



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:05 pm BST

PDB ID : 2AG0
Title : Crystal structure of Benzaldehyde lyase (BAL)- native
Authors : Mosbacher, T.G.; Mueller, M.; Schulz, G.E.
Deposited on : 2005-07-26
Resolution : 2.58 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

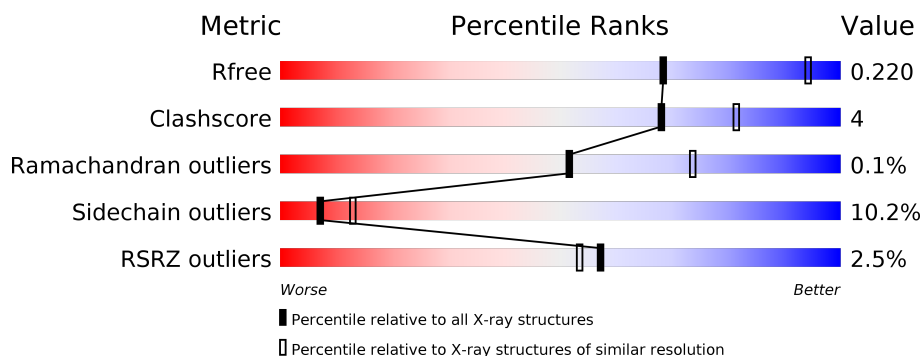
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 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	563	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	563	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	563	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	D	563	<div> <div>0%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>••</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16902 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.

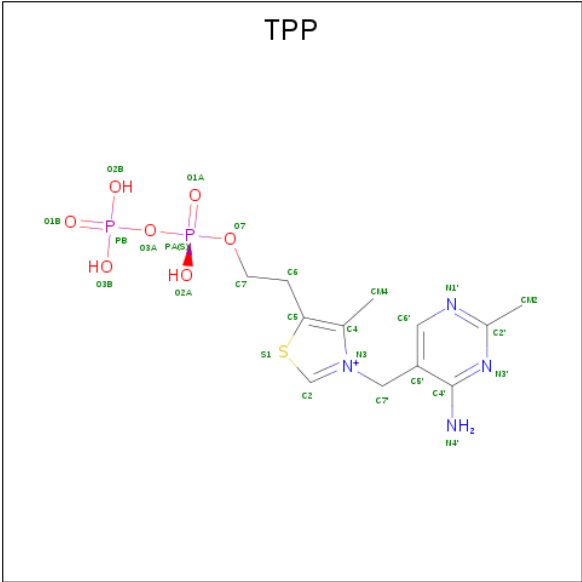
- Molecule 1 is a protein called benzaldehyde lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	B	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	C	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	D	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

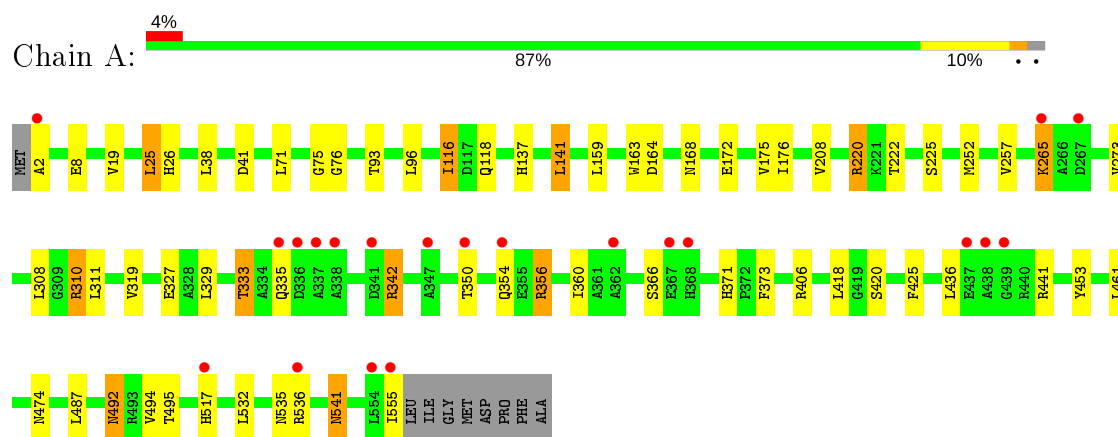
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	80	Total	O	0	0
			80	80		
4	C	132	Total	O	0	0
			132	132		
4	D	167	Total	O	0	0
			167	167		

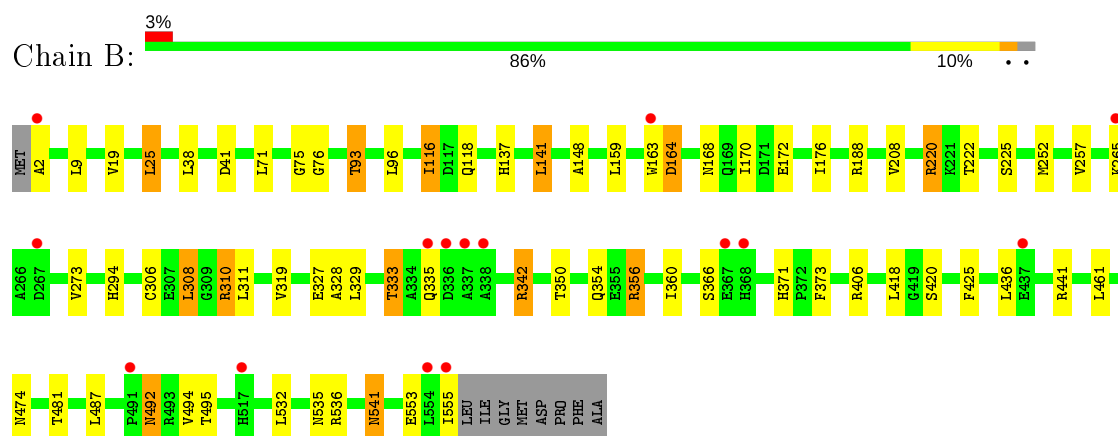
3 Residue-property plots [i](#)

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 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.

