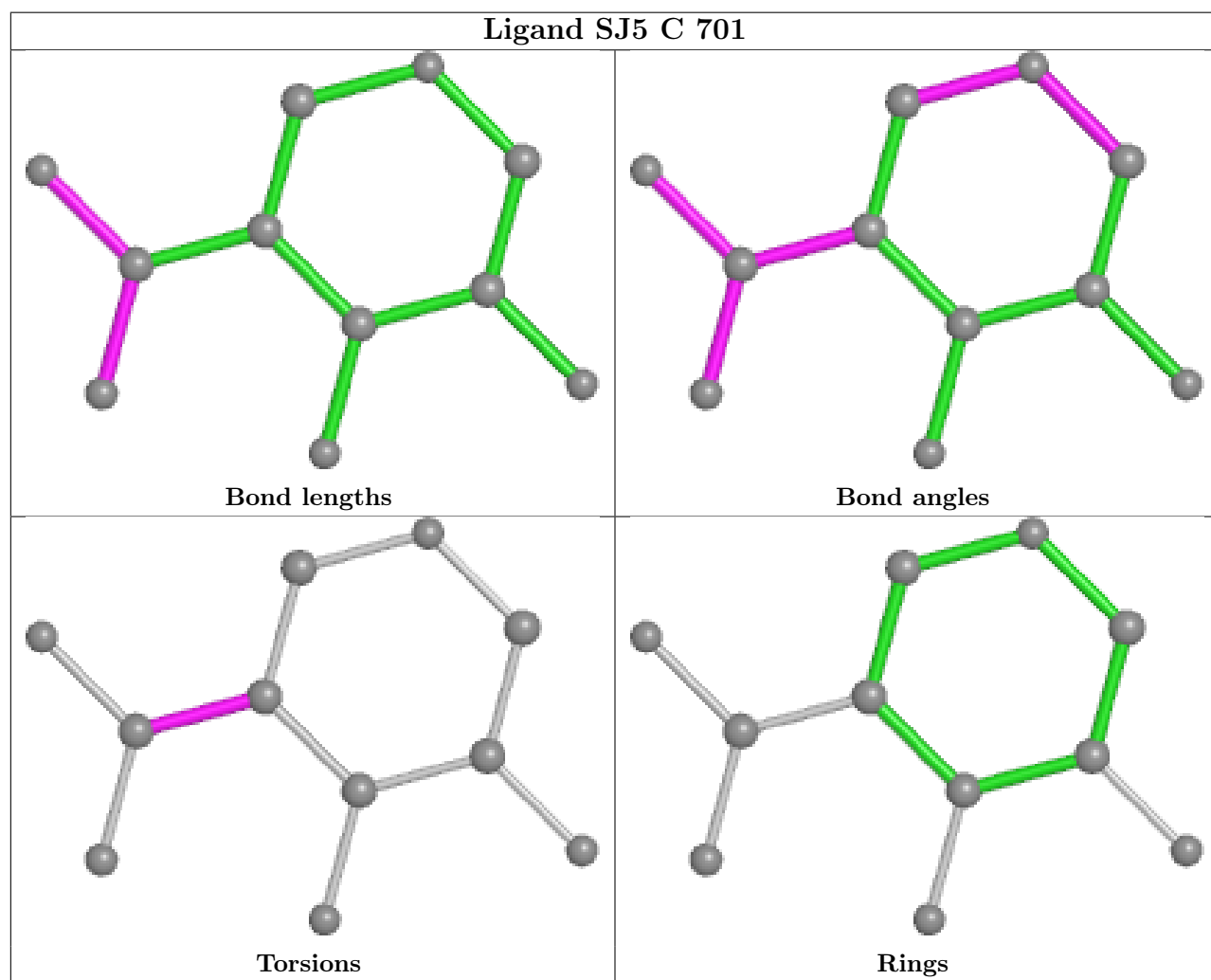
There are no ring outliers.

