



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 AM UTC

PDB ID : 5RW0 / pdb_00005rw0
Title : PanDDA analysis group deposition – Crystal Structure of DHTKD1 in complex with Z2444997446
Authors : Bezerra, G.A.; Foster, W.R.; Bailey, H.J.; Shrestha, L.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Yue, W.W.
Deposited on : 2020-10-27
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

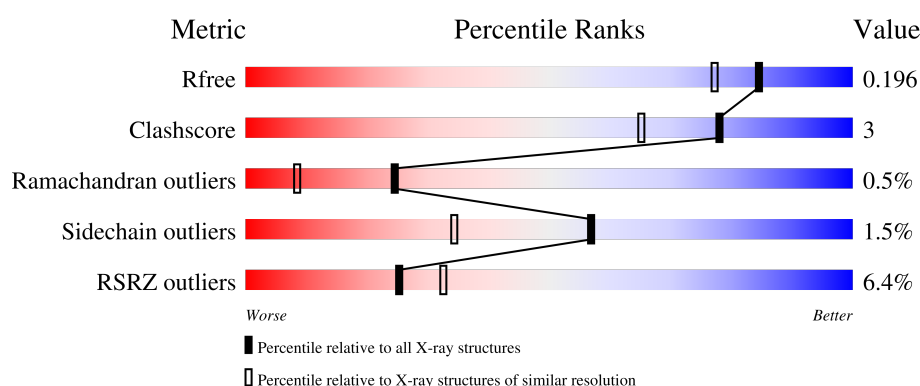
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	898	4% 89% 6% . .
1	B	898	8% 89% 8% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	WGD	A	1002	X	-	-	-
2	WGD	A	1003	X	-	-	-
2	WGD	B	1002	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15420 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 Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	867	Total	C	N	O	S	0	5	0
			6775	4317	1169	1249	40			
1	B	867	Total	C	N	O	S	0	2	0
			6740	4296	1163	1243	38			

There are 46 discrepancies between the modelled and reference sequences:

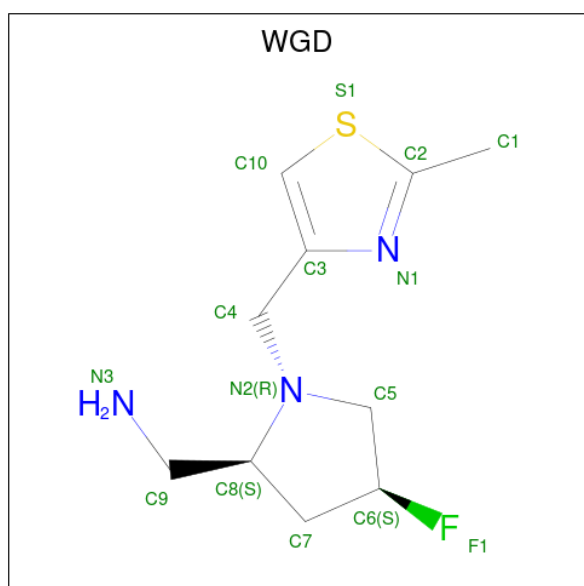
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP Q96HY7
A	23	HIS	-	expression tag	UNP Q96HY7
A	24	HIS	-	expression tag	UNP Q96HY7
A	25	HIS	-	expression tag	UNP Q96HY7
A	26	HIS	-	expression tag	UNP Q96HY7
A	27	HIS	-	expression tag	UNP Q96HY7
A	28	HIS	-	expression tag	UNP Q96HY7
A	29	SER	-	expression tag	UNP Q96HY7
A	30	SER	-	expression tag	UNP Q96HY7
A	31	GLY	-	expression tag	UNP Q96HY7
A	32	VAL	-	expression tag	UNP Q96HY7
A	33	ASP	-	expression tag	UNP Q96HY7
A	34	LEU	-	expression tag	UNP Q96HY7
A	35	GLY	-	expression tag	UNP Q96HY7
A	36	THR	-	expression tag	UNP Q96HY7
A	37	GLU	-	expression tag	UNP Q96HY7
A	38	ASN	-	expression tag	UNP Q96HY7
A	39	LEU	-	expression tag	UNP Q96HY7
A	40	TYR	-	expression tag	UNP Q96HY7
A	41	PHE	-	expression tag	UNP Q96HY7
A	42	GLN	-	expression tag	UNP Q96HY7
A	43	SER	-	expression tag	UNP Q96HY7
A	44	MET	-	expression tag	UNP Q96HY7
B	22	MET	-	initiating methionine	UNP Q96HY7

Continued on next page...

Continued from previous page...