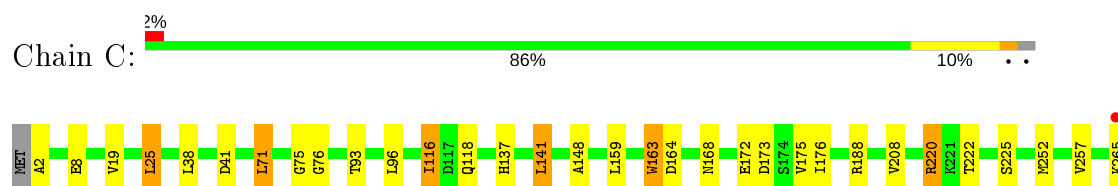
- Molecule 1: benzaldehyde lyase

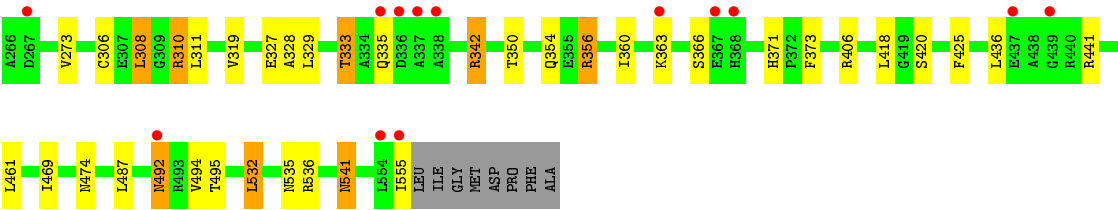


- Molecule 1: benzaldehyde lyase

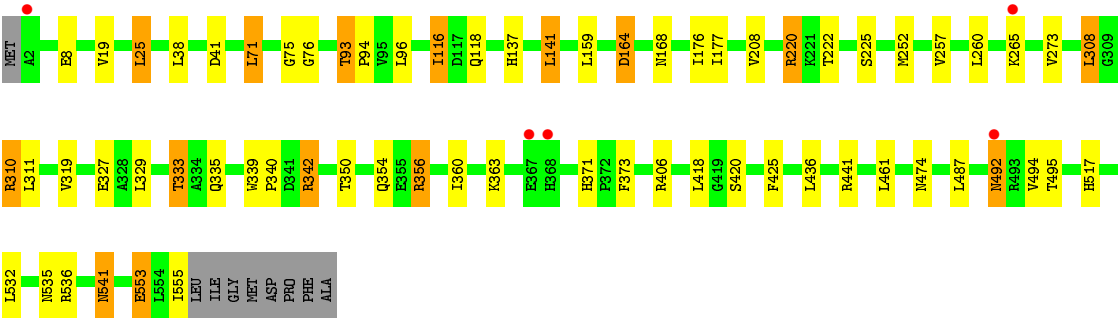
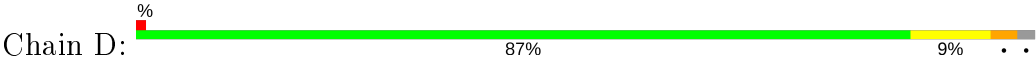


- Molecule 1: benzaldehyde lyase





● Molecule 1: benzaldehyde lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.72Å 154.72Å 200.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.58 19.95 – 2.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.58) 98.2 (19.95-2.58)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.220 0.200 , 0.220	Depositor DCC
R_{free} test set	4281 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16902	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/4162	0.68	3/5677 (0.1%)
1	B	0.53	0/4162	0.68	4/5677 (0.1%)
1	C	0.60	0/4162	0.70	4/5677 (0.1%)
1	D	0.62	0/4162	0.71	4/5677 (0.1%)
All	All	0.58	0/16648	0.69	15/22708 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ASP	N-CA-CB	-7.98	96.24	110.60
1	C	164	ASP	N-CA-CB	-7.45	97.18	110.60
1	A	164	ASP	N-CA-CB	-7.43	97.22	110.60
1	D	553	GLU	CB-CA-C	-7.01	96.38	110.40
1	B	163	TRP	CB-CA-C	-6.98	96.44	110.40
1	D	25	LEU	CA-CB-CG	6.48	130.20	115.30
1	D	164	ASP	N-CA-CB	-6.32	99.22	110.60
1	C	163	TRP	CB-CA-C	-6.13	98.14	110.40
1	A	25	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	163	TRP	CB-CA-C	-5.92	98.55	110.40
1	B	25	LEU	CA-CB-CG	5.72	128.46	115.30
1	C	25	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	553	GLU	CB-CA-C	-5.57	99.25	110.40
1	C	71	LEU	CA-CB-CG	5.40	127.73	115.30
1	D	71	LEU	CA-CB-CG	5.25	127.37	115.30

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	4079	0	4069	27	2
1	B	4079	0	4069	32	0
1	C	4079	0	4069	31	1
1	D	4079	0	4069	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	0	0
3	B	26	0	16	0	0
3	C	26	0	16	0	0
3	D	26	0	16	1	0
4	A	99	0	0	4	0
4	B	80	0	0	4	0
4	C	132	0	0	1	0
4	D	167	0	0	13	0
All	All	16902	0	16340	123	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 4.

