



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2019 – 06:08 AM EDT

PDB ID : 2C97
Title : LUMAZINE SYNTHASE FROM MYCOBACTERIUM TUBERCULOSIS
BOUND TO 4-(6- chloro-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)bu
tyl phosphate
Authors : Morgunova, E.; Illarionov, B.; Jin, G.; Haase, I.; Fischer, M.; Cushman, M.;
Bacher, A.; Ladenstein, R.
Deposited on : 2005-12-09
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

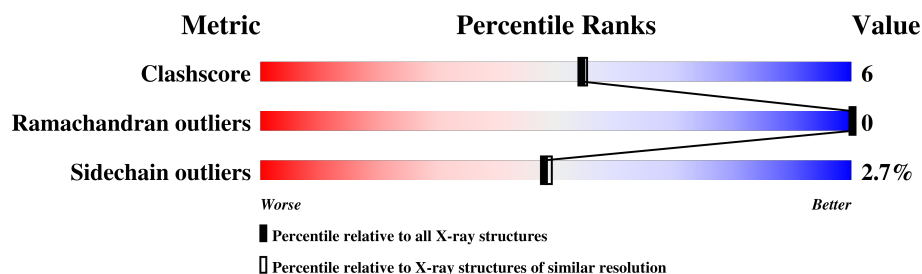
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	160	78% 14% • 8%
1	B	160	80% 11% • 8%
1	C	160	78% 13% 9%
1	D	160	81% 9% • 8%
1	E	160	83% 8% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DTD	E	1166	X	-	-	-

2 Entry composition [i](#)

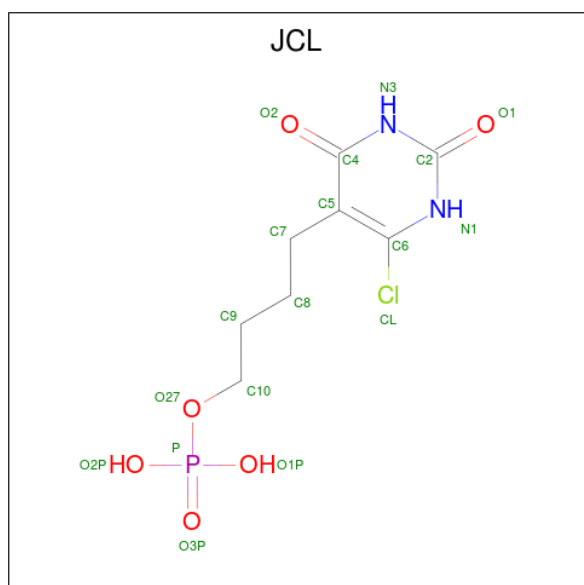
There are 7 unique types of molecules in this entry. The entry contains 5998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	B	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	C	146	Total	C	N	O	S	0	0	0
			1054	651	193	207	3			
1	D	147	Total	C	N	O	S	0	0	0
			1062	655	194	210	3			
1	E	146	Total	C	N	O	S	0	0	0
			1054	651	193	207	3			

- Molecule 2 is 4-(6-CHLORO-2,4-DIOXO-1,2,3,4-TETRAHYDOPYRIMIDIN-5-YL) BUTYL PHOSPHATE (three-letter code: JCL) (formula: C₈H₁₂ClN₂O₆P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	P	0	0
			18	8	1	2	6	1		

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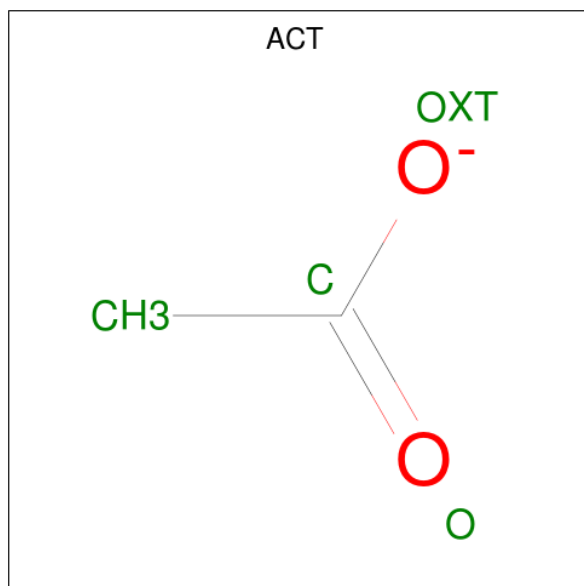
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	P	0	0
			18	8	1	2	6	1		
2	C	1	Total	C	Cl	N	O	P	0	0
			18	8	1	2	6	1		
2	D	1	Total	C	Cl	N	O	P	0	0
			18	8	1	2	6	1		
2	E	1	Total	C	Cl	N	O	P	0	0
			18	8	1	2	6	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

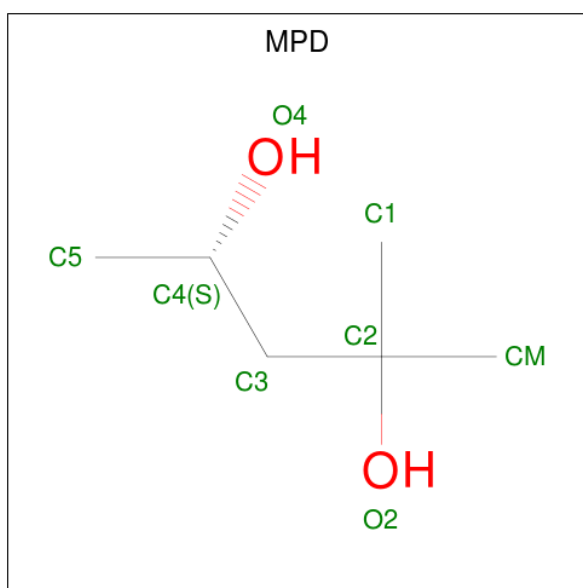
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	K	0	0
			4	4		
3	A	4	Total	K	0	0
			4	4		
3	D	2	Total	K	0	0
			2	2		
3	C	3	Total	K	0	0
			3	3		
3	E	3	Total	K	0	0
			3	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