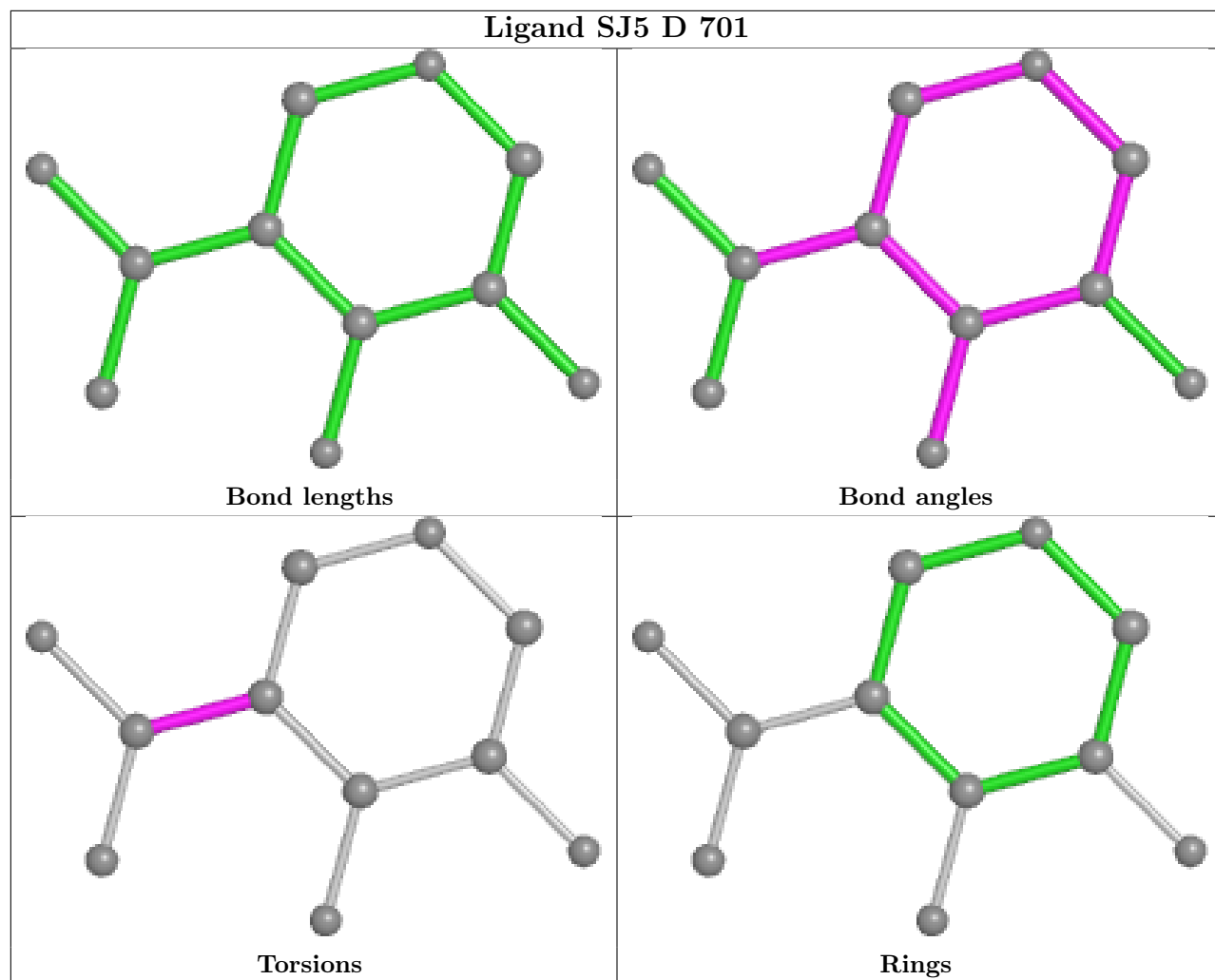
1 monomer is involved in 1 short contact:

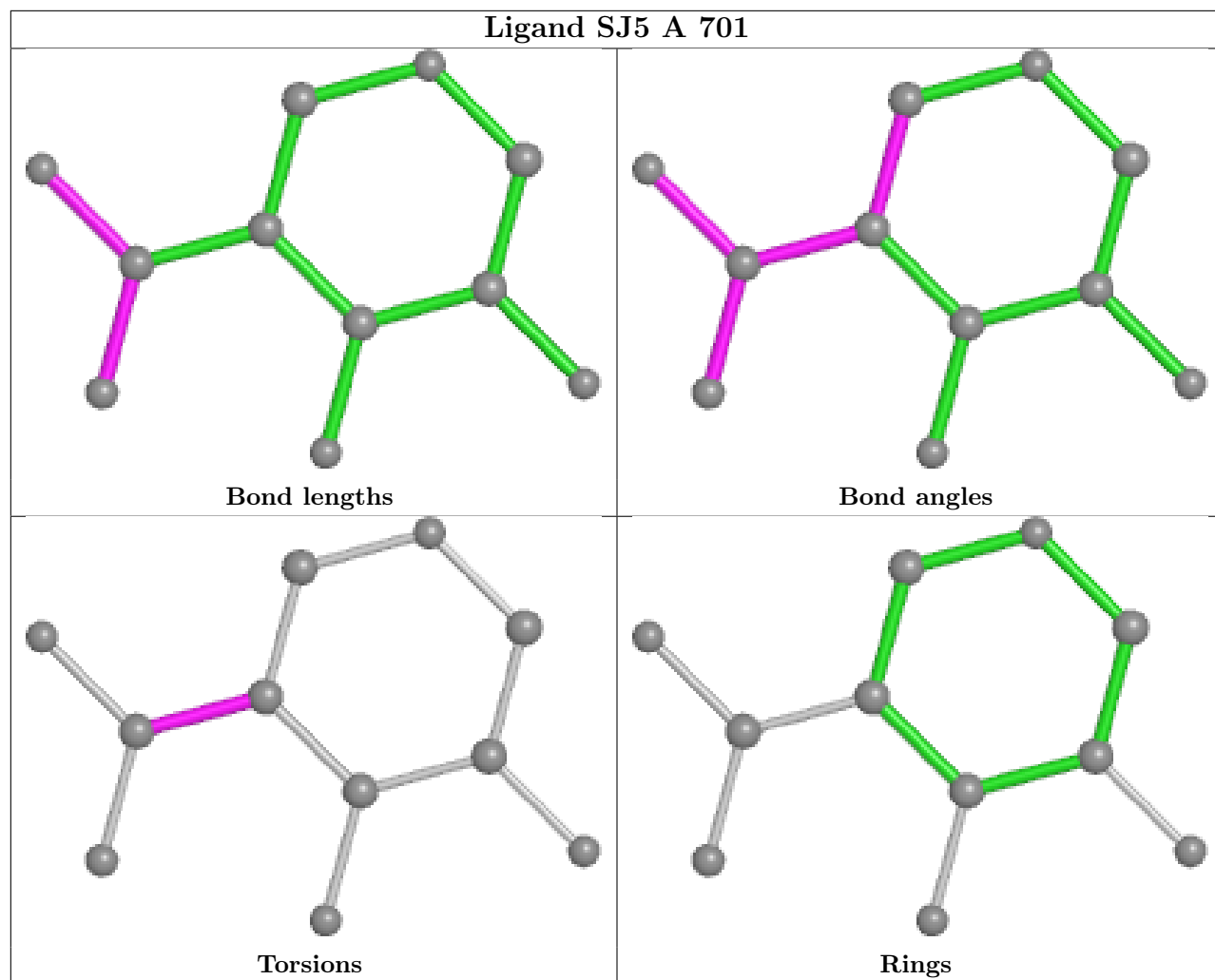


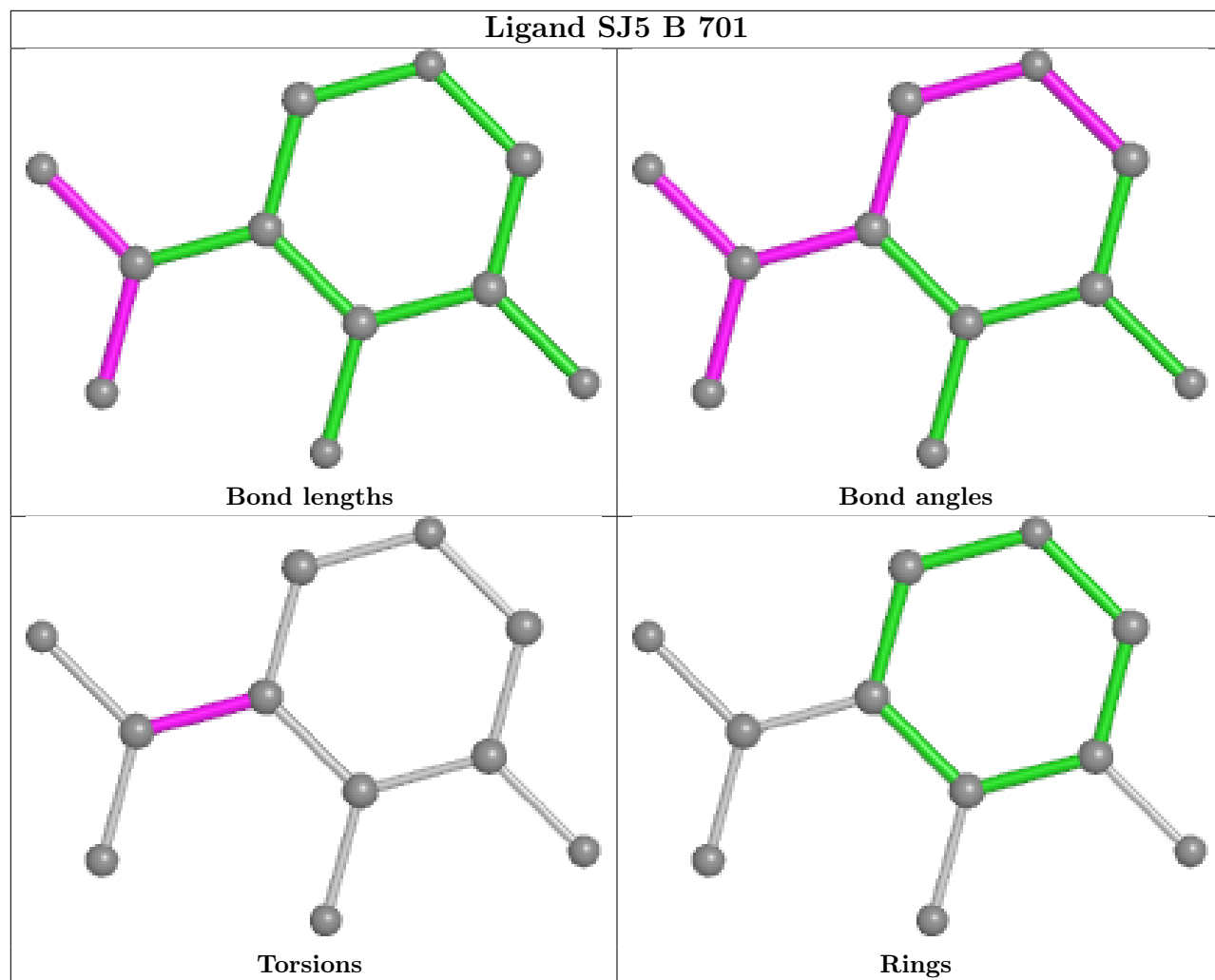
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	SJ5	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	620/670 (92%)	-0.52	8 (1%) 77 80	9, 15, 30, 59	0
1	B	620/670 (92%)	-0.49	9 (1%) 73 77	8, 15, 31, 62	0
1	C	620/670 (92%)	-0.26	12 (1%) 66 69	10, 20, 37, 63	0
1	D	620/670 (92%)	-0.23	14 (2%) 60 61	10, 21, 38, 70	0
