Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2023 – 02:14 AM JST

PDB ID	:	7YAN
Title	:	UDP-glucuronosyltransferase2B17 C-terminal domain
Authors	:	Wang, C.Y.; Zhang, L.
Deposited on	:	2022-06-28
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

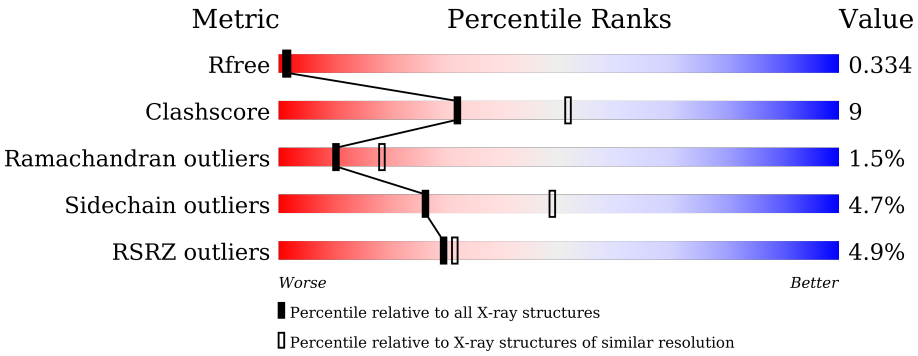
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	188	3% 70% 15% • 13%
1	B	188	5% 69% 16% •• 13%
1	C	188	3% 68% 16% •• 13%
1	D	188	6% 70% 14% •• 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	C	501	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5138 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 UDP-glucuronosyltransferase 2B17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1265	806	217	234	8			
1	B	164	Total	C	N	O	S	0	0	0
			1265	806	217	234	8			
1	C	164	Total	C	N	O	S	0	0	0
			1265	806	217	234	8			
1	D	163	Total	C	N	O	S	0	0	0
			1257	800	216	233	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	MET	-	initiating methionine	UNP O75795
A	265	GLY	-	expression tag	UNP O75795
A	266	HIS	-	expression tag	UNP O75795
A	267	HIS	-	expression tag	UNP O75795
A	268	HIS	-	expression tag	UNP O75795
A	269	HIS	-	expression tag	UNP O75795
A	270	HIS	-	expression tag	UNP O75795
A	271	HIS	-	expression tag	UNP O75795
A	272	GLU	-	expression tag	UNP O75795
A	273	ASN	-	expression tag	UNP O75795
A	274	LEU	-	expression tag	UNP O75795
A	275	TYR	-	expression tag	UNP O75795
A	276	PHE	-	expression tag	UNP O75795
A	277	GLN	-	expression tag	UNP O75795
A	278	GLY	-	expression tag	UNP O75795
A	279	HIS	-	expression tag	UNP O75795
A	280	MET	-	expression tag	UNP O75795
A	281	ALA	-	expression tag	UNP O75795
A	282	SER	-	expression tag	UNP O75795
A	283	MET	-	expression tag	UNP O75795
B	264	MET	-	initiating methionine	UNP O75795

Continued on next page...

Continued from previous page...

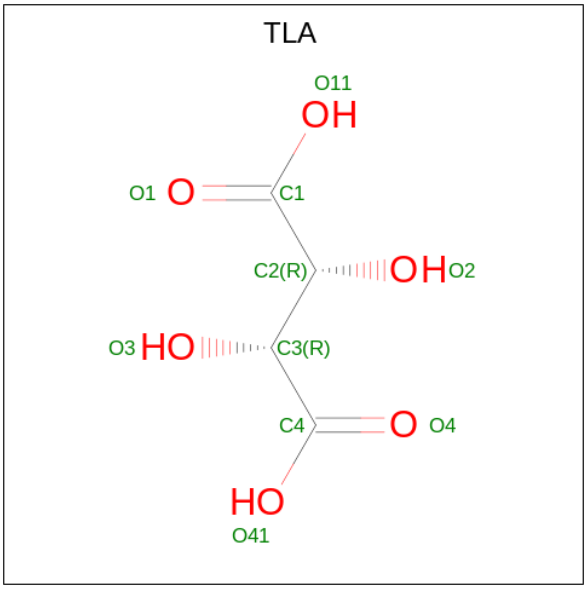
Chain	Residue	Modelled	Actual	Comment	Reference
B	265	GLY	-	expression tag	UNP O75795
B	266	HIS	-	expression tag	UNP O75795
B	267	HIS	-	expression tag	UNP O75795
B	268	HIS	-	expression tag	UNP O75795
B	269	HIS	-	expression tag	UNP O75795
B	270	HIS	-	expression tag	UNP O75795
B	271	HIS	-	expression tag	UNP O75795
B	272	GLU	-	expression tag	UNP O75795
B	273	ASN	-	expression tag	UNP O75795
B	274	LEU	-	expression tag	UNP O75795
B	275	TYR	-	expression tag	UNP O75795
B	276	PHE	-	expression tag	UNP O75795
B	277	GLN	-	expression tag	UNP O75795
B	278	GLY	-	expression tag	UNP O75795
B	279	HIS	-	expression tag	UNP O75795
B	280	MET	-	expression tag	UNP O75795
B	281	ALA	-	expression tag	UNP O75795
B	282	SER	-	expression tag	UNP O75795
B	283	MET	-	expression tag	UNP O75795
C	264	MET	-	initiating methionine	UNP O75795
C	265	GLY	-	expression tag	UNP O75795
C	266	HIS	-	expression tag	UNP O75795
C	267	HIS	-	expression tag	UNP O75795
C	268	HIS	-	expression tag	UNP O75795
C	269	HIS	-	expression tag	UNP O75795
C	270	HIS	-	expression tag	UNP O75795
C	271	HIS	-	expression tag	UNP O75795
C	272	GLU	-	expression tag	UNP O75795
C	273	ASN	-	expression tag	UNP O75795
C	274	LEU	-	expression tag	UNP O75795
C	275	TYR	-	expression tag	UNP O75795
C	276	PHE	-	expression tag	UNP O75795
C	277	GLN	-	expression tag	UNP O75795
C	278	GLY	-	expression tag	UNP O75795
C	279	HIS	-	expression tag	UNP O75795
C	280	MET	-	expression tag	UNP O75795
C	281	ALA	-	expression tag	UNP O75795
C	282	SER	-	expression tag	UNP O75795
C	283	MET	-	expression tag	UNP O75795
D	264	MET	-	initiating methionine	UNP O75795
D	265	GLY	-	expression tag	UNP O75795
D	266	HIS	-	expression tag	UNP O75795

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	267	HIS	-	expression tag	UNP O75795
D	268	HIS	-	expression tag	UNP O75795
D	269	HIS	-	expression tag	UNP O75795
D	270	HIS	-	expression tag	UNP O75795
D	271	HIS	-	expression tag	UNP O75795
D	272	GLU	-	expression tag	UNP O75795
D	273	ASN	-	expression tag	UNP O75795
D	274	LEU	-	expression tag	UNP O75795
D	275	TYR	-	expression tag	UNP O75795
D	276	PHE	-	expression tag	UNP O75795
D	277	GLN	-	expression tag	UNP O75795
D	278	GLY	-	expression tag	UNP O75795
D	279	HIS	-	expression tag	UNP O75795
D	280	MET	-	expression tag	UNP O75795
D	281	ALA	-	expression tag	UNP O75795
D	282	SER	-	expression tag	UNP O75795
D	283	MET	-	expression tag	UNP O75795