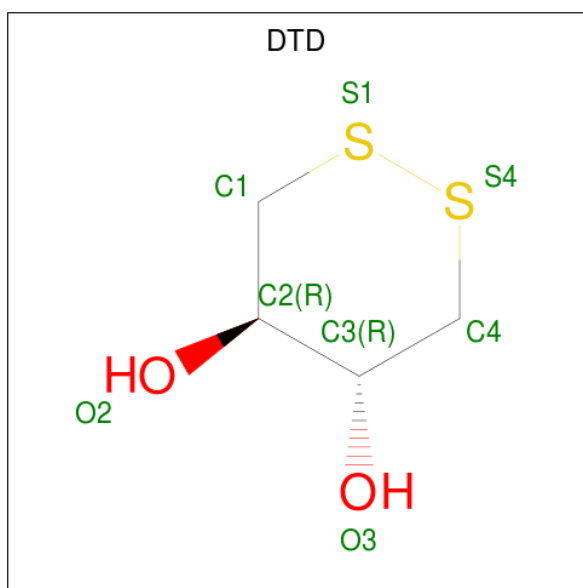
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is DITHIANE DIOL (three-letter code: DTD) (formula: $C_4H_8O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	O	S	0	0
			8	4	2	2		

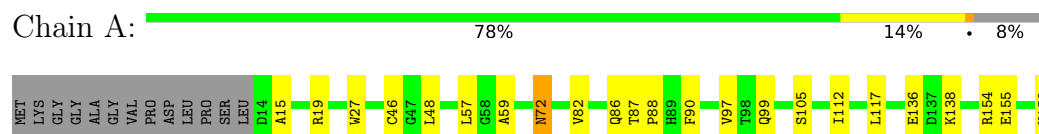
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	100	Total	O	0	0
			100	100		
7	C	81	Total	O	0	0
			81	81		
7	D	107	Total	O	0	0
			107	107		
7	E	110	Total	O	0	0
			110	110		

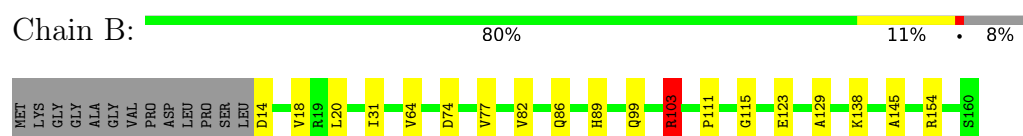
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

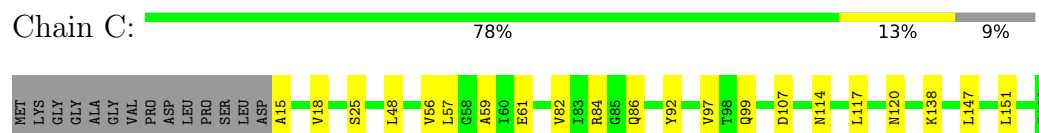
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



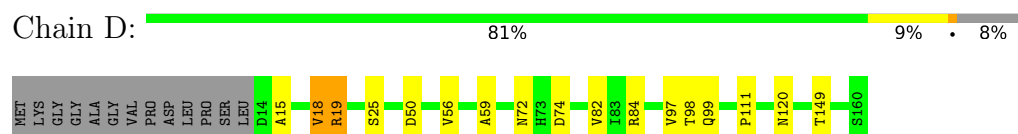
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



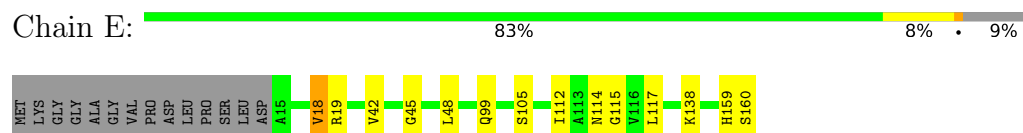
• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



• Molecule 1: 6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.64Å 82.24Å 86.35Å 90.00° 120.53° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 19.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.00) 90.3 (19.82-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.146 , 0.215 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5998	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JCL, MPD, ACT, K, DTD

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	0.53	0/1074	0.67	0/1467
1	B	0.54	0/1074	0.64	1/1467 (0.1%)
1	C	0.50	0/1066	0.59	0/1456
1	D	0.53	0/1074	0.65	1/1467 (0.1%)
1	E	0.55	0/1066	0.65	2/1456 (0.1%)
All	All	0.53	0/5354	0.64	4/7313 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	19	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	19	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	103	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	19	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1062	0	1073	18	0
1	B	1062	0	1073	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1054	0	1069	15	0
1	D	1062	0	1073	10	0
1	E	1054	0	1069	12	0
2	A	18	0	10	1	0
2	B	18	0	10	1	0
2	C	18	0	10	1	0
2	D	18	0	10	1	0
2	E	18	0	10	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
4	E	4	0	3	0	0
5	A	16	0	28	0	0
5	B	8	0	14	0	0
5	C	8	0	14	2	0
5	D	8	0	14	2	0
5	E	8	0	14	2	0
6	E	8	0	6	2	0
7	A	124	0	0	2	0
7	B	100	0	0	4	0
7	C	81	0	0	1	0
7	D	107	0	0	0	0
7	E	110	0	0	1	0
All	All	5998	0	5512	61	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 6.