All	All	2480/2680 (92%)	-0.38	43 (1%) 70 73	8, 18, 36, 70	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	342	SER	5.3
1	C	235	ASP	5.2
1	D	343	ARG	5.1
1	A	303	THR	4.9
1	C	342	SER	4.8
1	C	343	ARG	4.6
1	D	303	THR	4.5
1	D	274	GLY	4.3
1	A	342	SER	4.3
1	D	-1	ASN	4.2
1	B	343	ARG	4.2
1	C	274	GLY	4.1
1	A	343	ARG	4.0
1	A	274	GLY	3.9
1	C	303	THR	3.9
1	C	298	ARG	3.9
1	D	298	ARG	3.8
1	B	298	ARG	3.6
1	B	342	SER	3.6
1	D	216	GLY	3.4
1	D	297	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	3.0
1	B	303	THR	3.0
1	D	235	ASP	3.0
1	C	-1	ASN	2.8
1	A	298	ARG	2.7
1	C	383	TYR	2.6
1	A	235	ASP	2.6
1	B	274	GLY	2.5
1	D	344	ILE	2.4
1	C	297	GLU	2.4
1	C	234	GLY	2.4
1	B	297	GLU	2.4
1	D	383	TYR	2.3
1	B	383	TYR	2.3
1	C	285	GLU	2.3
1	C	565	ASN	2.3
1	D	124	ALA	2.3
1	A	485	ASP	2.2
1	D	487	GLU	2.2
1	B	334	PRO	2.2
1	A	297	GLU	2.2
1	D	219	CYS	2.1

## 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, 95<sup>th</sup> 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.