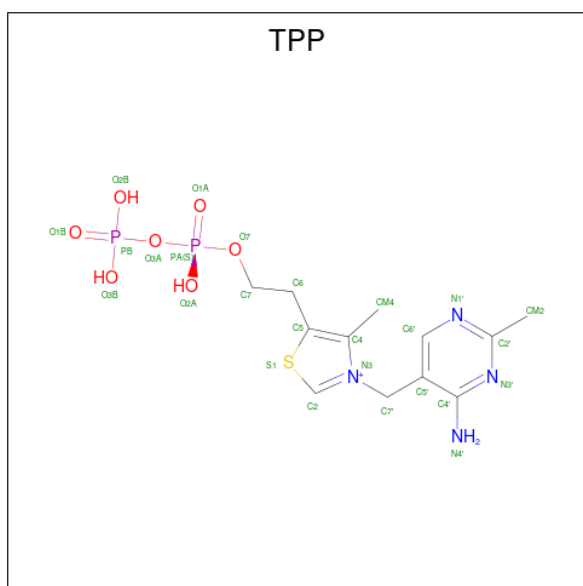
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q96HY7
B	24	HIS	-	expression tag	UNP Q96HY7
B	25	HIS	-	expression tag	UNP Q96HY7
B	26	HIS	-	expression tag	UNP Q96HY7
B	27	HIS	-	expression tag	UNP Q96HY7
B	28	HIS	-	expression tag	UNP Q96HY7
B	29	SER	-	expression tag	UNP Q96HY7
B	30	SER	-	expression tag	UNP Q96HY7
B	31	GLY	-	expression tag	UNP Q96HY7
B	32	VAL	-	expression tag	UNP Q96HY7
B	33	ASP	-	expression tag	UNP Q96HY7
B	34	LEU	-	expression tag	UNP Q96HY7
B	35	GLY	-	expression tag	UNP Q96HY7
B	36	THR	-	expression tag	UNP Q96HY7
B	37	GLU	-	expression tag	UNP Q96HY7
B	38	ASN	-	expression tag	UNP Q96HY7
B	39	LEU	-	expression tag	UNP Q96HY7
B	40	TYR	-	expression tag	UNP Q96HY7
B	41	PHE	-	expression tag	UNP Q96HY7
B	42	GLN	-	expression tag	UNP Q96HY7
B	43	SER	-	expression tag	UNP Q96HY7
B	44	MET	-	expression tag	UNP Q96HY7

- Molecule 2 is 1-[(2S,4S)-4-fluoro-1-[(2-methyl-1,3-thiazol-4-yl)methyl]pyrrolidin-2-yl]methanamine (CCD ID: WGD) (formula: C₁₀H₁₆FN₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	S	0	0
			15	10	1	3	1		
2	A	1	Total	C	F	N	S	0	0
			15	10	1	3	1		
2	A	1	Total	C	F	N	S	0	0
			15	10	1	3	1		
2	B	1	Total	C	F	N	S	0	0
			15	10	1	3	1		
2	B	1	Total	C	F	N	S	0	0
			15	10	1	3	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

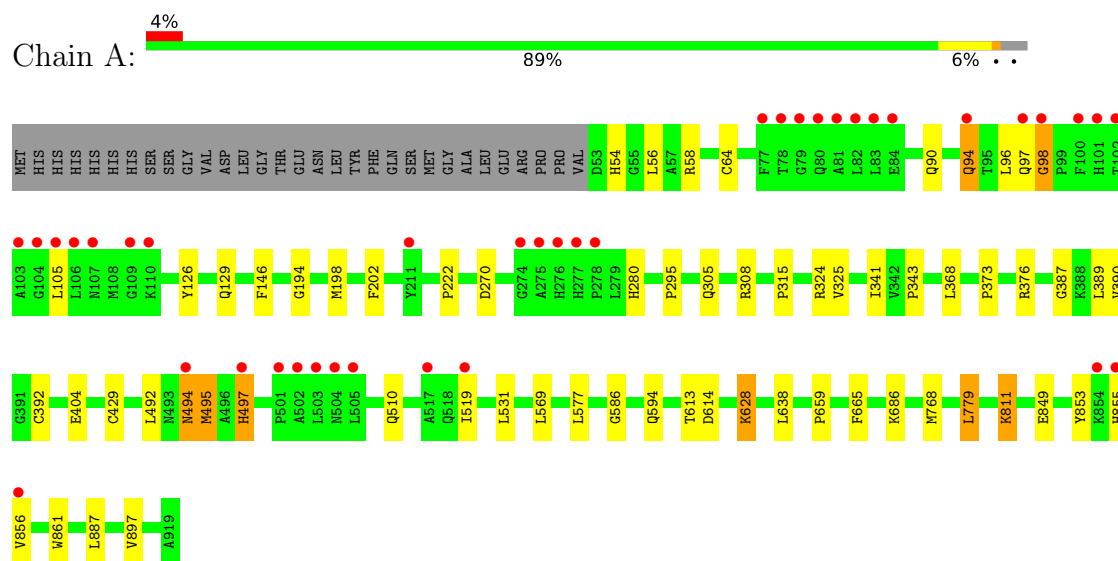
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	999	Total 999	O 999	0	0
5	B	776	Total 776	O 776	0	0