All (61) 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:B:99:GLN:HE22	1:C:99:GLN:HA	1.59	0.67
5:C:1165:MPD:HM1	5:C:1165:MPD:O4	1.97	0.65
1:B:99:GLN:NE2	7:B:2058:HOH:O	2.28	0.64
1:E:45:GLY:CA	6:E:1166:DTD:O2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:H	1:A:72:ASN:HD22	1.45	0.62
1:A:72:ASN:N	1:A:72:ASN:HD22	1.97	0.62
1:B:123:GLU:HG3	7:B:2076:HOH:O	2.02	0.59
1:B:89:HIS:CE1	1:C:114:ASN:HD21	2.20	0.59
1:B:115:GLY:HA2	1:B:138:LYS:HD3	1.85	0.57
1:C:86:GLN:HG2	7:C:2044:HOH:O	2.03	0.57
1:E:114:ASN:OD1	5:E:1165:MPD:H31	2.05	0.57
1:A:105:SER:HB3	1:A:112:ILE:HG12	1.88	0.56
1:A:86:GLN:HG2	7:A:2063:HOH:O	2.07	0.55
1:E:42:VAL:HA	6:E:1166:DTD:O3	2.07	0.55
1:C:99:GLN:HE22	1:D:99:GLN:HA	1.73	0.53
1:C:117:LEU:HD23	1:C:138:LYS:HD3	1.91	0.53
1:D:84:ARG:NH1	1:D:120:ASN:OD1	2.40	0.53
1:D:82:VAL:HA	2:D:701:JCL:CL	2.45	0.53
1:A:99:GLN:HA	1:E:99:GLN:HE22	1.74	0.52
1:A:136:GLU:OE2	1:A:138:LYS:HE2	2.10	0.52
1:E:105:SER:HB3	1:E:112:ILE:HG12	1.93	0.51
1:A:87:THR:HB	1:A:88:PRO:HD2	1.93	0.50
1:E:117:LEU:HD21	1:E:138:LYS:HG3	1.93	0.49
1:D:98:THR:HG23	5:D:1164:MPD:H11	1.95	0.49
1:C:84:ARG:NH1	1:C:120:ASN:OD1	2.46	0.48
1:E:114:ASN:HB2	5:E:1165:MPD:H52	1.96	0.48
1:C:15:ALA:HB2	1:C:151:LEU:HD11	1.96	0.48
1:A:59:ALA:HB1	1:A:97:VAL:HG21	1.96	0.47
5:C:1165:MPD:CM	5:C:1165:MPD:O4	2.62	0.47
1:D:99:GLN:HE22	1:E:99:GLN:HA	1.78	0.47
1:D:25:SER:HA	1:D:56:VAL:O	2.15	0.46
1:B:31:ILE:HG23	1:B:129:ALA:HB2	1.98	0.46
1:A:15:ALA:HB3	1:A:46:CYS:HB3	1.97	0.46
1:B:103:ARG:NH2	1:C:107:ASP:OD2	2.36	0.45
1:C:82:VAL:HA	2:C:701:JCL:CL	2.53	0.45
1:C:61:GLU:HG2	1:D:149:THR:OG1	2.17	0.45
1:A:87:THR:HB	1:A:88:PRO:CD	2.47	0.45
1:A:57:LEU:HD23	1:B:145:ALA:HB2	1.98	0.45
1:C:59:ALA:HB1	1:C:97:VAL:HG21	1.99	0.44
1:C:57:LEU:HB3	1:C:61:GLU:OE1	2.18	0.43
1:A:27:TRP:HZ2	7:B:2089:HOH:O	2.01	0.43
1:E:18:VAL:HG22	1:E:48:LEU:HD11	2.01	0.43
1:B:86:GLN:HG2	7:B:2050:HOH:O	2.18	0.43
1:A:82:VAL:HA	2:A:701:JCL:CL	2.57	0.42
1:D:15:ALA:HB1	1:D:18:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:SER:HA	1:C:56:VAL:O	2.19	0.42
1:C:48:LEU:HD11	1:C:147:LEU:HD21	2.01	0.42
1:B:82:VAL:HA	2:B:701:JCL:CL	2.56	0.42
1:C:92:TYR:HB3	5:D:1164:MPD:H12	2.01	0.42
1:A:155:GLU:O	1:A:159:HIS:HE1	2.03	0.42
1:A:72:ASN:ND2	1:A:72:ASN:N	2.67	0.42
1:E:138:LYS:HG2	7:E:2093:HOH:O	2.20	0.42
1:A:82:VAL:HG12	1:A:90:PHE:CD1	2.55	0.42
1:E:115:GLY:HA2	1:E:138:LYS:HE3	2.01	0.41
1:B:20:LEU:HD11	1:B:77:VAL:HG23	2.01	0.41
1:A:117:LEU:HD21	1:A:138:LYS:HG3	2.02	0.41
1:A:15:ALA:N	7:A:2002:HOH:O	2.43	0.41
1:B:74:ASP:O	1:B:111:PRO:HD2	2.20	0.41
1:E:159:HIS:HB2	1:E:160:SER:HB3	2.03	0.41
1:D:59:ALA:HB1	1:D:97:VAL:HG21	2.04	0.40
1:D:74:ASP:O	1:D:111:PRO:HD2	2.21	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	145/160 (91%)	142 (98%)	3 (2%)	0	100	100
1	B	145/160 (91%)	141 (97%)	4 (3%)	0	100	100
1	C	144/160 (90%)	142 (99%)	2 (1%)	0	100	100
1	D	145/160 (91%)	142 (98%)	3 (2%)	0	100	100
1	E	144/160 (90%)	143 (99%)	1 (1%)	0	100	100
All	All	723/800 (90%)	710 (98%)	13 (2%)	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	111/120 (92%)	107 (96%)	4 (4%)	38	36
1	B	111/120 (92%)	106 (96%)	5 (4%)	30	26
1	C	110/120 (92%)	109 (99%)	1 (1%)	81	85
1	D	111/120 (92%)	107 (96%)	4 (4%)	38	36
1	E	110/120 (92%)	109 (99%)	1 (1%)	81	85
All	All	553/600 (92%)	538 (97%)	15 (3%)	48	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	48	LEU
1	A	72	ASN
1	A	154	ARG
1	B	14	ASP
1	B	18	VAL
1	B	64	VAL
1	B	103	ARG
1	B	154	ARG
1	C	18	VAL
1	D	18	VAL
1	D	19	ARG
1	D	50	ASP
1	D	72	ASN
1	E	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	159	HIS
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	89	HIS
1	B	99	GLN
1	B	114	ASN
1	B	159	HIS
1	C	99	GLN
1	C	159	HIS
1	D	72	ASN
1	D	99	GLN
1	D	114	ASN
1	D	159	HIS
1	E	99	GLN
1	E	159	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 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	$\# Z > 2$
4	ACT	A	1165	-	1,3,3	1.38	0	0,3,3	0.00	-
5	MPD	A	1166	-	7,7,7	0.25	0	9,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	A	1167	-	7,7,7	0.32	0	9,10,10	0.70	0
2	JCL	A	701	-	15,18,18	0.97	1 (6%)	17,25,25	3.12	8 (47%)
5	MPD	B	1165	-	7,7,7	0.31	0	9,10,10	0.56	0
4	ACT	B	632	-	1,3,3	1.46	0	0,3,3	0.00	-
2	JCL	B	701	-	15,18,18	1.03	2 (13%)	17,25,25	2.70	4 (23%)
4	ACT	C	1164	-	1,3,3	1.19	0	0,3,3	0.00	-
5	MPD	C	1165	-	7,7,7	0.36	0	9,10,10	0.77	0
2	JCL	C	701	-	15,18,18	1.10	1 (6%)	17,25,25	3.32	10 (58%)
4	ACT	D	1163	-	1,3,3	1.45	0	0,3,3	0.00	-
5	MPD	D	1164	-	7,7,7	0.31	0	9,10,10	0.34	0
2	JCL	D	701	-	15,18,18	1.09	2 (13%)	17,25,25	2.73	7 (41%)
4	ACT	E	1164	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
5	MPD	E	1165	-	7,7,7	0.30	0	9,10,10	0.53	0
6	DTD	E	1166	1	6,8,8	0.99	1 (16%)	6,10,10	9.27	6 (100%)
2	JCL	E	701	-	15,18,18	1.11	2 (13%)	17,25,25	3.09	7 (41%)