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0

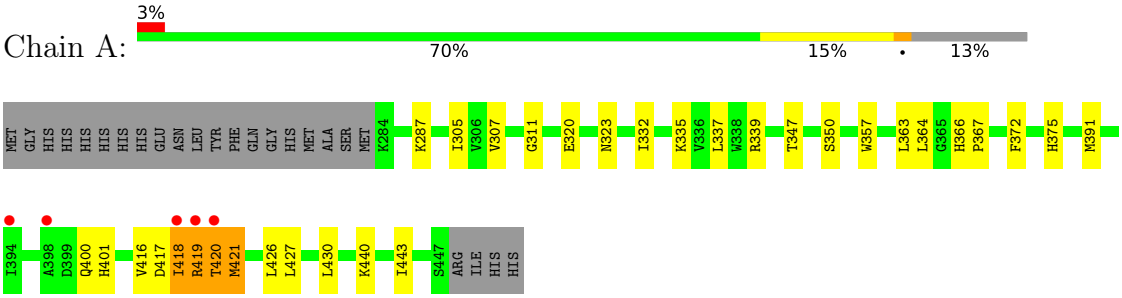
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	14	Total O 14 14	0	0
3	C	13	Total O 13 13	0	0
3	D	10	Total O 10 10	0	0

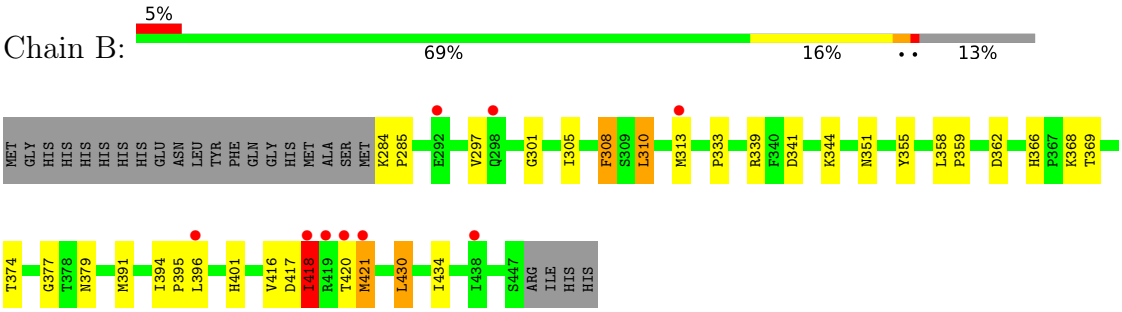
3 Residue-property plots (i)

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.

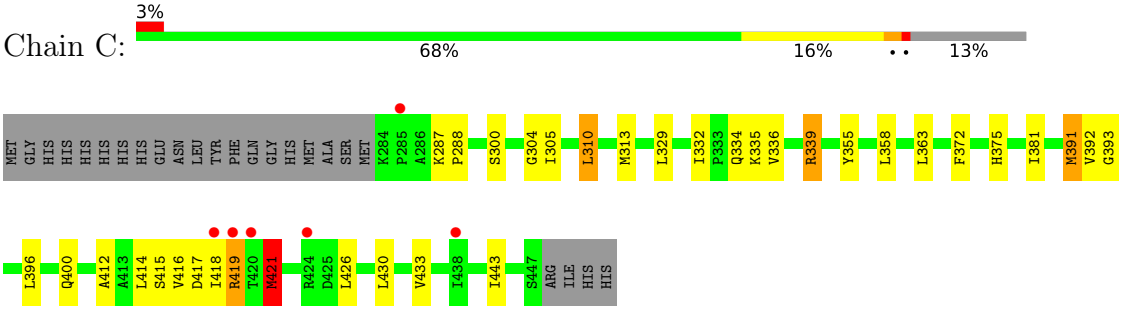
• Molecule 1: UDP-glucuronosyltransferase 2B17



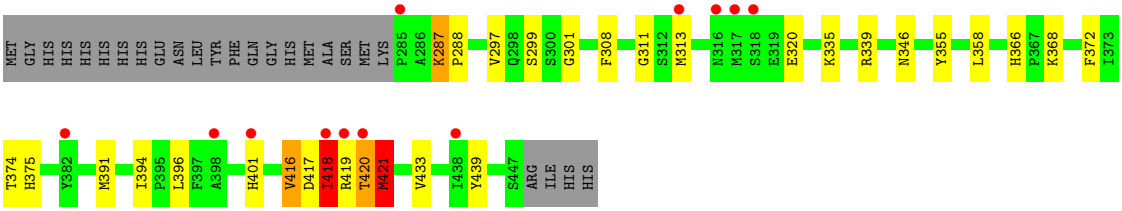
• Molecule 1: UDP-glucuronosyltransferase 2B17



• Molecule 1: UDP-glucuronosyltransferase 2B17



• Molecule 1: UDP-glucuronosyltransferase 2B17


MET GLY HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY HIS MET ALA SER MET LYS P285 A286 K287 P288 V297 Q298 S299 S300 G301 F308 G311 S312 M313 N316 M317 S318 E319 E320 K335 R339 N346 Y355 L358 H366 P367 K368 F372 I373
T374 H375 Y382 M391 I394 P395 L396 F397 A398 H401 V416 D417 I418 R419 T420 M421 V433 I438 Y439 S447 ARG ILE HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.15Å 57.31Å 74.07Å 99.25° 94.72° 90.12°	Depositor
Resolution (Å)	19.11 – 2.50 19.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.11-2.50) 76.6 (19.11-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.49Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.268 , 0.331 0.270 , 0.334	Depositor DCC
R_{free} test set	1012 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 5.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TLA

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	0.68	0/1292	0.79	0/1744
1	B	0.68	0/1292	0.81	0/1744
1	C	0.69	0/1292	0.80	0/1744
1	D	0.68	0/1284	0.80	0/1734
All	All	0.68	0/5160	0.80	0/6966

There are no bond length outliers.

There are no bond angle outliers.

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	1265	0	1287	21	0
1	B	1265	0	1287	33	0
1	C	1265	0	1287	21	0
1	D	1257	0	1276	23	0
2	A	10	0	4	0	0
2	B	10	0	4	2	0
2	C	10	0	4	2	0
2	D	10	0	4	0	0
3	A	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	0	0
3	C	13	0	0	0	0
3	D	10	0	0	0	0
All	All	5138	0	5153	91	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 9.