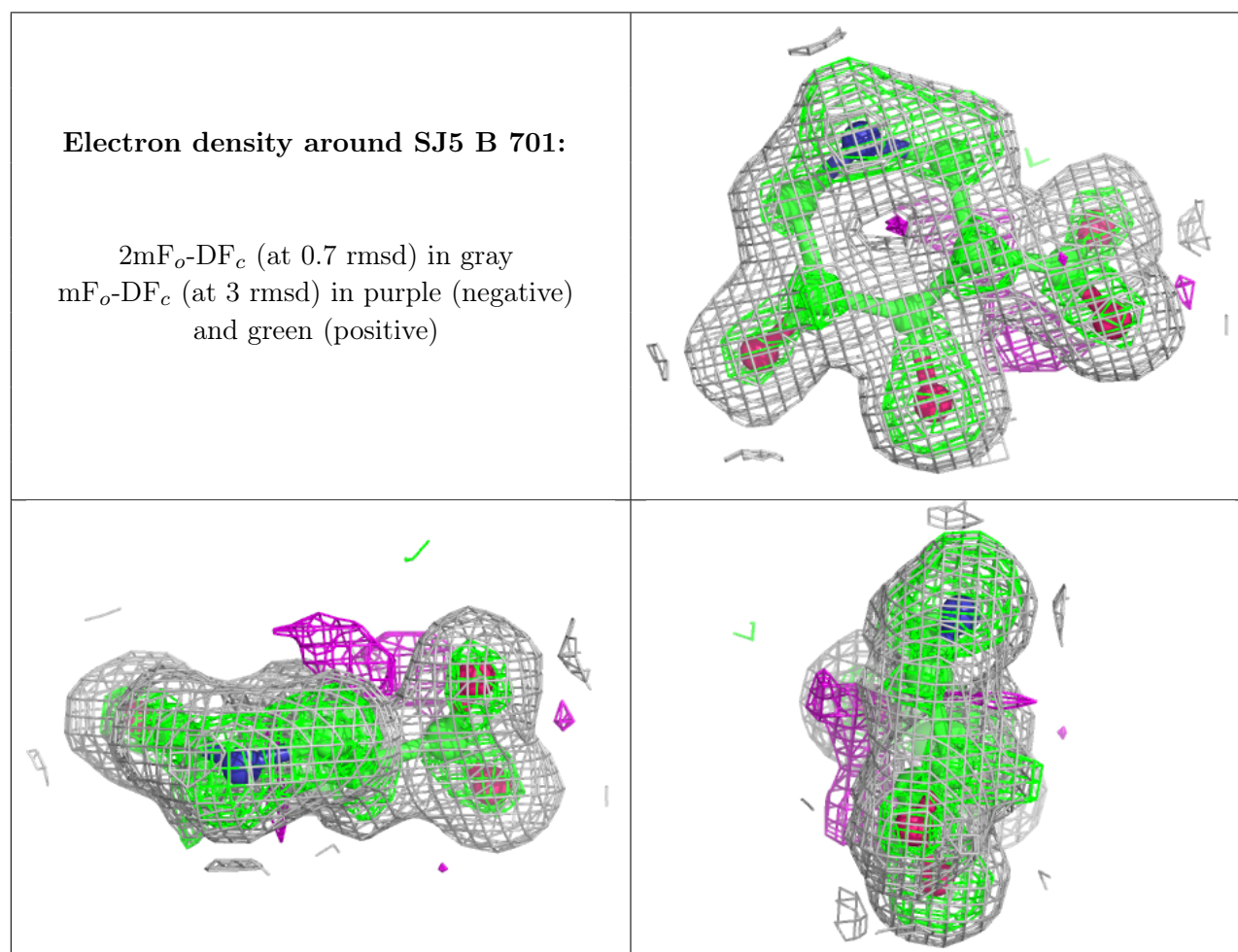
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SJ5	B	701	11/11	0.94	0.16	20,20,20,20	0

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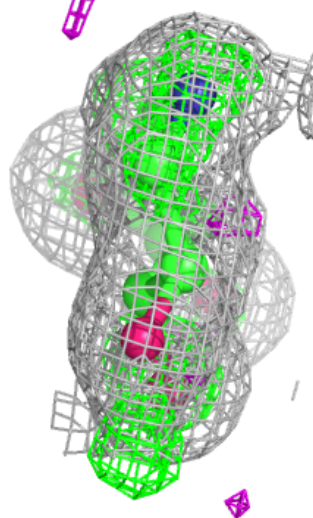
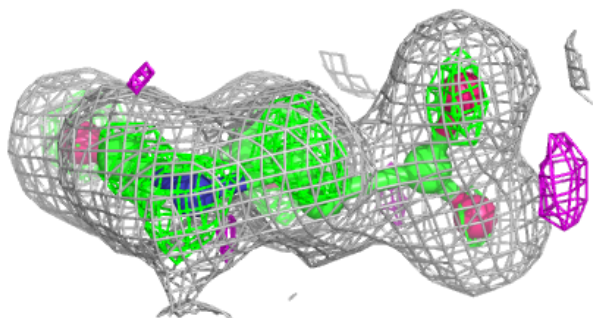
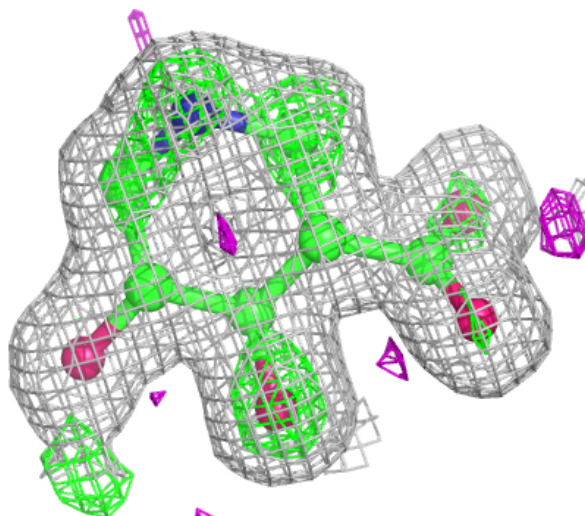