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
5	MPD	A	1166	-	-	1/5/5/5	-
5	MPD	A	1167	-	-	0/5/5/5	-
2	JCL	A	701	-	-	7/9/9/9	0/1/1/1
5	MPD	B	1165	-	-	1/5/5/5	-
2	JCL	B	701	-	-	1/9/9/9	0/1/1/1
5	MPD	C	1165	-	-	3/5/5/5	-
2	JCL	C	701	-	-	8/9/9/9	0/1/1/1
5	MPD	D	1164	-	-	3/5/5/5	-
2	JCL	D	701	-	-	0/9/9/9	0/1/1/1
5	MPD	E	1165	-	-	0/5/5/5	-
6	DTD	E	1166	1	2/2/2/2	-	0/0/1/1
2	JCL	E	701	-	-	6/9/9/9	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	JCL	C2-N1	-2.90	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	JCL	C2-N1	-2.89	1.32	1.38
2	D	701	JCL	C2-N1	-2.80	1.32	1.38
2	B	701	JCL	C2-N1	-2.63	1.33	1.38
2	A	701	JCL	C2-N1	-2.38	1.33	1.38
4	E	1164	ACT	CH3-C	2.22	1.51	1.48
6	E	1166	DTD	C3-C2	2.20	1.55	1.52
2	E	701	JCL	C4-N3	2.17	1.36	1.33
2	D	701	JCL	C4-N3	2.12	1.36	1.33
2	B	701	JCL	C4-N3	2.02	1.36	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1166	DTD	O2-C2-C3	11.47	135.36	110.20
6	E	1166	DTD	O3-C3-C2	11.36	135.12	110.20
2	A	701	JCL	C4-N3-C2	9.78	123.40	115.14
2	E	701	JCL	C4-N3-C2	9.76	123.38	115.14
2	C	701	JCL	C4-N3-C2	9.11	122.83	115.14
6	E	1166	DTD	O3-C3-C4	-8.90	94.57	109.91
2	D	701	JCL	C4-N3-C2	8.41	122.24	115.14
2	B	701	JCL	C4-N3-C2	8.32	122.16	115.14
6	E	1166	DTD	C4-C3-C2	8.31	128.86	112.45
6	E	1166	DTD	C1-C2-C3	7.32	126.92	112.45
6	E	1166	DTD	O2-C2-C1	-7.29	97.35	109.91
2	C	701	JCL	C5-C6-N1	-5.59	121.42	126.63
2	C	701	JCL	C2-N1-C6	4.44	121.23	115.53
2	E	701	JCL	C5-C6-N1	-4.15	122.76	126.63
2	B	701	JCL	C2-N1-C6	4.05	120.72	115.53
2	A	701	JCL	O27-C10-C9	3.94	122.20	108.99
2	B	701	JCL	C5-C6-N1	-3.84	123.05	126.63
2	C	701	JCL	C8-C7-C5	3.78	120.07	112.79
2	D	701	JCL	C2-N1-C6	3.66	120.22	115.53
2	D	701	JCL	C5-C6-N1	-3.57	123.30	126.63
2	E	701	JCL	C2-N1-C6	3.45	119.95	115.53
2	A	701	JCL	C5-C6-N1	-3.27	123.58	126.63
2	E	701	JCL	O1P-P-O27	-3.13	98.41	106.73
2	A	701	JCL	C2-N1-C6	3.09	119.50	115.53
2	E	701	JCL	P-O27-C10	3.07	126.74	118.30
2	D	701	JCL	O27-C10-C9	2.91	118.75	108.99
2	C	701	JCL	O27-C10-C9	2.80	118.36	108.99
2	B	701	JCL	O27-C10-C9	2.79	118.35	108.99
2	A	701	JCL	P-O27-C10	2.79	125.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	JCL	C8-C7-C5	2.76	118.10	112.79
2	C	701	JCL	C9-C8-C7	-2.69	103.06	113.76
2	E	701	JCL	O27-C10-C9	2.60	117.72	108.99
2	D	701	JCL	C8-C7-C5	2.53	117.66	112.79
2	C	701	JCL	O1P-P-O27	-2.44	100.24	106.73
2	C	701	JCL	P-O27-C10	2.43	124.99	118.30
2	A	701	JCL	O1P-P-O27	-2.35	100.47	106.73
2	C	701	JCL	O2P-P-O1P	2.32	116.58	107.57
2	A	701	JCL	O2P-P-O1P	2.30	116.51	107.57
2	E	701	JCL	O2P-P-O1P	2.23	116.22	107.57
2	C	701	JCL	C7-C5-C6	2.15	125.35	121.83
2	D	701	JCL	P-O27-C10	2.12	124.14	118.30
2	D	701	JCL	C7-C5-C4	2.00	125.01	120.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	1166	DTD	C3
6	E	1166	DTD	C2

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	JCL	C4-C5-C7-C8
2	A	701	JCL	C10-O27-P-O1P
2	A	701	JCL	C10-O27-P-O2P
2	E	701	JCL	C10-O27-P-O3P
5	C	1165	MPD	O2-C2-C3-C4
5	C	1165	MPD	CM-C2-C3-C4
2	C	701	JCL	C4-C5-C7-C8
2	C	701	JCL	C10-O27-P-O1P
2	C	701	JCL	C10-O27-P-O2P
2	C	701	JCL	C7-C8-C9-C10
2	A	701	JCL	O27-C10-C9-C8
2	C	701	JCL	O27-C10-C9-C8
2	A	701	JCL	C7-C8-C9-C10
2	A	701	JCL	C10-O27-P-O3P
2	C	701	JCL	C10-O27-P-O3P
2	A	701	JCL	C6-C5-C7-C8
2	C	701	JCL	C6-C5-C7-C8
2	E	701	JCL	C5-C7-C8-C9
2	E	701	JCL	O27-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	B	1165	MPD	O2-C2-C3-C4
2	E	701	JCL	C10-O27-P-O1P
2	C	701	JCL	C5-C7-C8-C9
5	D	1164	MPD	CM-C2-C3-C4
5	A	1166	MPD	CM-C2-C3-C4
2	E	701	JCL	C7-C8-C9-C10
5	D	1164	MPD	O2-C2-C3-C4
2	E	701	JCL	C10-O27-P-O2P
2	B	701	JCL	C5-C7-C8-C9
5	D	1164	MPD	C2-C3-C4-O4
5	C	1165	MPD	C2-C3-C4-O4