All (91) 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:401:HIS:NE2	1:D:418:ILE:HG12	1.87	0.89
1:B:401:HIS:NE2	1:B:418:ILE:HG12	1.93	0.83
1:D:287:LYS:N	1:D:287:LYS:HD3	2.03	0.73
1:C:310:LEU:HB2	2:C:501:TLA:O41	1.90	0.71
1:B:420:THR:OG1	1:B:421:MET:N	2.21	0.70
1:C:417:ASP:O	1:C:419:ARG:N	2.26	0.69
1:B:301:GLY:O	1:B:368:LYS:NZ	2.25	0.69
1:B:284:LYS:CG	1:B:285:PRO:HD3	2.23	0.68
1:A:287:LYS:HE3	1:B:285:PRO:O	1.95	0.67
1:D:287:LYS:N	1:D:287:LYS:CD	2.61	0.64
1:D:313:MET:HB3	1:D:396:LEU:CD1	2.28	0.63
1:D:420:THR:O	1:D:421:MET:HB3	1.99	0.60
1:A:417:ASP:HA	1:A:421:MET:HB2	1.84	0.60
1:B:333:PRO:HA	1:D:346:ASN:HD22	1.66	0.59
1:B:351:ASN:HD21	1:D:346:ASN:ND2	2.00	0.58
1:C:310:LEU:HD12	2:C:501:TLA:O41	2.05	0.57
1:B:333:PRO:HA	1:D:346:ASN:ND2	2.19	0.57
1:B:284:LYS:HG3	1:B:285:PRO:HD3	1.87	0.56
1:B:313:MET:HB3	1:B:396:LEU:CD1	2.35	0.56
1:B:417:ASP:HA	1:B:421:MET:HB2	1.88	0.56
1:C:300:SER:HB2	1:C:304:GLY:O	2.06	0.56
1:A:337:LEU:HD12	1:A:337:LEU:N	2.22	0.54
1:D:301:GLY:O	1:D:368:LYS:NZ	2.38	0.54
1:B:359:PRO:HB2	1:B:362:ASP:HB2	1.90	0.54
1:C:392:VAL:HA	1:C:414:LEU:O	2.08	0.54
1:B:284:LYS:CB	1:B:285:PRO:CD	2.87	0.53
1:B:284:LYS:CB	1:B:285:PRO:HD3	2.39	0.53
1:C:417:ASP:HA	1:C:421:MET:HB2	1.90	0.53
1:A:440:LYS:O	1:A:443:ILE:HG22	2.09	0.52
1:D:401:HIS:NE2	1:D:418:ILE:CG1	2.68	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PHE:O	1:A:391:MET:HA	2.11	0.51
1:D:299:SER:OG	1:D:335:LYS:HE2	2.10	0.51
1:A:366:HIS:ND1	1:A:367:PRO:HD2	2.25	0.51
1:B:355:TYR:CG	1:B:358:LEU:HD21	2.46	0.51
1:C:412:ALA:HB1	1:C:443:ILE:HD13	1.94	0.49
1:B:351:ASN:HD21	1:D:346:ASN:CG	2.16	0.49
1:C:305:ILE:HA	1:C:335:LYS:O	2.12	0.49
1:D:287:LYS:HD3	1:D:287:LYS:H	1.78	0.49
1:C:372:PHE:O	1:C:391:MET:HA	2.13	0.48
1:D:374:THR:HG21	1:D:391:MET:CE	2.43	0.48
1:C:329:LEU:HD22	1:C:336:VAL:HG11	1.94	0.48
1:D:311:GLY:HA2	1:D:375:HIS:NE2	2.28	0.48
1:B:377:GLY:HA3	2:B:501:TLA:O11	2.14	0.47
1:D:394:ILE:HG22	1:D:416:VAL:HG12	1.96	0.47
1:A:426:LEU:O	1:A:430:LEU:HG	2.14	0.47
1:A:287:LYS:CE	1:B:285:PRO:O	2.62	0.47
1:D:297:VAL:HG11	1:D:366:HIS:CE1	2.50	0.46
1:D:417:ASP:HA	1:D:421:MET:HB2	1.97	0.46
1:A:357:TRP:HA	1:B:379:ASN:OD1	2.15	0.46
1:B:284:LYS:CG	1:B:285:PRO:CD	2.91	0.46
1:B:308:PHE:CZ	1:B:394:ILE:HD11	2.51	0.46
1:B:310:LEU:HB2	2:B:501:TLA:O2	2.16	0.46
1:D:372:PHE:O	1:D:391:MET:HA	2.16	0.46
1:B:395:PRO:HG2	1:B:401:HIS:CD2	2.51	0.45
1:B:297:VAL:HG11	1:B:366:HIS:CE1	2.51	0.45
1:B:416:VAL:HG13	1:B:421:MET:HG3	1.97	0.45
1:B:374:THR:HG21	1:B:391:MET:CE	2.47	0.44
1:A:311:GLY:HA2	1:A:375:HIS:NE2	2.32	0.44
1:A:416:VAL:CG1	1:A:417:ASP:N	2.81	0.44
1:C:287:LYS:HB2	1:C:288:PRO:CD	2.48	0.44
1:B:430:LEU:O	1:B:434:ILE:HG13	2.18	0.44
1:D:313:MET:CB	1:D:396:LEU:CD1	2.96	0.43
1:A:305:ILE:HA	1:A:335:LYS:O	2.18	0.43
1:C:375:HIS:O	1:C:400:GLN:HB3	2.19	0.43
1:B:310:LEU:HD23	1:B:310:LEU:O	2.19	0.43
1:C:332:ILE:HG23	1:C:334:GLN:OE1	2.18	0.43
1:A:416:VAL:HG13	1:A:421:MET:SD	2.58	0.43
1:C:426:LEU:O	1:C:430:LEU:HB2	2.19	0.43
1:A:401:HIS:NE2	1:A:418:ILE:HG12	2.34	0.43
1:C:381:ILE:HG12	1:C:391:MET:HE3	2.00	0.43
1:C:313:MET:CB	1:C:396:LEU:CD1	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASN:O	1:A:347:THR:OG1	2.37	0.42
1:B:420:THR:HG1	1:B:421:MET:H	1.60	0.42
1:C:358:LEU:HD22	1:C:363:LEU:HD11	2.00	0.42
1:C:430:LEU:HD12	1:C:430:LEU:HA	1.84	0.42
1:A:416:VAL:CG1	1:A:421:MET:SD	3.08	0.42
1:B:284:LYS:HB2	1:B:285:PRO:HD3	2.02	0.42
1:C:393:GLY:O	1:C:415:SER:HA	2.20	0.42
1:A:375:HIS:O	1:A:400:GLN:HB3	2.19	0.42
1:C:416:VAL:CG1	1:C:417:ASP:N	2.83	0.42
1:A:364:LEU:HD21	1:A:372:PHE:CD1	2.54	0.42
1:B:297:VAL:CG1	1:B:366:HIS:CE1	3.03	0.41
1:D:355:TYR:CG	1:D:358:LEU:HD21	2.55	0.41
1:B:305:ILE:HG13	1:B:369:THR:HA	2.02	0.41
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.95	0.41
1:A:332:ILE:HD11	1:A:427:LEU:HD12	2.02	0.41
1:A:419:ARG:O	1:A:420:THR:C	2.59	0.41
1:A:307:VAL:HG21	1:A:363:LEU:HB3	2.03	0.41
1:D:420:THR:O	1:D:421:MET:CB	2.68	0.40
1:C:339:ARG:HA	1:C:355:TYR:O	2.22	0.40
1:D:433:VAL:HA	1:D:439:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