All (123) 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:420:SER:HB3	4:B:5023:HOH:O	1.39	1.18
1:D:420:SER:HB3	4:D:5045:HOH:O	1.01	1.17
1:D:517:HIS:HB3	4:D:5162:HOH:O	1.60	1.02
1:B:354:GLN:HE22	1:B:406:ARG:HH12	1.03	1.01
1:D:420:SER:CB	4:D:5045:HOH:O	1.69	0.98
1:C:354:GLN:HE22	1:C:406:ARG:HH12	1.15	0.94
1:D:354:GLN:HE22	1:D:406:ARG:HH12	1.13	0.94
1:A:354:GLN:HE22	1:A:406:ARG:HH12	1.15	0.93
1:B:354:GLN:NE2	1:B:406:ARG:HH12	1.66	0.92
1:D:342:ARG:HH11	1:D:342:ARG:HG3	1.34	0.92
1:C:342:ARG:HH11	1:C:342:ARG:HG3	1.36	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HH11	1:B:342:ARG:HG3	1.35	0.91
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.36	0.90
1:D:354:GLN:NE2	1:D:406:ARG:HH12	1.71	0.88
1:C:354:GLN:NE2	1:C:406:ARG:HH12	1.74	0.85
1:A:354:GLN:NE2	1:A:406:ARG:HH12	1.73	0.85
1:D:342:ARG:CG	1:D:342:ARG:HH11	1.90	0.84
1:B:342:ARG:CG	1:B:342:ARG:HH11	1.92	0.81
1:C:342:ARG:HH11	1:C:342:ARG:CG	1.94	0.81
1:A:342:ARG:HH11	1:A:342:ARG:CG	1.95	0.78
1:A:371:HIS:HD2	1:A:373:PHE:H	1.29	0.78
1:D:371:HIS:HD2	1:D:373:PHE:H	1.29	0.78
1:B:371:HIS:HD2	1:B:373:PHE:H	1.33	0.74
1:C:371:HIS:HD2	1:C:373:PHE:H	1.34	0.74
1:D:517:HIS:HE1	4:D:5180:HOH:O	1.76	0.69
1:A:420:SER:OG	1:B:76:GLY:HA3	1.94	0.67
1:A:116:ILE:HD11	1:A:118:GLN:HE21	1.60	0.66
1:B:116:ILE:HD11	1:B:118:GLN:HE21	1.61	0.66
1:A:8:GLU:HG2	4:A:5026:HOH:O	1.95	0.66
1:C:310:ARG:HG3	1:C:311:LEU:HG	1.80	0.64
1:D:220:ARG:HD3	1:D:327:GLU:OE1	1.99	0.63
1:D:8:GLU:HG2	4:D:5126:HOH:O	1.97	0.63
1:C:220:ARG:HD3	1:C:327:GLU:OE1	1.99	0.63
1:B:93:THR:HG21	4:B:5033:HOH:O	1.97	0.62
1:A:2:ALA:HA	1:A:172:GLU:OE1	1.99	0.62
1:A:76:GLY:HA3	1:B:420:SER:OG	1.99	0.62
1:C:420:SER:OG	1:D:76:GLY:HA3	1.99	0.62
1:B:354:GLN:HE22	1:B:406:ARG:NH1	1.87	0.61
1:A:310:ARG:HG3	1:A:311:LEU:HG	1.82	0.61
1:A:220:ARG:HD3	1:A:327:GLU:OE1	2.01	0.61
1:D:342:ARG:HD3	4:D:5133:HOH:O	2.00	0.60
1:B:220:ARG:HD3	1:B:327:GLU:OE1	2.00	0.60
1:C:116:ILE:HD11	1:C:118:GLN:HE21	1.66	0.60
1:A:453:TYR:HB3	4:A:5025:HOH:O	2.00	0.60
1:B:310:ARG:HG3	1:B:311:LEU:HG	1.83	0.60
1:D:354:GLN:HE22	1:D:406:ARG:NH1	1.95	0.59
1:D:116:ILE:HD11	1:D:118:GLN:HE21	1.67	0.59
1:D:310:ARG:HG3	1:D:311:LEU:HG	1.86	0.58
1:B:2:ALA:HA	1:B:172:GLU:OE1	2.04	0.58
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.64	0.56
1:D:177:ILE:HD11	4:D:5131:HOH:O	2.07	0.55
1:D:342:ARG:CD	4:D:5133:HOH:O	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASN:ND2	1:A:492:ASN:H	2.05	0.55
1:C:342:ARG:CG	1:C:342:ARG:NH1	2.62	0.54
1:B:420:SER:CB	4:B:5023:HOH:O	2.21	0.54
1:A:492:ASN:H	1:A:492:ASN:HD22	1.57	0.53
1:B:342:ARG:CG	1:B:342:ARG:NH1	2.61	0.53
1:C:356:ARG:O	1:C:360:ILE:HG12	2.09	0.53
1:C:8:GLU:HG2	4:C:5117:HOH:O	2.07	0.53
1:A:356:ARG:O	1:A:360:ILE:HG12	2.08	0.52
1:D:492:ASN:ND2	1:D:492:ASN:H	2.07	0.52
1:B:137:HIS:HB3	1:B:141:LEU:HD22	1.91	0.52
1:B:492:ASN:H	1:B:492:ASN:ND2	2.08	0.52
1:A:354:GLN:HE22	1:A:406:ARG:NH1	1.97	0.52
1:B:356:ARG:O	1:B:360:ILE:HG12	2.10	0.51
1:C:492:ASN:ND2	1:C:492:ASN:H	2.08	0.51
1:D:553:GLU:O	1:D:553:GLU:CG	2.59	0.51
1:A:329:LEU:O	1:A:333:THR:HB	2.10	0.50
1:C:2:ALA:HA	1:C:172:GLU:OE1	2.11	0.50
1:C:492:ASN:H	1:C:492:ASN:HD22	1.60	0.50
1:C:535:ASN:O	1:C:536:ARG:HG3	2.12	0.50
1:D:116:ILE:HD13	4:D:5149:HOH:O	2.10	0.50
1:A:342:ARG:HD3	4:A:5074:HOH:O	2.12	0.50
1:B:492:ASN:HD22	1:B:492:ASN:H	1.59	0.50
1:D:356:ARG:O	1:D:360:ILE:HG12	2.12	0.50
1:B:75:GLY:H	1:B:118:GLN:HE22	1.60	0.49
1:D:137:HIS:HB3	1:D:141:LEU:HD22	1.95	0.49
1:C:354:GLN:HE22	1:C:406:ARG:NH1	1.97	0.49
1:D:474:ASN:HD22	1:D:541:ASN:HD21	1.60	0.49
1:D:517:HIS:CD2	4:D:5203:HOH:O	2.66	0.48
1:B:329:LEU:O	1:B:333:THR:HB	2.14	0.48
1:A:371:HIS:CD2	1:A:373:PHE:H	2.20	0.48
1:D:93:THR:HG21	4:D:5046:HOH:O	2.14	0.48
1:A:137:HIS:HB3	1:A:141:LEU:HD22	1.96	0.48
1:D:492:ASN:H	1:D:492:ASN:HD22	1.61	0.47
1:C:137:HIS:HB3	1:C:141:LEU:HD22	1.96	0.47
1:A:75:GLY:H	1:A:118:GLN:HE22	1.63	0.47
1:A:535:ASN:O	1:A:536:ARG:HG3	2.16	0.46
1:A:342:ARG:CD	4:A:5074:HOH:O	2.64	0.46
1:C:163:TRP:CD1	1:C:163:TRP:O	2.68	0.46
1:A:26:HIS:CD2	1:B:481:THR:HB	2.51	0.46
1:B:294:HIS:HD2	4:B:5053:HOH:O	1.99	0.45
1:C:75:GLY:H	1:C:118:GLN:HE22	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:CG	1:D:342:ARG:NH1	2.60	0.44
1:D:93:THR:HA	1:D:94:PRO:HD3	1.92	0.44
1:D:75:GLY:H	1:D:118:GLN:HE22	1.65	0.44
1:C:76:GLY:HA3	1:D:420:SER:OG	2.17	0.44
1:C:329:LEU:O	1:C:333:THR:HB	2.17	0.43
1:D:339:TRP:HA	1:D:340:PRO:HD3	1.92	0.43
1:B:474:ASN:HD22	1:B:541:ASN:HD21	1.67	0.43
1:C:474:ASN:HD22	1:C:541:ASN:HD21	1.65	0.43
1:B:75:GLY:H	1:B:118:GLN:NE2	2.16	0.43
1:B:354:GLN:NE2	1:B:406:ARG:NH1	2.49	0.42
1:D:329:LEU:O	1:D:333:THR:HB	2.19	0.42
1:B:188:ARG:HD3	1:B:328:ALA:HB2	2.01	0.42
1:D:535:ASN:O	1:D:536:ARG:HG3	2.19	0.42
1:B:148:ALA:HB2	1:C:306:CYS:SG	2.59	0.42
1:A:474:ASN:HD22	1:A:541:ASN:HD21	1.68	0.42
1:D:553:GLU:O	1:D:553:GLU:HG2	2.19	0.42
1:B:535:ASN:O	1:B:536:ARG:HG3	2.19	0.42
1:C:188:ARG:HD3	1:C:328:ALA:HB2	2.02	0.42
1:D:363:LYS:HB3	1:D:363:LYS:HE2	1.85	0.42
1:C:363:LYS:HB3	1:C:363:LYS:HE2	1.89	0.41
1:D:492:ASN:N	1:D:492:ASN:HD22	2.18	0.41
1:C:371:HIS:CD2	1:C:373:PHE:H	2.25	0.41
1:C:354:GLN:NE2	1:C:406:ARG:NH1	2.56	0.41
3:D:632:TPP:H62	3:D:632:TPP:HM41	1.89	0.41
1:B:9:LEU:HD11	1:B:170:ILE:HD11	2.02	0.41
1:D:177:ILE:CD1	4:D:5131:HOH:O	2.68	0.41
1:B:306:CYS:SG	1:C:148:ALA:HB2	2.62	0.40
1:C:75:GLY:H	1:C:118:GLN:NE2	2.19	0.40
1:D:517:HIS:HD2	4:D:5203:HOH:O	2.04	0.40
1:C:469:ILE:CD1	1:C:532:LEU:HD13	2.51	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)
1:A:265:LYS:O	1:A:265:LYS:O[6_555]	2.13	0.07
1:A:517:HIS:CD2	1:C:173:ASP:OD1[4_545]	2.14	0.06