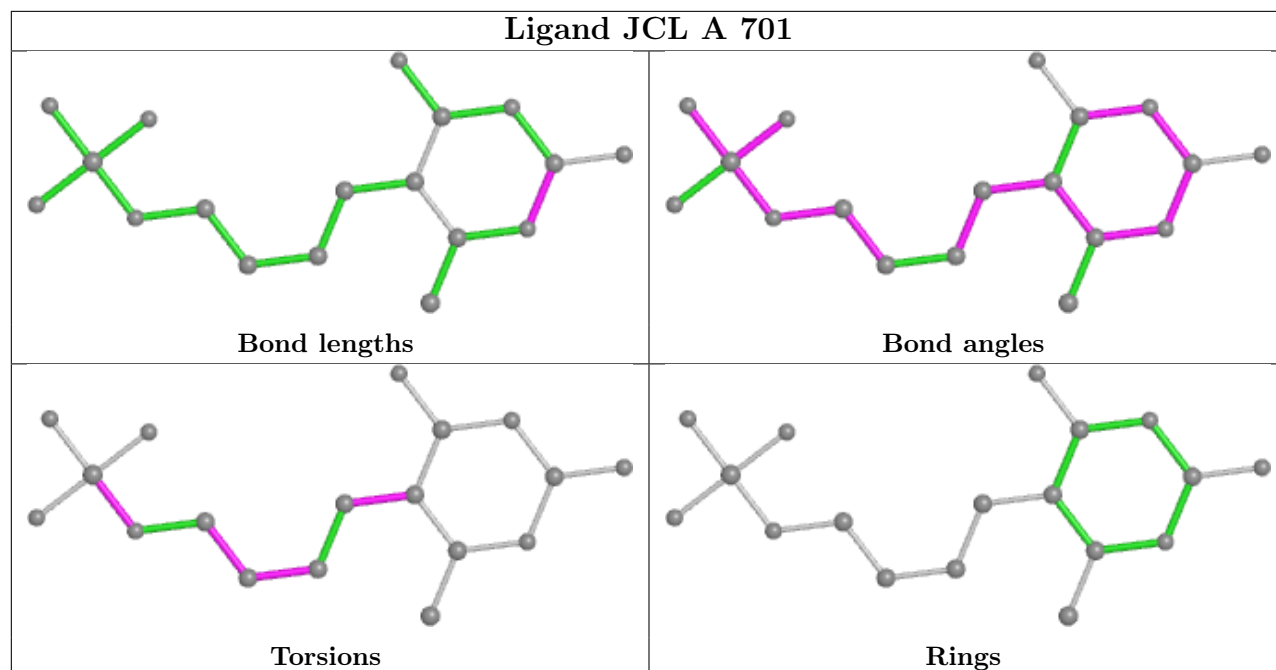
There are no ring outliers.

8 monomers are involved in 12 short contacts:

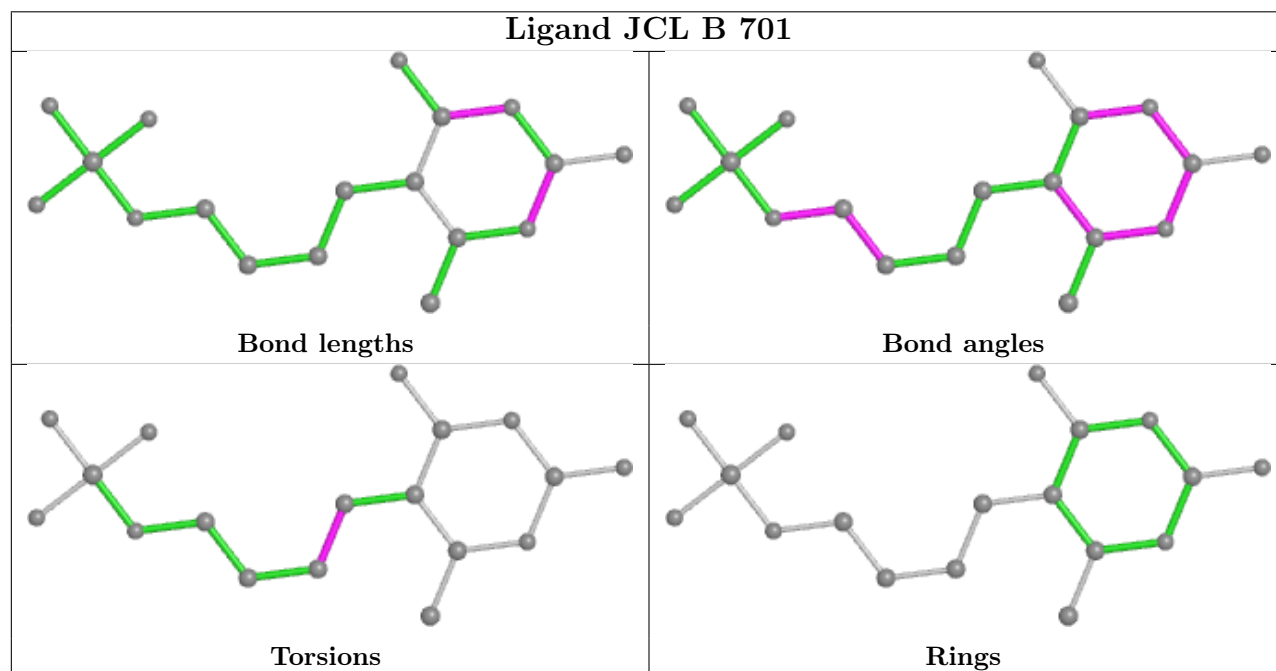
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	JCL	1	0
2	B	701	JCL	1	0
5	C	1165	MPD	2	0
2	C	701	JCL	1	0
5	D	1164	MPD	2	0
2	D	701	JCL	1	0
5	E	1165	MPD	2	0
6	E	1166	DTD	2	0

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.