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	162/188 (86%)	152 (94%)	7 (4%)	3 (2%)	8 13
1	B	162/188 (86%)	150 (93%)	10 (6%)	2 (1%)	13 24
1	C	162/188 (86%)	153 (94%)	7 (4%)	2 (1%)	13 24
1	D	161/188 (86%)	151 (94%)	7 (4%)	3 (2%)	8 13
All	All	647/752 (86%)	606 (94%)	31 (5%)	10 (2%)	10 18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	MET
1	C	418	ILE
1	D	421	MET
1	A	418	ILE
1	B	421	MET
1	A	420	THR
1	C	421	MET
1	D	418	ILE
1	D	288	PRO
1	B	418	ILE

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	138/160 (86%)	134 (97%)	4 (3%)	42	69
1	B	138/160 (86%)	131 (95%)	7 (5%)	24	45
1	C	138/160 (86%)	132 (96%)	6 (4%)	29	53
1	D	138/160 (86%)	129 (94%)	9 (6%)	17	33
All	All	552/640 (86%)	526 (95%)	26 (5%)	26	49

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	GLU
1	A	339	ARG
1	A	350	SER
1	A	419	ARG
1	B	308	PHE
1	B	310	LEU
1	B	339	ARG
1	B	341	ASP
1	B	344	LYS
1	B	418	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	430	LEU
1	C	310	LEU
1	C	339	ARG
1	C	391	MET
1	C	419	ARG
1	C	421	MET
1	C	433	VAL
1	D	287	LYS
1	D	308	PHE
1	D	320	GLU
1	D	339	ARG
1	D	416	VAL
1	D	418	ILE
1	D	419	ARG
1	D	420	THR
1	D	421	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
1	B	351	ASN
1	B	442	ASN
1	D	331	GLN
1	D	406	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 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	TLA	B	501	-	9,9,9	1.21	1 (11%)	12,12,12	1.23	1 (8%)
2	TLA	D	501	-	9,9,9	1.00	0	12,12,12	1.70	4 (33%)
2	TLA	C	501	-	9,9,9	1.55	2 (22%)	12,12,12	1.90	4 (33%)
2	TLA	A	501	-	9,9,9	1.29	1 (11%)	12,12,12	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	B	501	-	-	4/12/12/12	-
2	TLA	D	501	-	-	2/12/12/12	-
2	TLA	C	501	-	-	8/12/12/12	-
2	TLA	A	501	-	-	6/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	TLA	C3-C4	-2.83	1.48	1.52
2	C	501	TLA	O41-C4	-2.46	1.22	1.30
2	B	501	TLA	O41-C4	-2.23	1.23	1.30
2	A	501	TLA	O2-C2	2.18	1.46	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	TLA	C3-C2-C1	3.91	118.61	109.87
2	D	501	TLA	O41-C4-C3	3.74	123.37	113.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	TLA	O4-C4-C3	-2.88	114.05	121.63
2	C	501	TLA	O11-C1-C2	2.86	121.00	113.27
2	C	501	TLA	O2-C2-C1	-2.45	105.54	110.66
2	C	501	TLA	O2-C2-C3	-2.41	105.44	110.23
2	B	501	TLA	O41-C4-O4	-2.35	118.75	124.09
2	D	501	TLA	O11-C1-O1	-2.33	118.79	124.09
2	D	501	TLA	O11-C1-C2	2.24	119.32	113.27

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TLA	C1-C2-C3-C4
2	C	501	TLA	C1-C2-C3-O3
2	C	501	TLA	C1-C2-C3-C4
2	C	501	TLA	O2-C2-C3-C4
2	A	501	TLA	O2-C2-C3-O3
2	C	501	TLA	O2-C2-C3-O3
2	C	501	TLA	O1-C1-C2-O2
2	C	501	TLA	O11-C1-C2-O2
2	A	501	TLA	O2-C2-C3-C4
2	C	501	TLA	O3-C3-C4-O4
2	C	501	TLA	O3-C3-C4-O41
2	A	501	TLA	O1-C1-C2-O2
2	A	501	TLA	O11-C1-C2-O2
2	A	501	TLA	C1-C2-C3-O3
2	B	501	TLA	O3-C3-C4-O41
2	B	501	TLA	O3-C3-C4-O4
2	B	501	TLA	C2-C3-C4-O4
2	B	501	TLA	C2-C3-C4-O41
2	D	501	TLA	O1-C1-C2-C3
2	D	501	TLA	O11-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

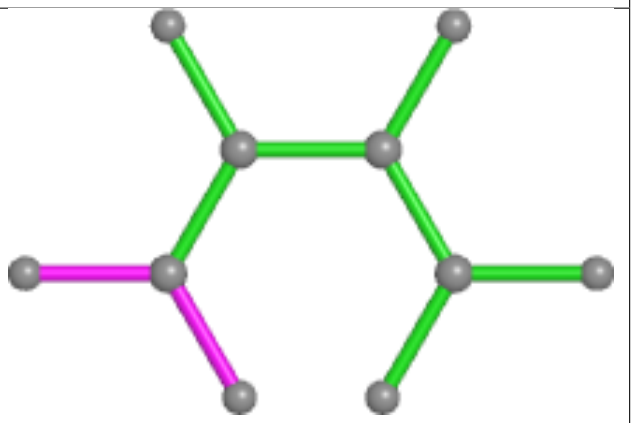
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	TLA	2	0
2	C	501	TLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

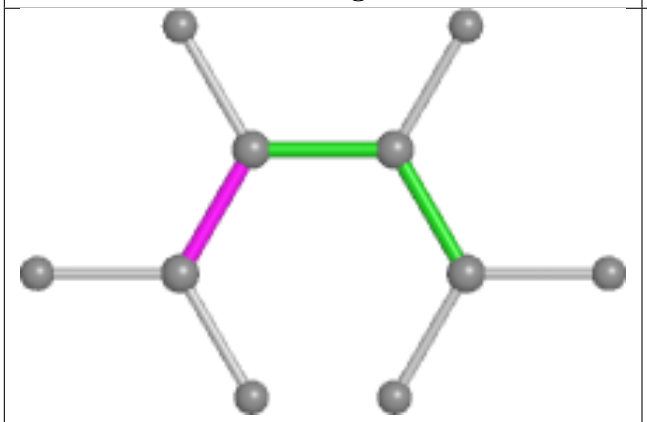
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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 TLA B 501