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	552/563 (98%)	535 (97%)	17 (3%)	0	100	100
1	B	552/563 (98%)	532 (96%)	19 (3%)	1 (0%)	47	69
1	C	552/563 (98%)	534 (97%)	17 (3%)	1 (0%)	47	69
1	D	552/563 (98%)	534 (97%)	17 (3%)	1 (0%)	47	69
All	All	2208/2252 (98%)	2135 (97%)	70 (3%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	308	LEU
1	C	308	LEU
1	D	308	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/419 (98%)	370 (90%)	42 (10%)	7	13
1	B	412/419 (98%)	370 (90%)	42 (10%)	7	13
1	C	412/419 (98%)	370 (90%)	42 (10%)	7	13
1	D	412/419 (98%)	370 (90%)	42 (10%)	7	13
All	All	1648/1676 (98%)	1480 (90%)	168 (10%)	7	13

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	25	LEU
1	A	38	LEU
1	A	41	ASP
1	A	71	LEU
1	A	93	THR
1	A	96	LEU
1	A	116	ILE
1	A	141	LEU
1	A	159	LEU
1	A	168	ASN
1	A	175	VAL
1	A	176	ILE
1	A	208	VAL
1	A	220	ARG
1	A	222	THR
1	A	225	SER
1	A	252	MET
1	A	257	VAL
1	A	265	LYS
1	A	273	VAL
1	A	308	LEU
1	A	310	ARG
1	A	319	VAL
1	A	333	THR
1	A	335	GLN
1	A	342	ARG
1	A	350	THR
1	A	356	ARG
1	A	366	SER
1	A	418	LEU
1	A	425	PHE
1	A	436	LEU
1	A	441	ARG
1	A	461	LEU
1	A	487	LEU
1	A	492	ASN
1	A	494	VAL
1	A	495	THR
1	A	532	LEU
1	A	541	ASN
1	A	555	ILE
1	B	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	25	LEU
1	B	38	LEU
1	B	41	ASP
1	B	71	LEU
1	B	93	THR
1	B	96	LEU
1	B	116	ILE
1	B	141	LEU
1	B	159	LEU
1	B	164	ASP
1	B	168	ASN
1	B	176	ILE
1	B	208	VAL
1	B	220	ARG
1	B	222	THR
1	B	225	SER
1	B	252	MET
1	B	257	VAL
1	B	265	LYS
1	B	273	VAL
1	B	308	LEU
1	B	310	ARG
1	B	319	VAL
1	B	333	THR
1	B	335	GLN
1	B	342	ARG
1	B	350	THR
1	B	356	ARG
1	B	366	SER
1	B	418	LEU
1	B	425	PHE
1	B	436	LEU
1	B	441	ARG
1	B	461	LEU
1	B	487	LEU
1	B	492	ASN
1	B	494	VAL
1	B	495	THR
1	B	532	LEU
1	B	541	ASN
1	B	555	ILE
1	C	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	25	LEU
1	C	38	LEU
1	C	41	ASP
1	C	71	LEU
1	C	93	THR
1	C	96	LEU
1	C	116	ILE
1	C	141	LEU
1	C	159	LEU
1	C	168	ASN
1	C	175	VAL
1	C	176	ILE
1	C	208	VAL
1	C	220	ARG
1	C	222	THR
1	C	225	SER
1	C	252	MET
1	C	257	VAL
1	C	265	LYS
1	C	273	VAL
1	C	308	LEU
1	C	310	ARG
1	C	319	VAL
1	C	333	THR
1	C	335	GLN
1	C	342	ARG
1	C	350	THR
1	C	356	ARG
1	C	366	SER
1	C	418	LEU
1	C	425	PHE
1	C	436	LEU
1	C	441	ARG
1	C	461	LEU
1	C	487	LEU
1	C	492	ASN
1	C	494	VAL
1	C	495	THR
1	C	532	LEU
1	C	541	ASN
1	C	555	ILE
1	D	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	25	LEU
1	D	38	LEU
1	D	41	ASP
1	D	71	LEU
1	D	93	THR
1	D	96	LEU
1	D	116	ILE
1	D	141	LEU
1	D	159	LEU
1	D	164	ASP
1	D	168	ASN
1	D	176	ILE
1	D	208	VAL
1	D	220	ARG
1	D	222	THR
1	D	225	SER
1	D	252	MET
1	D	257	VAL
1	D	260	LEU
1	D	265	LYS
1	D	273	VAL
1	D	308	LEU
1	D	310	ARG
1	D	319	VAL
1	D	333	THR
1	D	335	GLN
1	D	342	ARG
1	D	350	THR
1	D	356	ARG
1	D	418	LEU
1	D	425	PHE
1	D	436	LEU
1	D	441	ARG
1	D	461	LEU
1	D	487	LEU
1	D	492	ASN
1	D	494	VAL
1	D	495	THR
1	D	532	LEU
1	D	541	ASN
1	D	555	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	113	GLN
1	A	118	GLN
1	A	144	GLN
1	A	168	ASN
1	A	196	GLN
1	A	335	GLN
1	A	354	GLN
1	A	371	HIS
1	A	374	HIS
1	A	492	ASN
1	A	541	ASN
1	B	26	HIS
1	B	113	GLN
1	B	118	GLN
1	B	144	GLN
1	B	196	GLN
1	B	294	HIS
1	B	335	GLN
1	B	354	GLN
1	B	371	HIS
1	B	374	HIS
1	B	492	ASN
1	B	541	ASN
1	C	26	HIS
1	C	29	HIS
1	C	87	ASN
1	C	113	GLN
1	C	118	GLN
1	C	144	GLN
1	C	196	GLN
1	C	294	HIS
1	C	335	GLN
1	C	354	GLN
1	C	371	HIS
1	C	374	HIS
1	C	492	ASN
1	C	541	ASN
1	D	26	HIS
1	D	87	ASN
1	D	113	GLN
1	D	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	144	GLN
1	D	196	GLN
1	D	294	HIS
1	D	335	GLN
1	D	354	GLN
1	D	371	HIS
1	D	374	HIS
1	D	415	HIS
1	D	486	GLN
1	D	492	ASN
1	D	541	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	TPP	A	602	2	22,27,27	7.37	5 (22%)	29,40,40	1.89	9 (31%)
3	TPP	D	632	2	22,27,27	7.53	6 (27%)	29,40,40	2.67	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	C	622	2	22,27,27	7.38	5 (22%)	29,40,40	2.31	7 (24%)
3	TPP	B	612	2	22,27,27	6.33	6 (27%)	29,40,40	2.65	10 (34%)