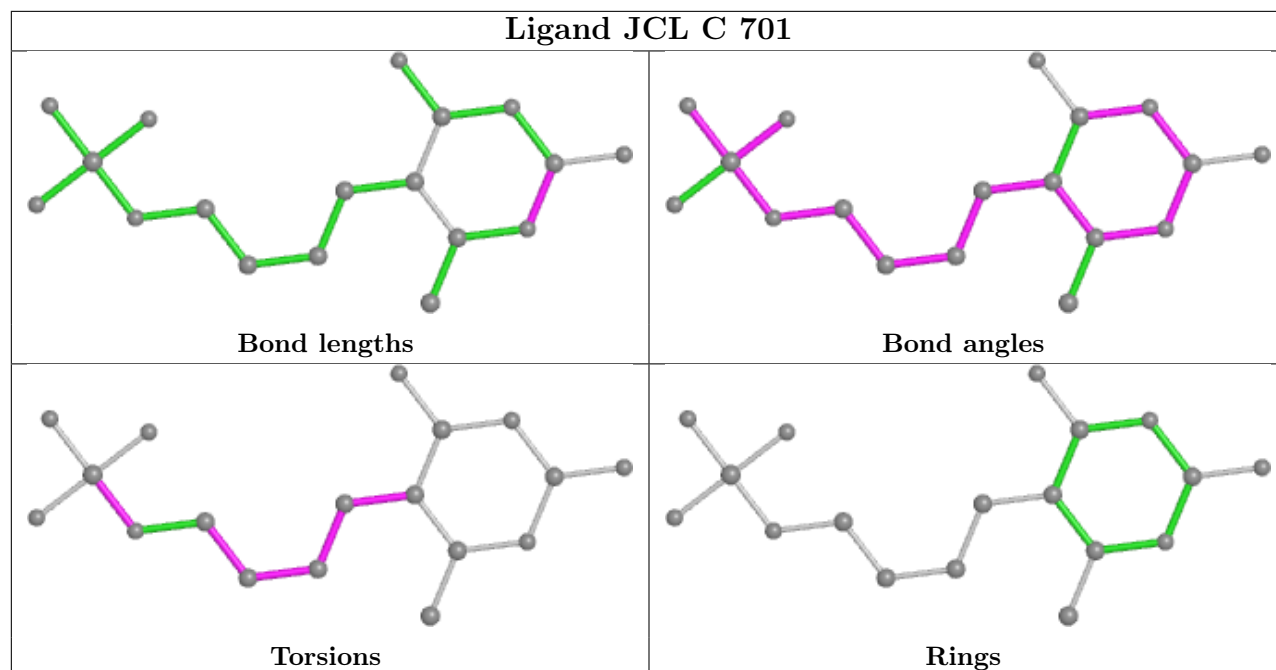
Ligand JCL A 701



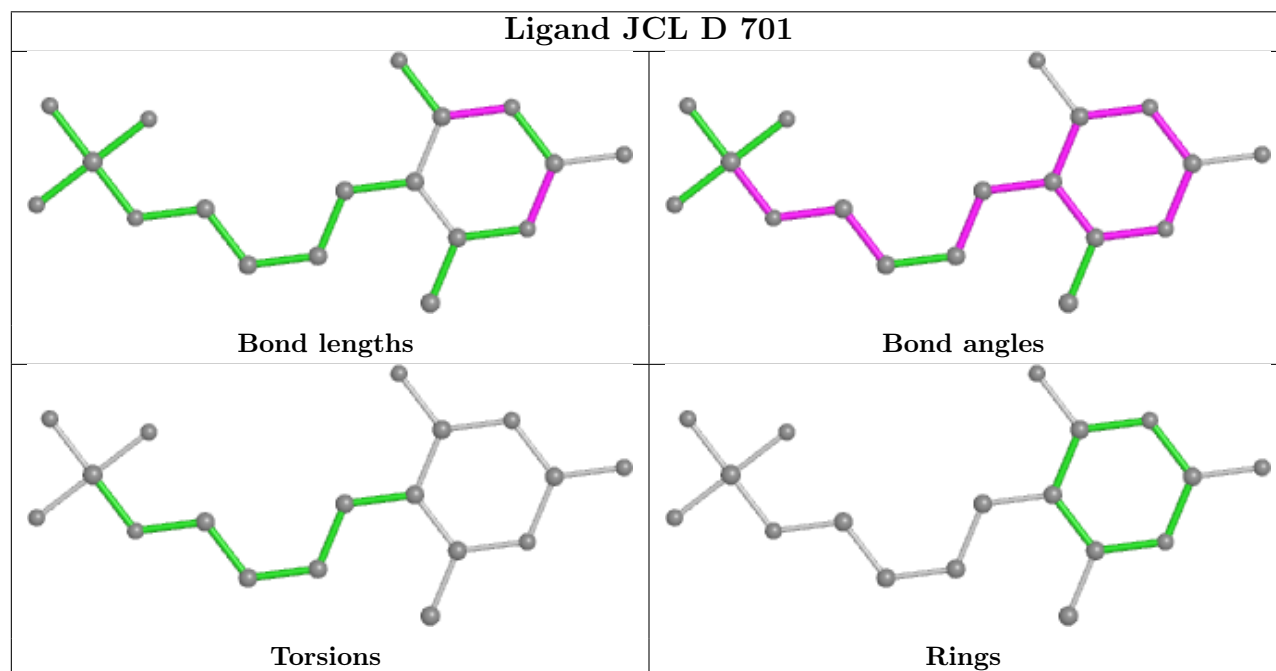
Ligand JCL B 701

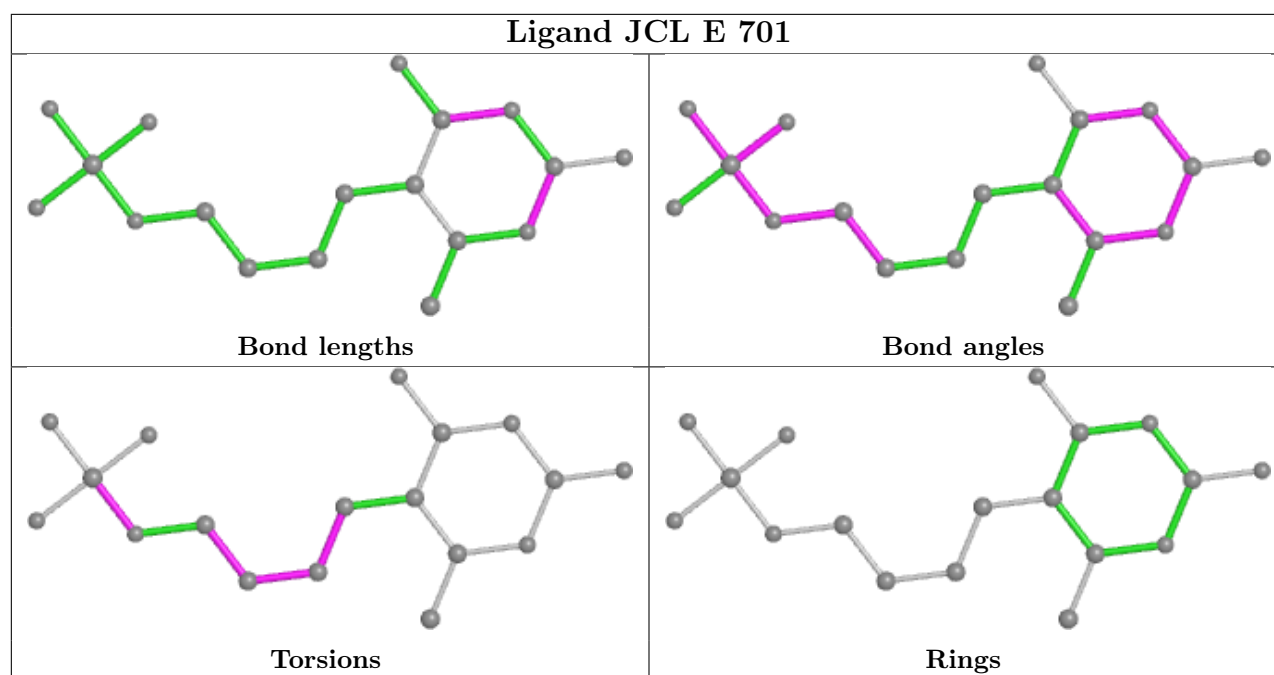


Ligand JCL C 701



Ligand JCL D 701