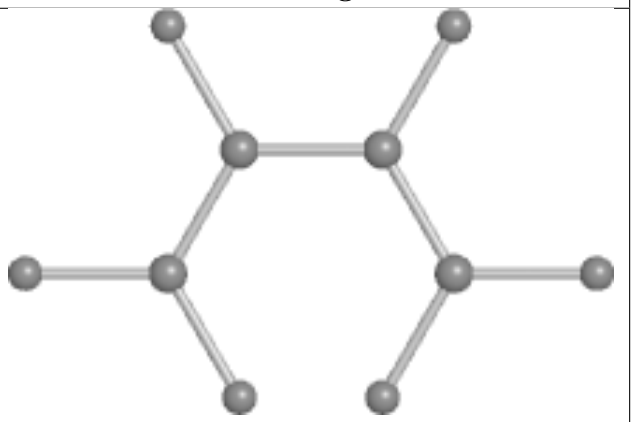
Bond lengths



Bond angles

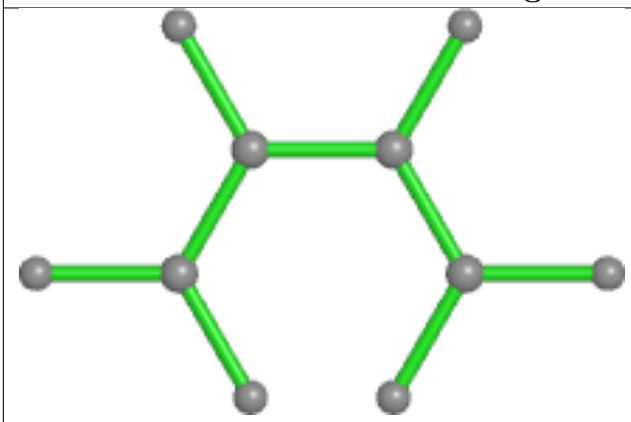


Torsions

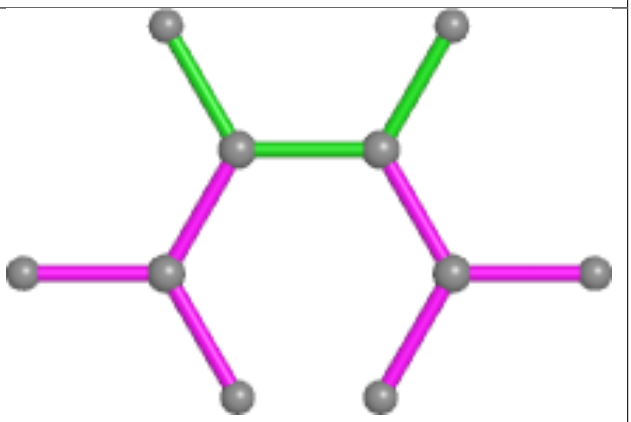


Rings

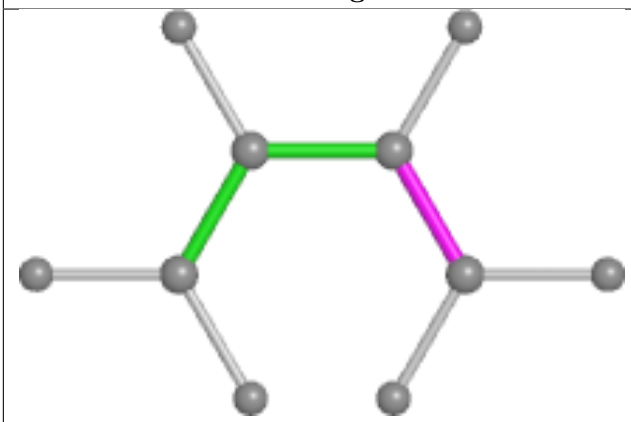
Ligand TLA D 501



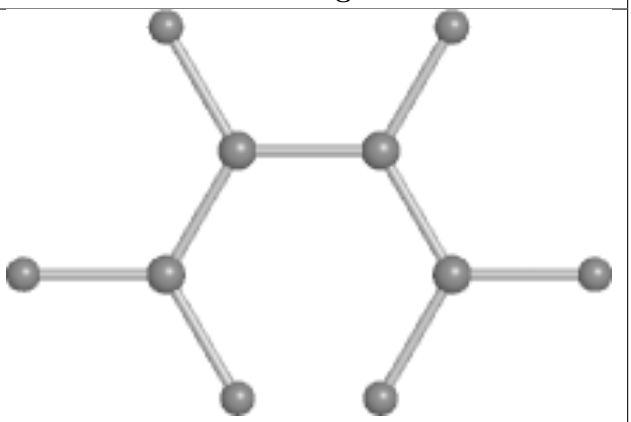
Bond lengths



Bond angles

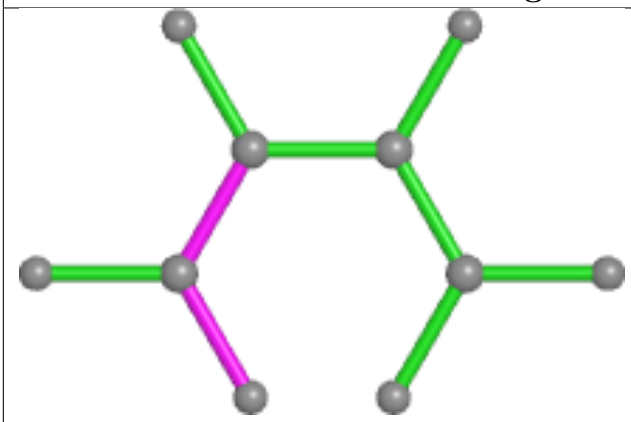


Torsions

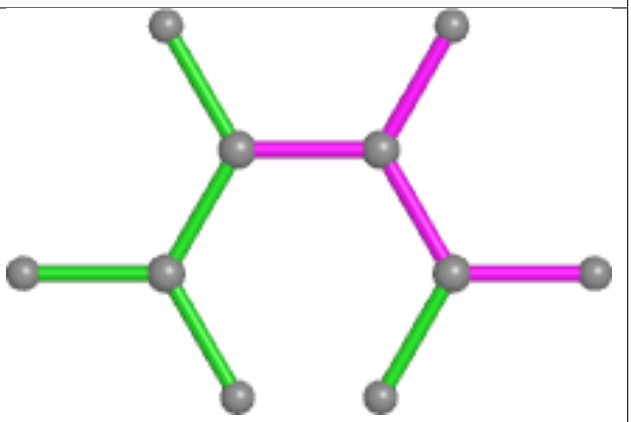


Rings

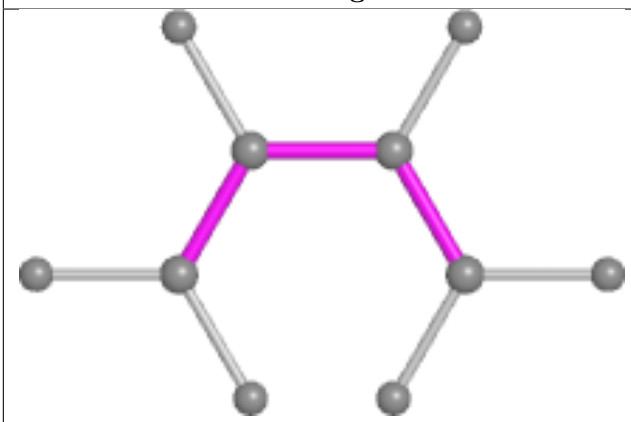
Ligand TLA C 501



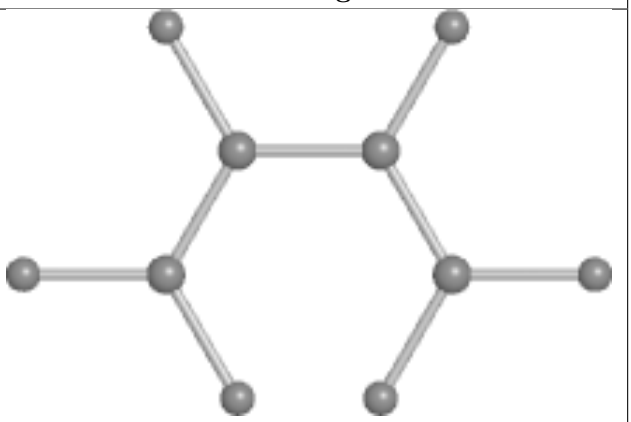
Bond lengths



Bond angles

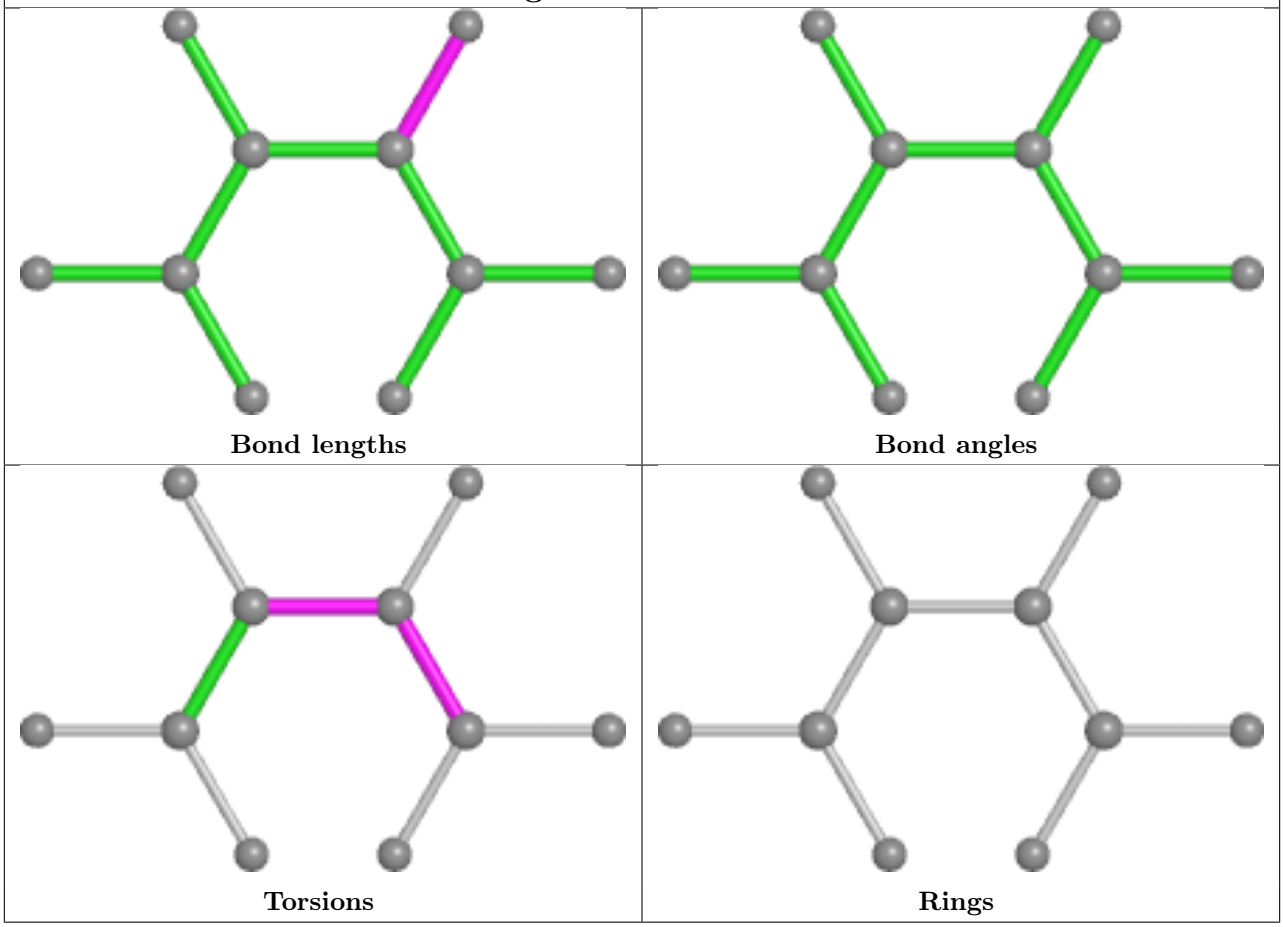


Torsions



Rings

Ligand TLA A 501



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^{th} 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	164/188 (87%)	0.25	5 (3%)	50	53	9, 15, 32, 53	0
1	B	164/188 (87%)	0.43	9 (5%)	25	26	8, 19, 39, 77	0