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
3	TPP	A	602	2	-	3/16/17/17	0/2/2/2
3	TPP	D	632	2	-	6/16/17/17	0/2/2/2
3	TPP	C	622	2	-	5/16/17/17	0/2/2/2
3	TPP	B	612	2	-	8/16/17/17	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	632	TPP	C6-C5	-32.98	1.36	1.50
3	A	602	TPP	C6-C5	-32.57	1.36	1.50
3	C	622	TPP	C6-C5	-32.56	1.36	1.50
3	B	612	TPP	C6-C5	-27.44	1.38	1.50
3	D	632	TPP	CM4-C4	-8.30	1.32	1.49
3	C	622	TPP	CM4-C4	-8.22	1.33	1.49
3	A	602	TPP	CM4-C4	-8.00	1.33	1.49
3	B	612	TPP	CM4-C4	-7.96	1.33	1.49
3	D	632	TPP	C2-N3	5.72	1.48	1.36
3	C	622	TPP	C2-N3	5.41	1.47	1.36
3	A	602	TPP	C2-N3	5.24	1.47	1.36
3	D	632	TPP	C4-N3	-5.22	1.35	1.39
3	B	612	TPP	C2-N3	5.09	1.46	1.36
3	A	602	TPP	C5'-C4'	4.39	1.50	1.42
3	C	622	TPP	C5'-C4'	4.03	1.49	1.42
3	D	632	TPP	C5'-C4'	3.85	1.49	1.42
3	C	622	TPP	C4-N3	-3.76	1.36	1.39
3	A	602	TPP	C4-N3	-3.74	1.36	1.39
3	B	612	TPP	C5'-C4'	3.70	1.49	1.42
3	B	612	TPP	C4-N3	-3.16	1.37	1.39
3	B	612	TPP	C2'-N1'	2.47	1.38	1.34
3	D	632	TPP	C2'-N1'	2.08	1.37	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	632	TPP	C6-C5-C4	-10.75	118.80	127.43
3	C	622	TPP	C6-C5-C4	-7.87	121.12	127.43
3	B	612	TPP	C7'-N3-C2	-6.63	113.37	125.35
3	B	612	TPP	C6-C5-C4	-6.38	122.31	127.43
3	B	612	TPP	CM2-C2'-N1'	5.16	122.82	117.14
3	A	602	TPP	C7'-N3-C2	-5.15	116.04	125.35
3	C	622	TPP	C7'-N3-C2	-5.11	116.12	125.35
3	B	612	TPP	C6'-N1'-C2'	4.97	124.42	115.96
3	D	632	TPP	CM2-C2'-N1'	4.47	122.06	117.14
3	D	632	TPP	C7'-N3-C2	-4.04	118.06	125.35
3	B	612	TPP	C5'-C6'-N1'	-3.92	117.28	123.82
3	C	622	TPP	C6'-N1'-C2'	3.61	122.11	115.96
3	A	602	TPP	C6'-N1'-C2'	3.60	122.09	115.96
3	D	632	TPP	C6'-N1'-C2'	3.46	121.84	115.96
3	A	602	TPP	C6-C5-C4	-3.41	124.69	127.43
3	B	612	TPP	C5-C4-N3	3.14	113.86	107.57
3	C	622	TPP	C5-C4-N3	3.14	113.85	107.57
3	D	632	TPP	C5-C4-N3	3.13	113.83	107.57
3	A	602	TPP	C5-C4-N3	2.97	113.52	107.57
3	A	602	TPP	CM2-C2'-N1'	2.84	120.26	117.14
3	D	632	TPP	N1'-C2'-N3'	-2.72	120.86	125.54
3	B	612	TPP	N1'-C2'-N3'	-2.67	120.95	125.54
3	A	602	TPP	N1'-C2'-N3'	-2.57	121.11	125.54
3	C	622	TPP	N1'-C2'-N3'	-2.54	121.17	125.54
3	C	622	TPP	N4'-C4'-N3'	2.45	120.50	117.03
3	B	612	TPP	CM4-C4-C5	-2.40	122.36	127.60
3	B	612	TPP	PA-O3A-PB	-2.27	125.04	132.83
3	C	622	TPP	CM4-C4-C5	-2.16	122.89	127.60
3	A	602	TPP	C5'-C6'-N1'	-2.10	120.32	123.82
3	B	612	TPP	C5'-C4'-N4'	-2.04	119.30	122.19
3	A	602	TPP	O3B-PB-O2B	2.01	115.34	107.64
3	A	602	TPP	PA-O3A-PB	-2.01	125.94	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	622	TPP	C7-O7-PA-O3A
3	D	632	TPP	C7-O7-PA-O3A
3	D	632	TPP	PA-O3A-PB-O3B
3	B	612	TPP	C6'-C5'-C7'-N3
3	B	612	TPP	C7-O7-PA-O3A
3	A	602	TPP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	632	TPP	PA-O3A-PB-O1B
3	B	612	TPP	PA-O3A-PB-O1B
3	B	612	TPP	C4'-C5'-C7'-N3
3	A	602	TPP	PA-O3A-PB-O3B
3	B	612	TPP	PA-O3A-PB-O3B
3	C	622	TPP	C7-O7-PA-O2A
3	D	632	TPP	C7-O7-PA-O1A
3	D	632	TPP	C7-O7-PA-O2A
3	B	612	TPP	C7-O7-PA-O2A
3	A	602	TPP	C4-C5-C6-C7
3	C	622	TPP	C4-C5-C6-C7
3	D	632	TPP	C4-C5-C6-C7
3	B	612	TPP	C4-C5-C6-C7
3	C	622	TPP	PA-O3A-PB-O1B
3	C	622	TPP	C7-O7-PA-O1A
3	B	612	TPP	C7-O7-PA-O1A