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SJ5	C	701	11/11	0.94	0.13	20,20,20,20	0
2	SJ5	A	701	11/11	0.96	0.13	20,20,20,20	0
2	SJ5	D	701	11/11	0.96	0.10	20,20,20,20	0

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 SJ5 C 701:**

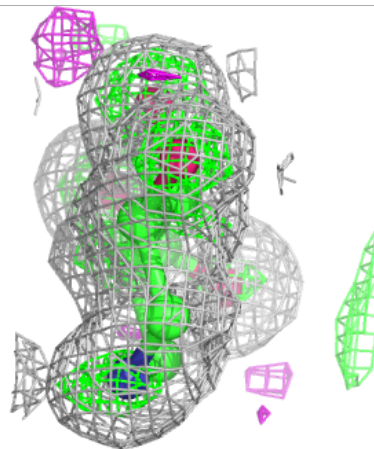
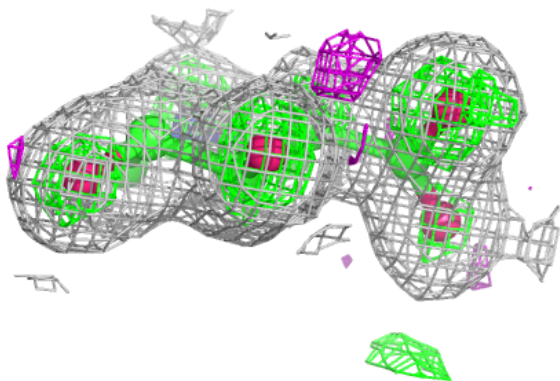
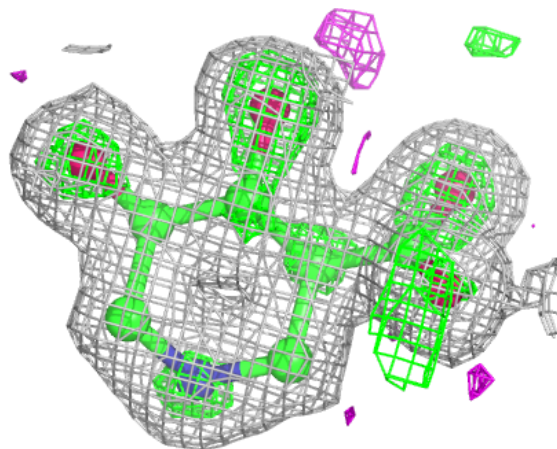
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

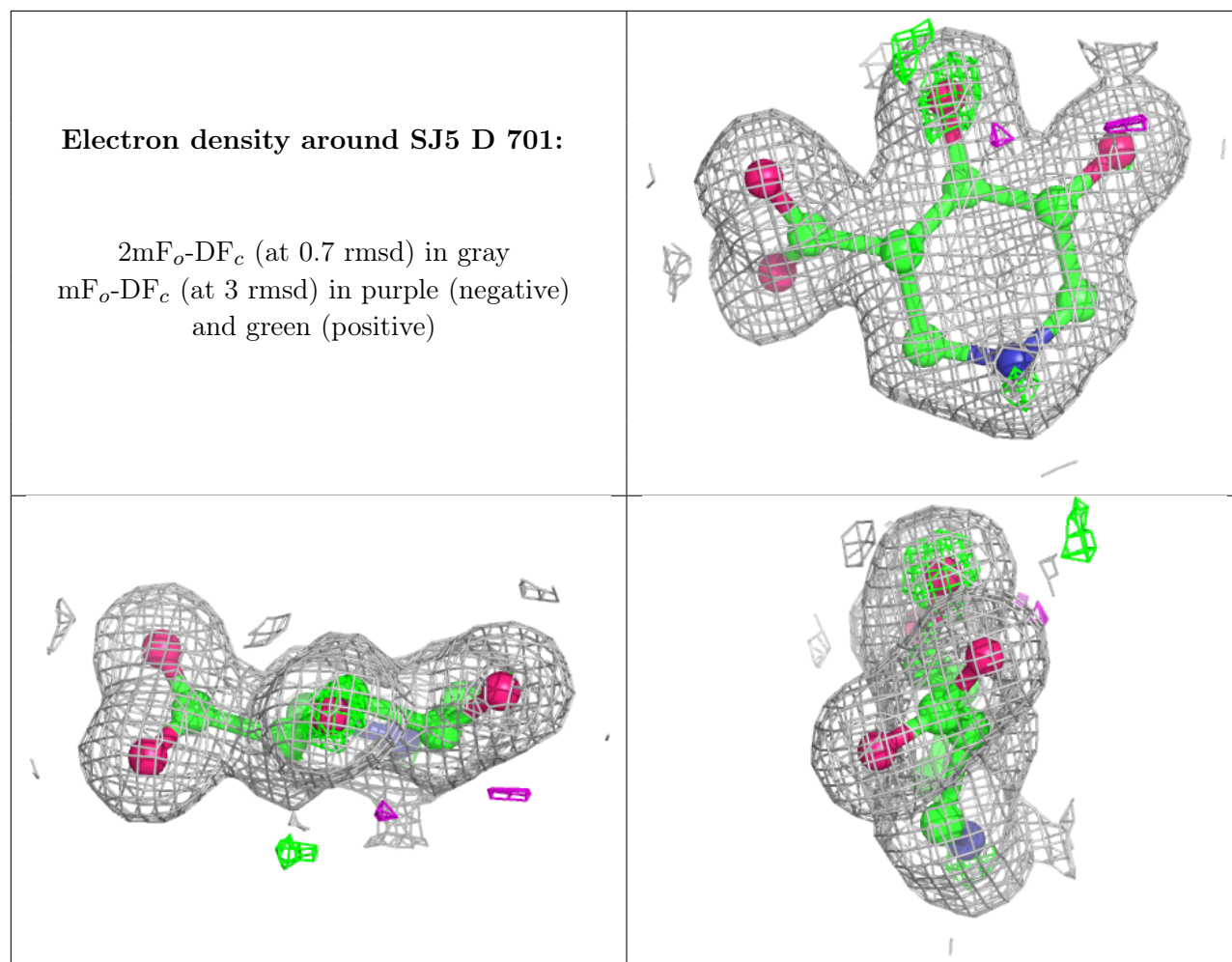




**Electron density around SJ5 A 701:**

$2mF_o-DF_c$  (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.