1	C	164/188 (87%)	0.22	6 (3%)	41	45	9, 16, 32, 55	0
1	D	163/188 (86%)	0.42	12 (7%)	14	15	10, 19, 36, 67	0
All	All	655/752 (87%)	0.33	32 (4%)	29	31	8, 17, 36, 77	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	ILE	8.5
1	B	420	THR	8.1
1	D	418	ILE	7.5
1	D	420	THR	7.2
1	C	418	ILE	6.0
1	A	418	ILE	5.7
1	B	419	ARG	5.2
1	A	420	THR	4.7
1	B	313	MET	4.0
1	C	420	THR	4.0
1	D	316	ASN	3.7
1	D	419	ARG	3.1
1	C	419	ARG	2.9
1	D	438	ILE	2.6
1	C	285	PRO	2.6
1	B	298	GLN	2.6
1	B	292	GLU	2.6
1	A	419	ARG	2.5
1	B	421	MET	2.5
1	A	398	ALA	2.5
1	A	394	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	396	LEU	2.3
1	C	438	ILE	2.3
1	D	285	PRO	2.3
1	D	398	ALA	2.2
1	B	438	ILE	2.2
1	D	401	HIS	2.1
1	D	318	SER	2.1
1	D	317	MET	2.1
1	D	313	MET	2.1
1	D	382	TYR	2.1
1	C	424	ARG	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)