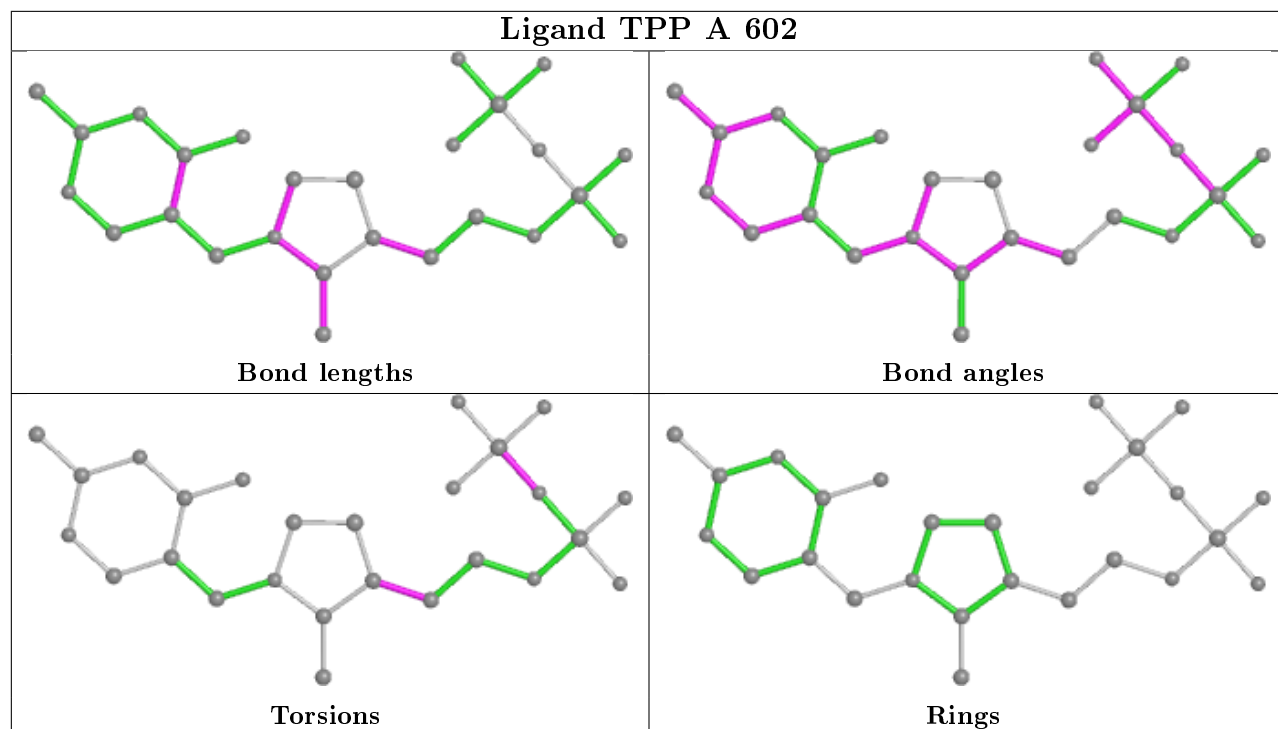
There are no ring outliers.

1 monomer is involved in 1 short contact:

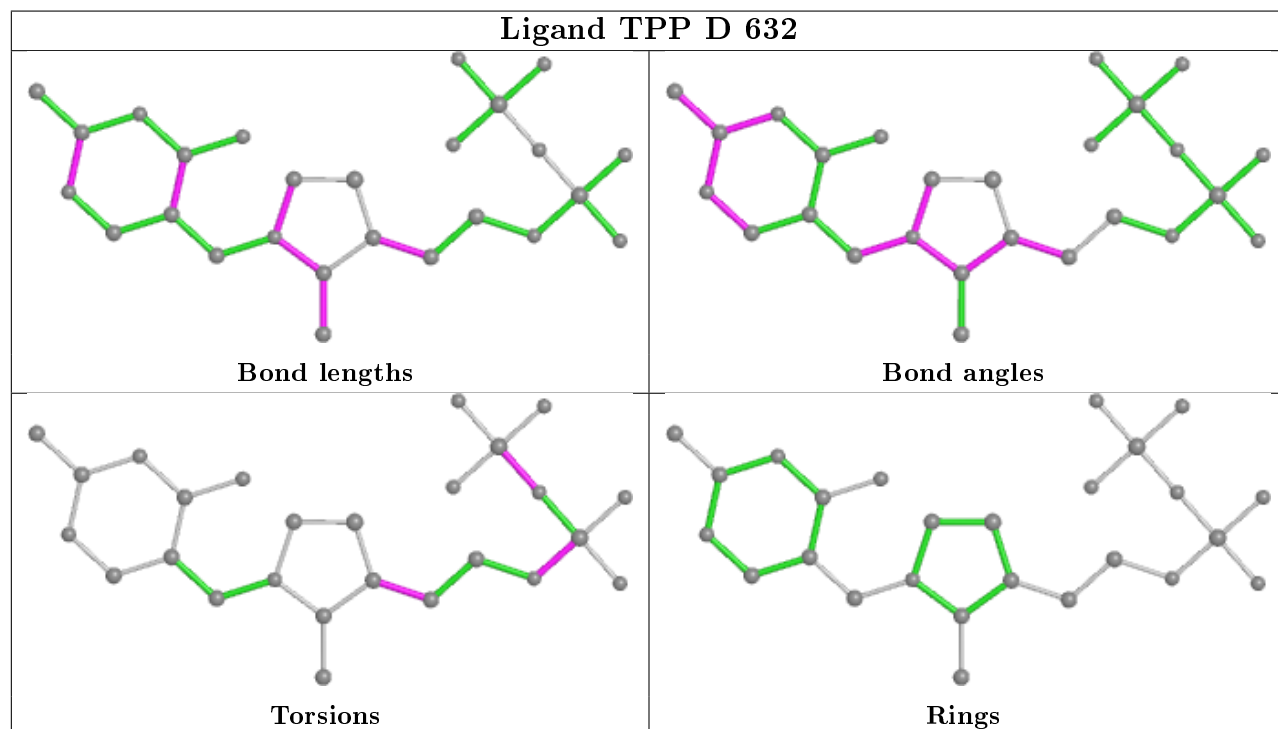
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	632	TPP	1	0