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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

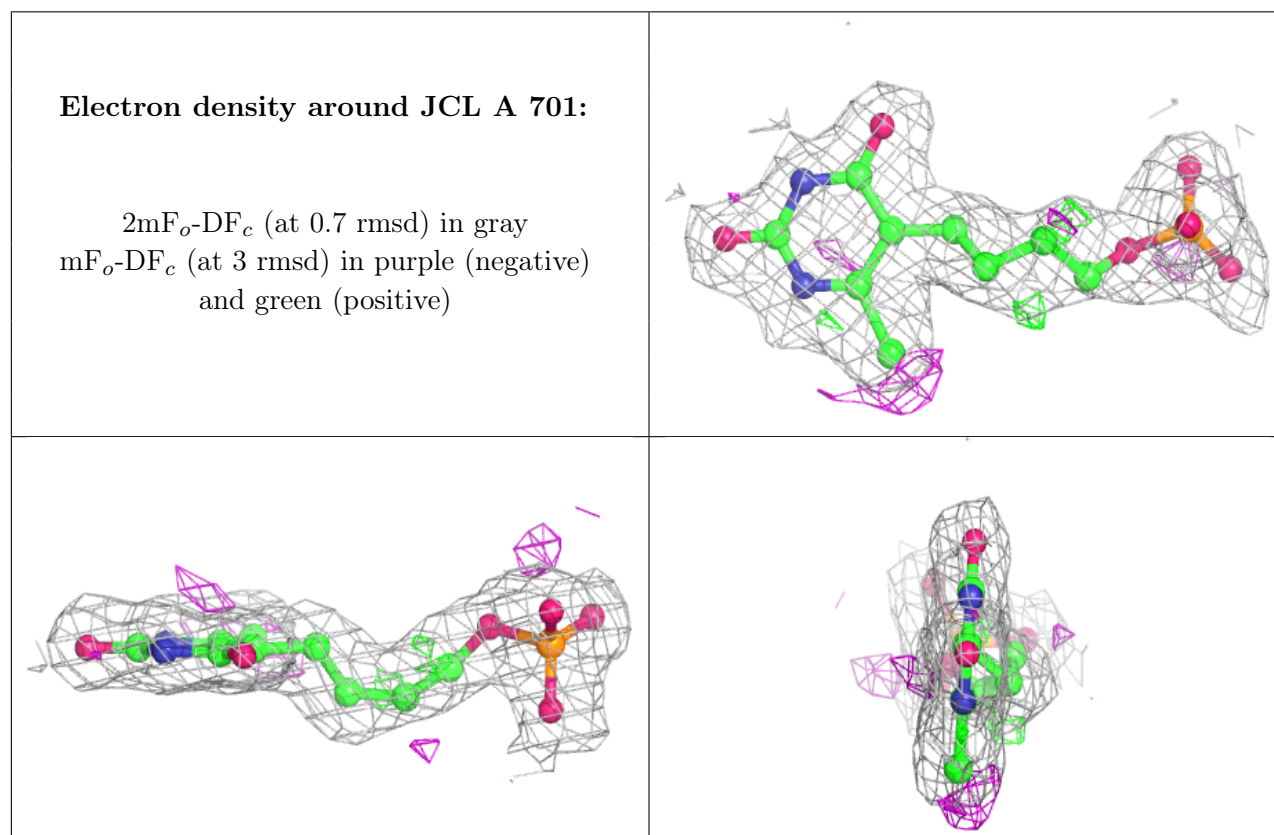
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