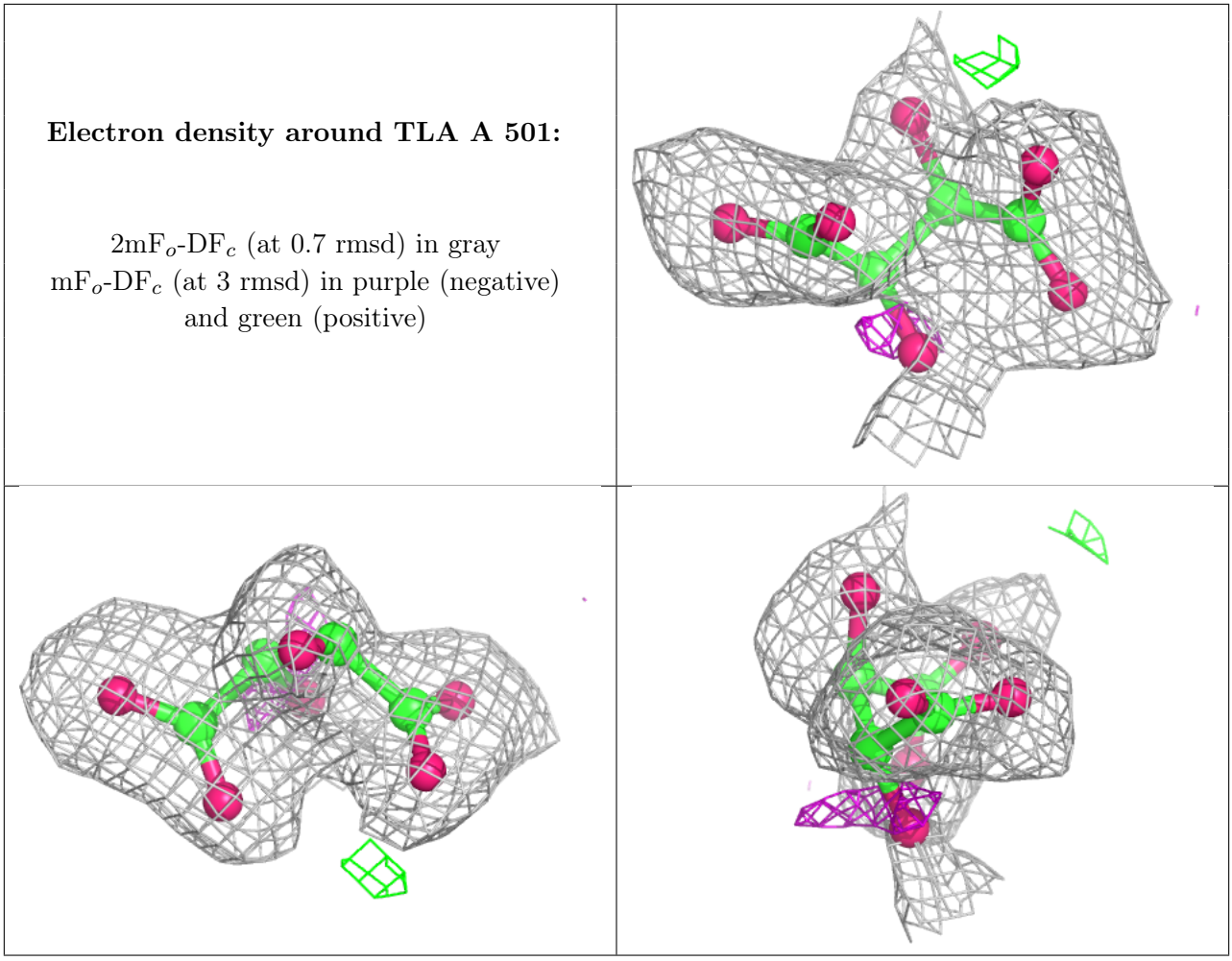
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TLA	A	501	10/10	0.82	0.20	16,17,18,20	0
2	TLA	C	501	10/10	0.88	0.16	19,20,21,24	0
2	TLA	D	501	10/10	0.92	0.14	11,12,13,13	0
2	TLA	B	501	10/10	0.94	0.10	14,14,15,15	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.

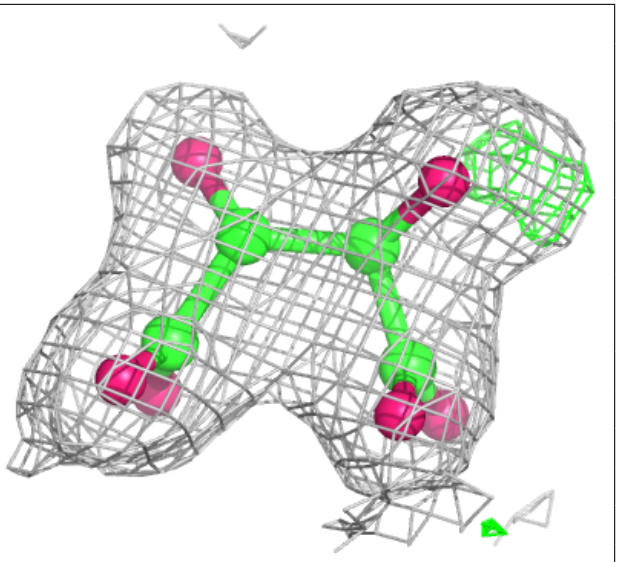
Electron density around TLA A 501:

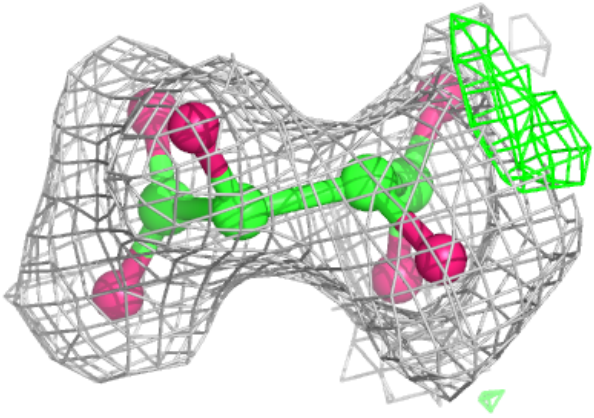
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

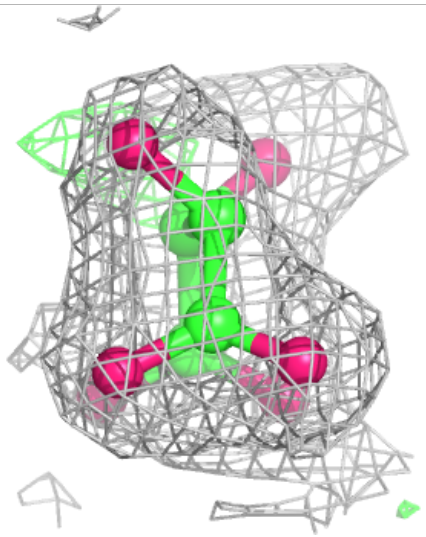


Electron density around TLA C 501:

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

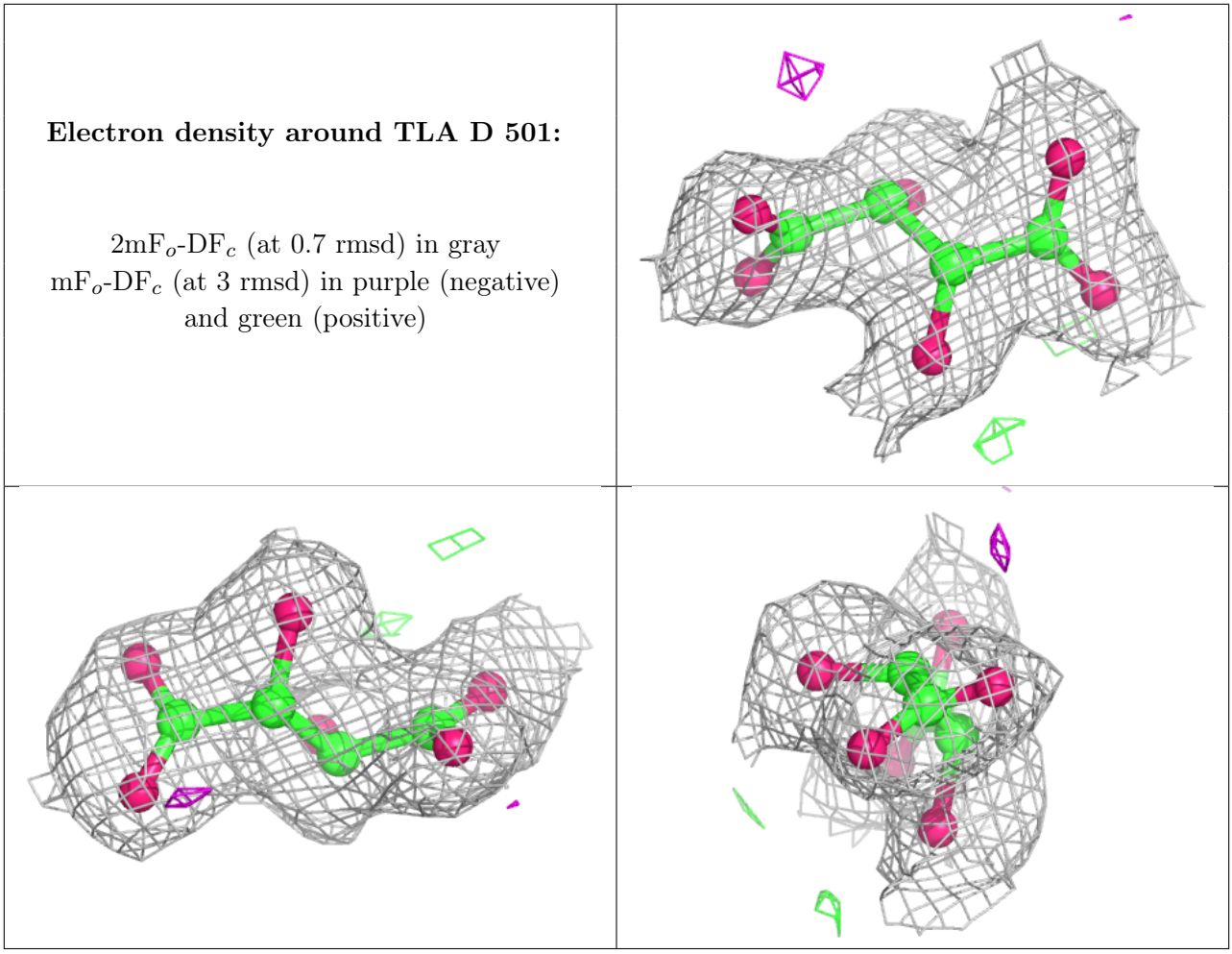






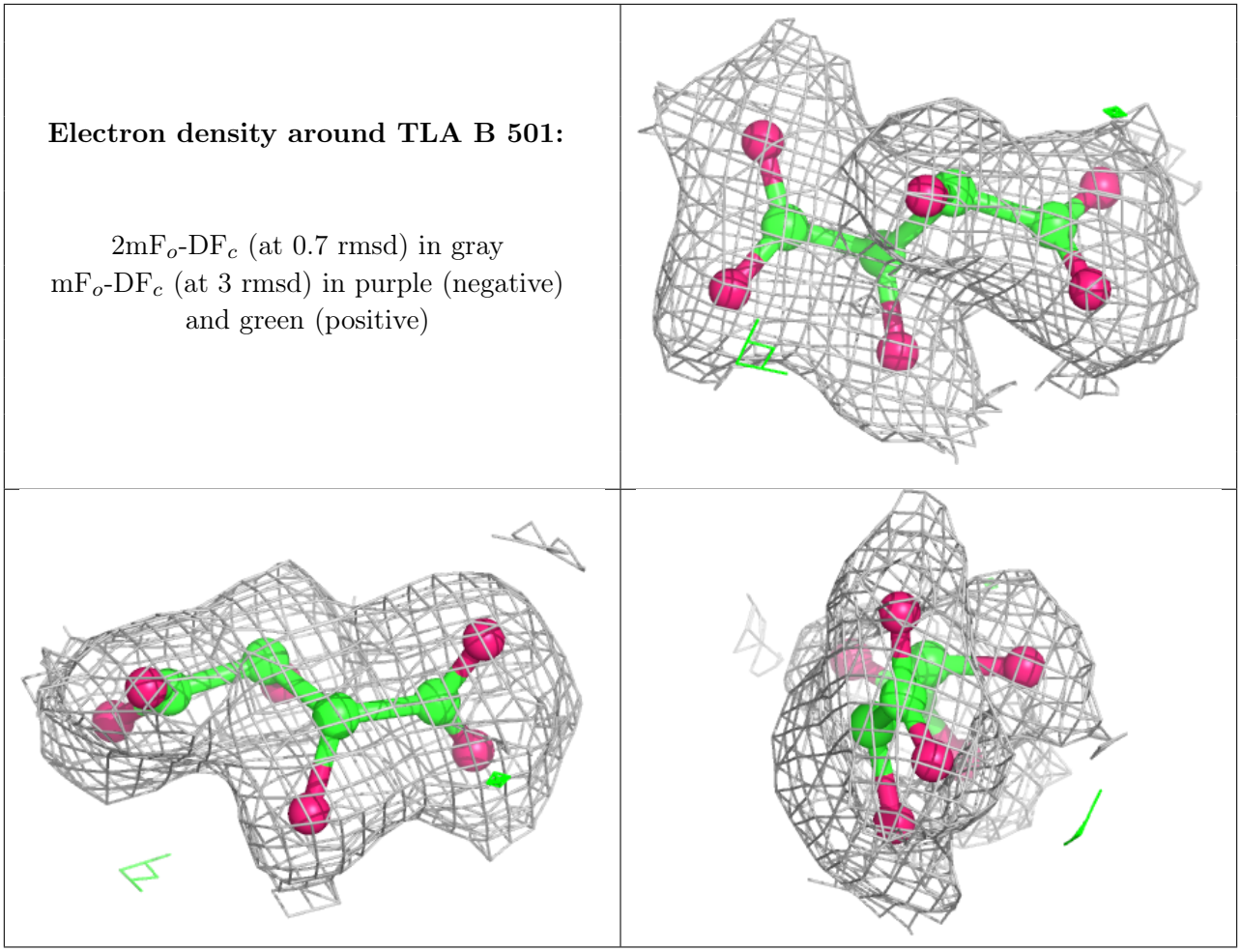
Electron density around TLA D 501:

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



Electron density around TLA B 501:

$2mF_o$-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.