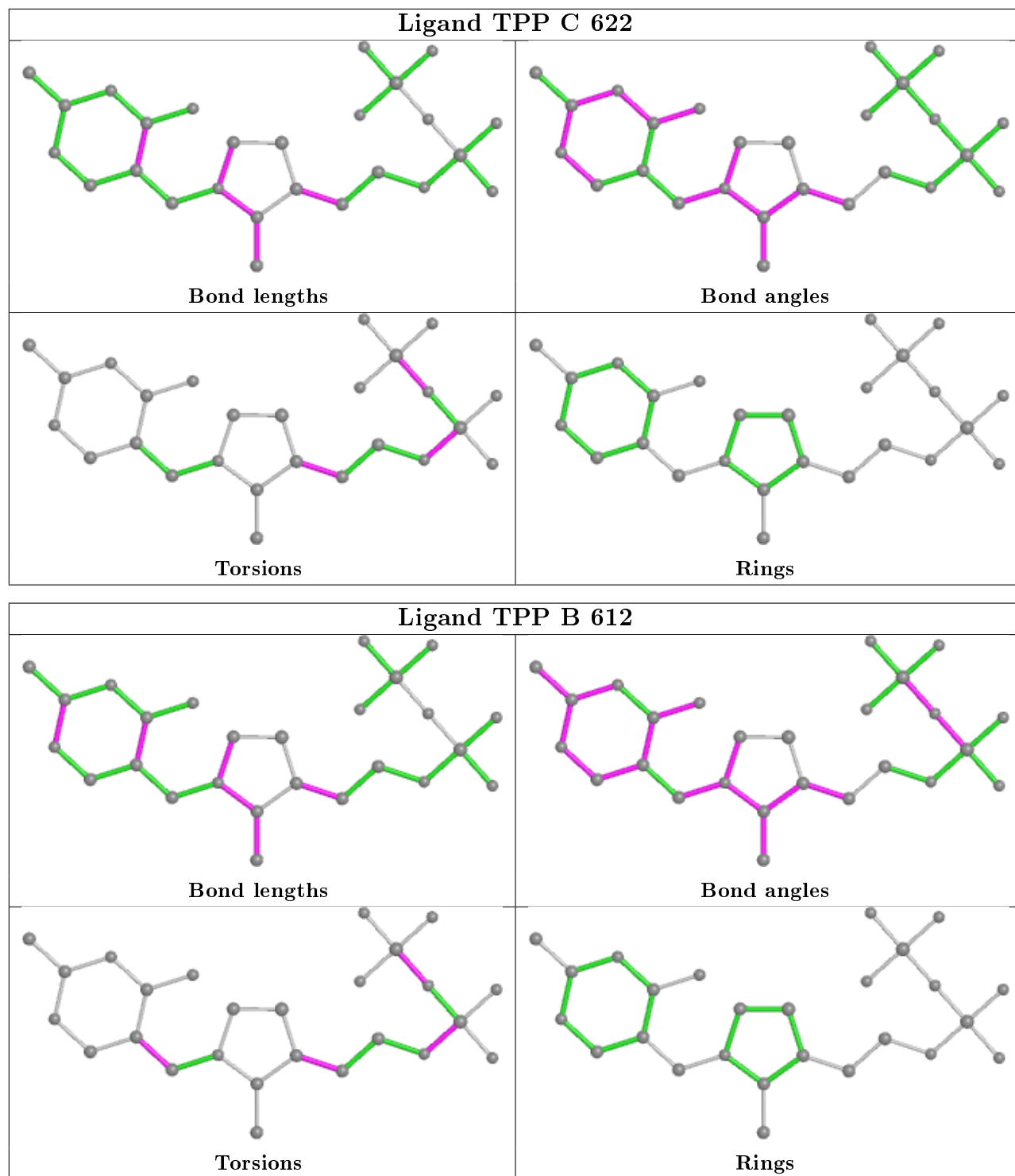
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand TPP A 602



Ligand TPP D 632





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/563 (98%)	-0.23	21 (3%) 40 36	18, 38, 68, 94	0
1	B	554/563 (98%)	-0.22	15 (2%) 54 51	22, 41, 66, 84	0
1	C	554/563 (98%)	-0.45	14 (2%) 57 53	15, 28, 49, 62	0
1	D	554/563 (98%)	-0.54	5 (0%) 84 83	14, 25, 38, 55	0
All	All	2216/2252 (98%)	-0.36	55 (2%) 57 53	14, 32, 62, 94	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ALA	7.7
1	A	368	HIS	7.5
1	B	335	GLN	6.6
1	A	337	ALA	5.4
1	B	368	HIS	5.1
1	C	368	HIS	5.0
1	D	368	HIS	4.8
1	C	338	ALA	4.7
1	B	336	ASP	4.6
1	C	335	GLN	4.3
1	A	554	LEU	4.2
1	A	265	LYS	3.9
1	A	335	GLN	3.9
1	B	337	ALA	3.8
1	A	367	GLU	3.8
1	A	555	ILE	3.8
1	A	336	ASP	3.5
1	B	265	LYS	3.5
1	B	2	ALA	3.1
1	A	338	ALA	2.9
1	A	437	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	265	LYS	2.8
1	A	439	GLY	2.8
1	D	265	LYS	2.7
1	A	536	ARG	2.7
1	A	341	ASP	2.7
1	A	362	ALA	2.7
1	A	267	ASP	2.7
1	A	517	HIS	2.7
1	C	555	ILE	2.7
1	D	2	ALA	2.6
1	C	336	ASP	2.6
1	B	555	ILE	2.5
1	A	350	THR	2.5
1	B	367	GLU	2.5
1	B	437	GLU	2.5
1	A	438	ALA	2.5
1	C	437	GLU	2.5
1	B	338	ALA	2.5
1	A	347	ALA	2.3
1	B	491	PRO	2.3
1	B	163	TRP	2.3
1	B	517	HIS	2.3
1	C	439	GLY	2.2
1	B	554	LEU	2.2
1	D	367	GLU	2.2
1	C	554	LEU	2.2
1	A	354	GLN	2.1
1	A	2	ALA	2.1
1	C	363	LYS	2.1
1	C	267	ASP	2.1
1	B	267	ASP	2.1
1	C	367	GLU	2.1
1	C	492	ASN	2.0
1	D	492	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