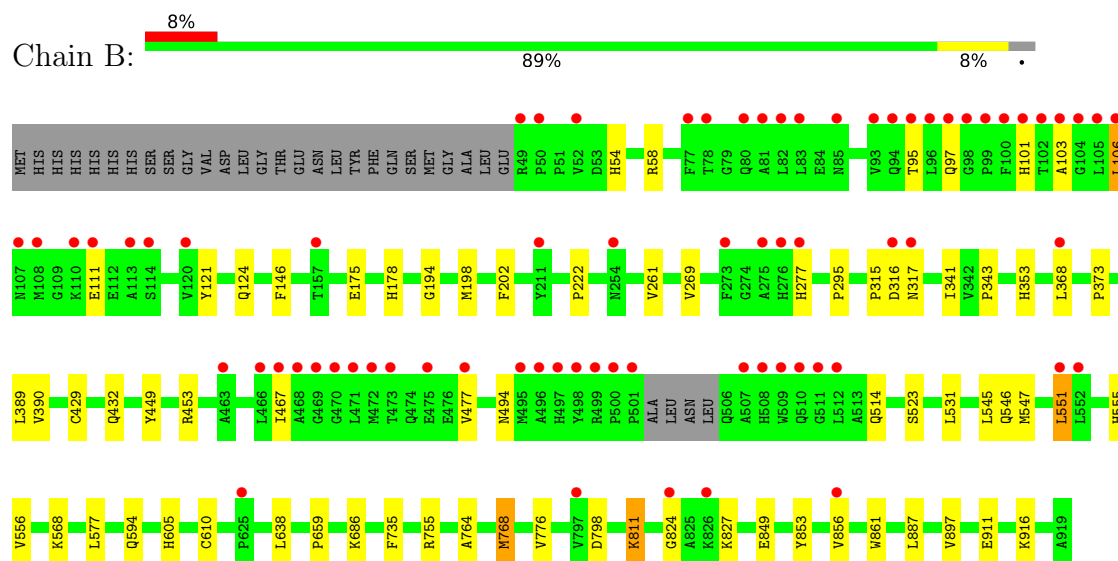
3 Residue-property plots [i](#)

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: Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial



- Molecule 1: Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.13Å 147.13Å 87.27Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	85.07 – 1.67 85.07 – 1.67	Depositor EDS
% Data completeness (in resolution range)	58.7 (85.07-1.67) 58.6 (85.07-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.67Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.161 , 0.187 0.169 , 0.196	Depositor DCC
R_{free} test set	6392 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15420	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: MG, WGD, 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	0.71	0/6959	1.02	3/9439 (0.0%)
1	B	0.71	2/6914 (0.0%)	1.01	7/9385 (0.1%)
All	All	0.71	2/13873 (0.0%)	1.02	10/18824 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLN	CA-C	9.69	1.57	1.52
1	B	768	MET	SD-CE	-5.93	1.64	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ASN	CA-CB-CG	7.34	119.94	112.60
1	B	316	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	798	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	495	MET	N-CA-C	5.21	117.36	111.11
1	B	764	ALA	N-CA-C	-5.15	99.36	108.23
1	A	665	PHE	N-CA-C	-5.15	101.36	109.50
1	B	261	VAL	CA-C-N	5.12	127.45	120.54
1	B	261	VAL	C-N-CA	5.12	127.45	120.54
1	B	315	PRO	CA-C-N	5.12	128.11	120.95
1	B	315	PRO	C-N-CA	5.12	128.11	120.95

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	6775	0	6624	41	0
1	B	6740	0	6571	36	0
2	A	45	0	0	2	0
2	B	30	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	3	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	999	0	0	2	0
5	B	776	0	0	1	0
All	All	15420	0	13227	74	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 3.