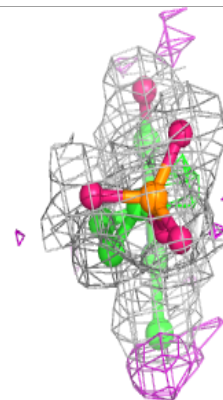
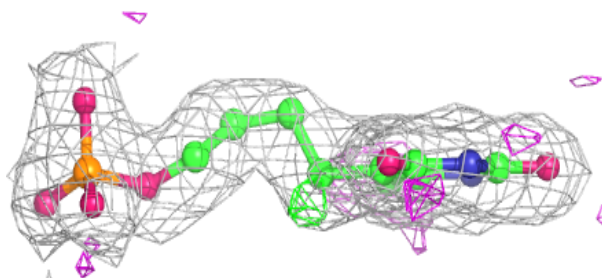
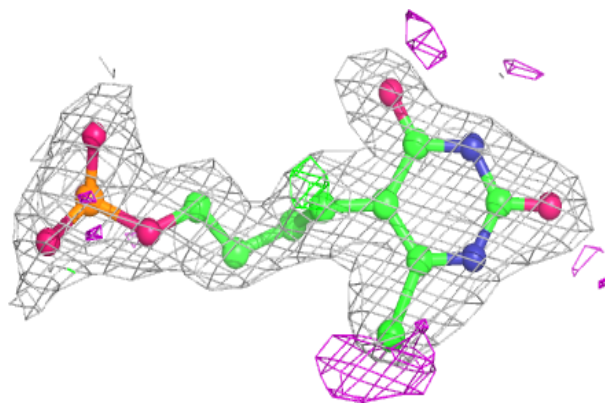
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

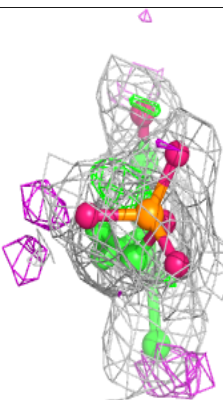
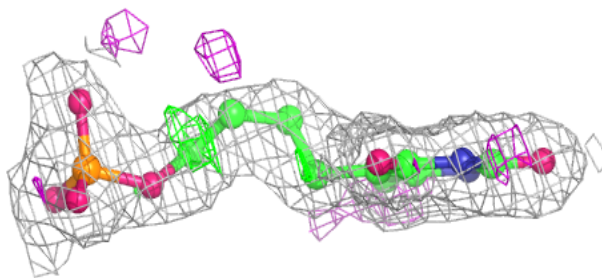
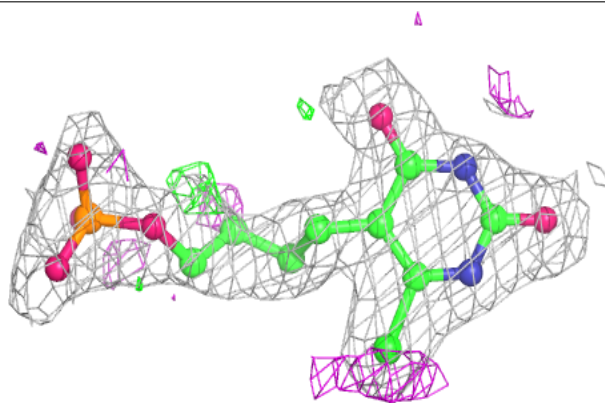


Electron density around JCL B 701:

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

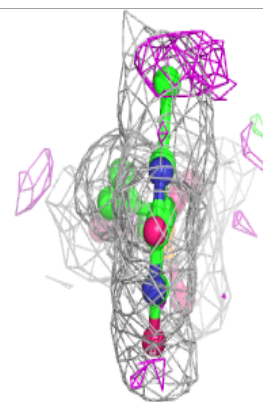
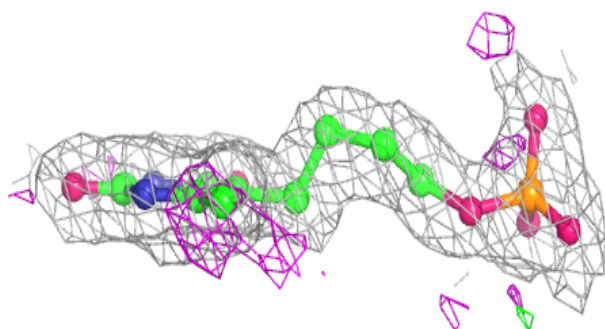
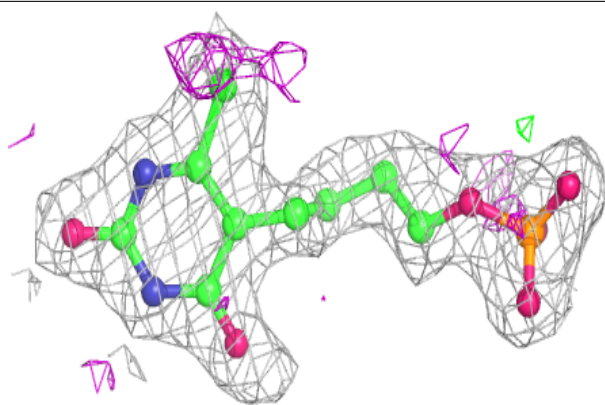
**Electron density around JCL E 701:**

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

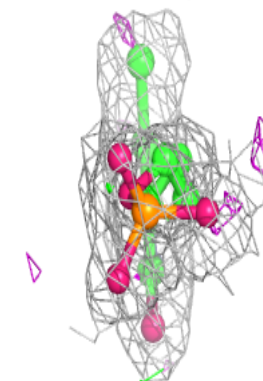
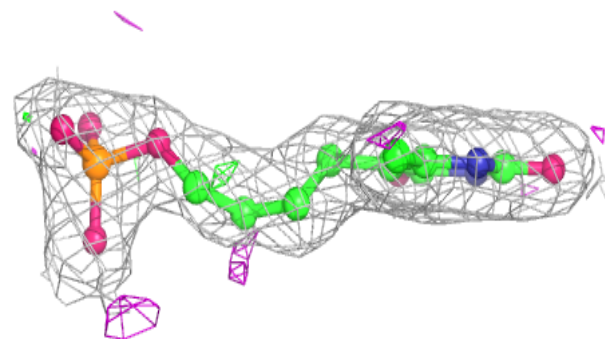
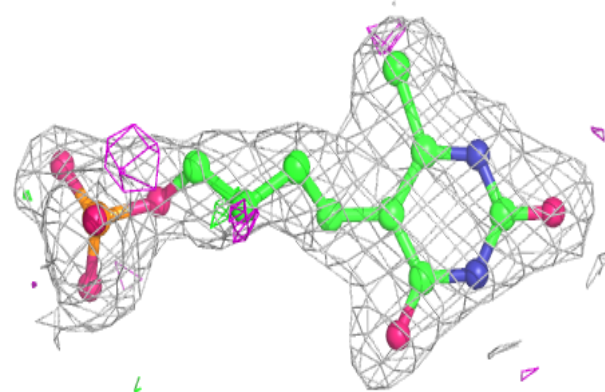


Electron density around JCL D 701:

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

**Electron density around JCL 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)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.