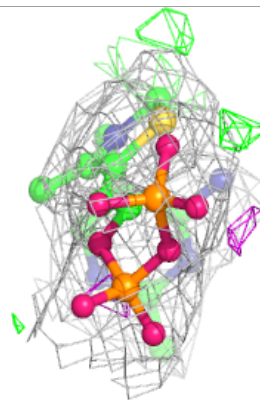
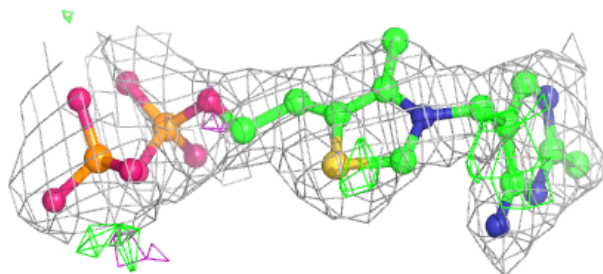
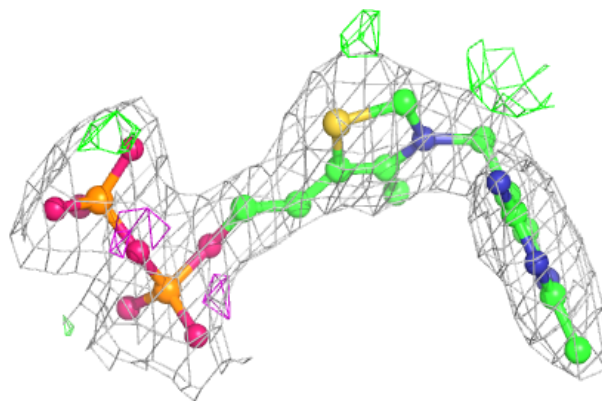
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.91	0.09	47,47,47,47	0
3	TPP	A	602	26/26	0.95	0.11	39,42,44,44	0
3	TPP	B	612	26/26	0.95	0.13	32,37,38,39	0
2	MG	B	611	1/1	0.96	0.05	31,31,31,31	0
2	MG	C	621	1/1	0.96	0.10	22,22,22,22	0
3	TPP	C	622	26/26	0.98	0.10	22,27,28,29	0
2	MG	D	631	1/1	0.98	0.09	18,18,18,18	0
3	TPP	D	632	26/26	0.98	0.09	16,18,20,21	0

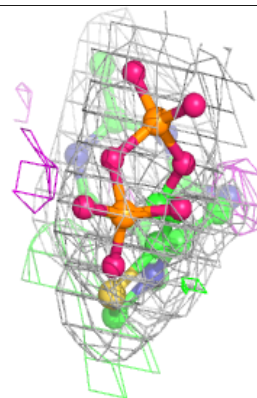
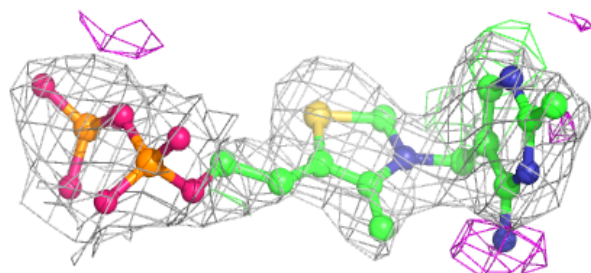
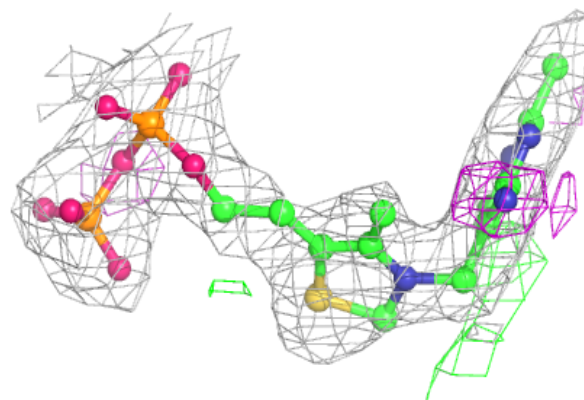
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 602:

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

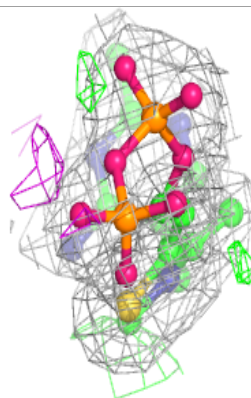
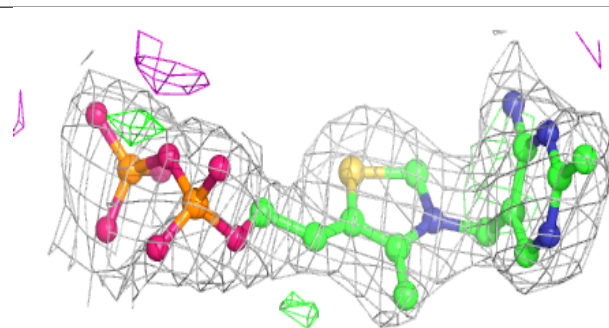
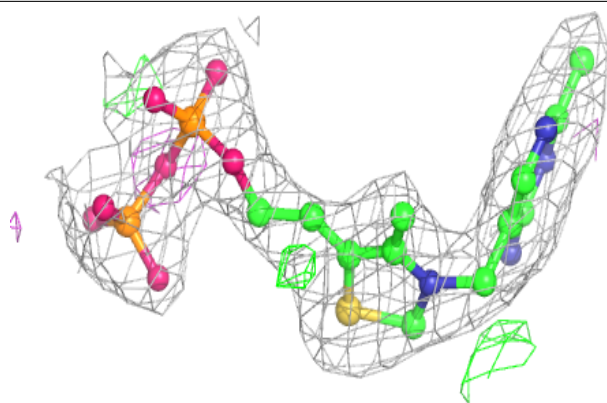
**Electron density around TPP B 612:**

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

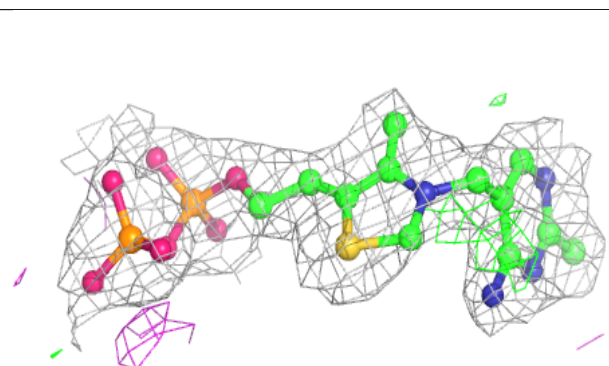
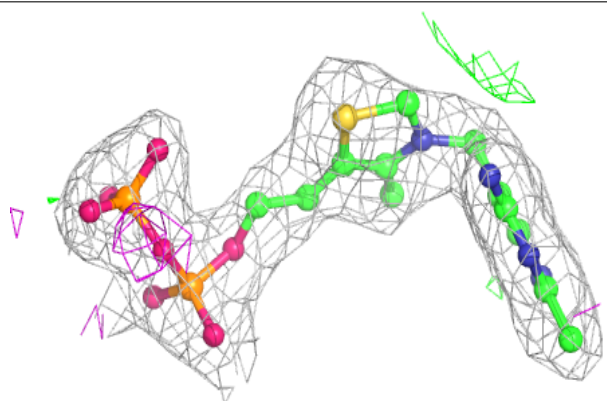


Electron density around TPP C 622:

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

**Electron density around TPP D 632:**

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



6.5 Other polymers

There are no such residues in this entry.