All (74) 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:A:54:HIS:CE1	1:B:95:THR:HG22	2.29	0.68
1:A:853:TYR:HA	1:A:855:HIS:CE1	2.30	0.67
1:B:824:GLY:O	1:B:827:LYS:HG2	1.96	0.66
1:A:54:HIS:HE1	1:B:95:THR:HG22	1.59	0.65
1:A:90:GLN:O	1:A:94:GLN:HG2	1.96	0.64
1:B:389:LEU:HD12	1:B:390:VAL:HG13	1.82	0.61
1:A:270:ASP:OD1	1:A:280[B]:HIS:ND1	2.34	0.61
1:A:389:LEU:HD12	1:A:390:VAL:HG13	1.82	0.60
1:A:768:MET:HE1	5:A:1143:HOH:O	2.01	0.59
1:A:315:PRO:HD2	2:A:1002:WGD:N3	2.19	0.58
1:A:492:LEU:HD12	1:A:495:MET:HE2	1.86	0.58
2:A:1001:WGD:N3	5:A:1104:HOH:O	2.32	0.58
1:B:432:GLN:O	1:B:453:ARG:NH1	2.35	0.58
1:A:96:LEU:HD23	1:B:54:HIS:NE2	2.21	0.56
1:B:551:LEU:HD21	1:B:605:HIS:CE1	2.43	0.54
1:A:494:ASN:HA	1:A:497[A]:HIS:CE1	2.42	0.54
1:A:569:LEU:HD21	1:A:779:LEU:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLN:O	1:A:98:GLY:O	2.26	0.53
1:B:853:TYR:HB3	1:B:856:VAL:HG23	1.89	0.53
1:A:853:TYR:HB3	1:A:856:VAL:HG23	1.91	0.53
1:B:368:LEU:HD23	1:B:373:PRO:HA	1.91	0.52
1:B:545:LEU:HG	1:B:610:CYS:HB2	1.90	0.52
1:B:853:TYR:HB3	1:B:856:VAL:CG2	2.40	0.52
1:A:494:ASN:ND2	1:A:497[B]:HIS:CD2	2.78	0.52
1:A:586:GLY:HA2	1:A:628:LYS:HG3	1.92	0.51
1:B:101:HIS:O	1:B:111:GLU:O	2.28	0.51
1:A:376:ARG:NH1	1:B:353:HIS:HD2	2.10	0.50
1:A:194:GLY:O	1:A:429:CYS:HB2	2.12	0.49
1:B:194:GLY:O	1:B:429:CYS:HB2	2.12	0.49
3:A:1004:TPP:HN42	3:A:1004:TPP:H2	1.77	0.49
1:A:594:GLN:OE1	3:B:1003:TPP:H6'	2.13	0.48
1:B:547:MET:SD	1:B:556:VAL:HG21	2.53	0.48
1:A:387:GLY:O	1:A:392[B]:CYS:HB2	2.14	0.48
1:A:343:PRO:HB3	1:A:389:LEU:HD21	1.97	0.47
3:A:1004:TPP:HN42	3:A:1004:TPP:C2	2.28	0.47
1:A:853:TYR:HB3	1:A:856:VAL:CG2	2.45	0.47
1:A:531:LEU:HD22	1:A:577:LEU:HB3	1.98	0.46
1:B:735:PHE:CE2	1:B:755:ARG:NH2	2.84	0.45
1:B:551:LEU:HD13	1:B:555:HIS:HB3	1.97	0.45
1:A:368:LEU:HD23	1:A:373:PRO:HA	1.98	0.45
1:B:449:TYR:HD2	1:B:453:ARG:NH1	2.15	0.45
1:A:198:MET:HE2	1:A:202:PHE:HE2	1.81	0.45
1:A:768:MET:HE2	1:A:811:LYS:HB2	1.99	0.45
1:A:897:VAL:HG11	1:B:686:LYS:HG3	1.98	0.44
1:B:198:MET:HE2	1:B:202:PHE:HE2	1.82	0.44
1:A:96:LEU:HD23	1:B:54:HIS:CE1	2.53	0.44
1:B:343:PRO:HB3	1:B:389:LEU:HD21	1.98	0.44
3:B:1003:TPP:HN42	3:B:1003:TPP:H2	1.82	0.44
1:B:768:MET:HE2	1:B:811:LYS:HB2	1.99	0.43
3:A:1004:TPP:H6'	1:B:594:GLN:OE1	2.18	0.43
1:B:175:GLU:OE2	1:B:178[B]:HIS:HD2	2.02	0.43
1:B:531:LEU:HD22	1:B:577:LEU:HB3	2.00	0.43
1:B:54:HIS:O	1:B:58:ARG:HG3	2.19	0.43
1:A:64:CYS:HG	1:A:126:TYR:HH	1.62	0.43
1:B:106:LEU:HG	1:B:121:TYR:CE2	2.54	0.42
1:A:376:ARG:NH1	1:B:353:HIS:CD2	2.87	0.42
1:A:861:TRP:HB2	1:A:887:LEU:HD13	2.01	0.42
1:B:467:ILE:HD11	1:B:477:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:HIS:O	1:A:58:ARG:HG3	2.19	0.42
1:A:129:GLN:HB2	1:A:404:GLU:HG3	2.02	0.41
1:A:308:ARG:O	1:A:324:ARG:NH2	2.51	0.41
1:A:295:PRO:HG3	1:A:341:ILE:HD11	2.03	0.41
1:A:613:THR:O	1:A:614:ASP:HB2	2.20	0.41
1:B:295:PRO:HG3	1:B:341:ILE:HD11	2.03	0.41
1:A:56:LEU:HD23	1:A:105:LEU:HD12	2.02	0.41
1:B:861:TRP:HB2	1:B:887:LEU:HD13	2.03	0.41
1:A:686:LYS:HG3	1:B:897:VAL:HG11	2.01	0.41
3:B:1003:TPP:HN42	3:B:1003:TPP:C2	2.34	0.41
1:A:64:CYS:SG	1:A:126:TYR:OH	2.76	0.41
1:B:514:GLN:NE2	5:B:1138:HOH:O	2.55	0.40
1:B:568:LYS:HA	1:B:776:VAL:HB	2.04	0.40
1:A:494:ASN:CG	1:A:497[B]:HIS:CD2	2.99	0.40
1:A:305:GLN:HG2	1:A:325:VAL:HB	2.03	0.40
1:B:916:LYS:HE3	1:B:916:LYS:HB2	1.83	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	870/898 (97%)	838 (96%)	28 (3%)	4 (0%)	24	8
1	B	865/898 (96%)	832 (96%)	29 (3%)	4 (0%)	24	8
All	All	1735/1796 (97%)	1670 (96%)	57 (3%)	8 (0%)	24	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	GLY
1	A	222	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	510	GLN
1	B	222	PRO
1	B	103	ALA
1	B	277	HIS
1	A	659	PRO
1	B	659	PRO

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	729/776 (94%)	719 (99%)	10 (1%)	59	36
1	B	723/776 (93%)	710 (98%)	13 (2%)	51	27
All	All	1452/1552 (94%)	1429 (98%)	23 (2%)	57	32

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	146	PHE
1	A	497[A]	HIS
1	A	497[B]	HIS
1	A	519	ILE
1	A	628	LYS
1	A	638	LEU
1	A	779	LEU
1	A	811	LYS
1	A	849	GLU
1	B	106	LEU
1	B	124	GLN
1	B	146	PHE
1	B	269	VAL
1	B	317	ASN
1	B	494	ASN
1	B	523	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	546	GLN
1	B	551	LEU
1	B	638	LEU
1	B	811	LYS
1	B	849	GLU
1	B	911	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	140	GLN
1	A	174	GLN
1	A	235	GLN
1	A	350	ASN
1	A	418	GLN
1	A	474	GLN
1	A	489	ASN
1	A	494	ASN
1	A	514	GLN
1	A	518	GLN
1	A	557	GLN
1	B	138	GLN
1	B	174	GLN
1	B	235	GLN
1	B	280	HIS
1	B	465	HIS
1	B	489	ASN
1	B	514	GLN
1	B	550	HIS
1	B	611	GLN
1	B	752	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	$\# Z > 2$
2	WGD	A	1002	-	16,16,16	0.27	0	19,22,22	1.53	3 (15%)
3	TPP	B	1003	4	26,27,27	0.55	0	38,40,40	0.69	0
2	WGD	B	1002	-	16,16,16	0.39	0	19,22,22	0.96	2 (10%)
2	WGD	A	1003	-	16,16,16	0.36	0	19,22,22	1.50	3 (15%)
3	TPP	A	1004	4	26,27,27	0.47	0	38,40,40	0.71	0
2	WGD	B	1001	-	16,16,16	0.34	0	19,22,22	0.74	0
2	WGD	A	1001	-	16,16,16	0.39	0	19,22,22	0.92	1 (5%)

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	WGD	A	1002	-	1/1/3/3	2/6/18/18	0/2/2/2
3	TPP	B	1003	4	-	1/17/17/17	0/2/2/2
2	WGD	A	1001	-	-	0/6/18/18	0/2/2/2
2	WGD	B	1002	-	1/1/3/3	1/6/18/18	0/2/2/2
3	TPP	A	1004	4	-	3/17/17/17	0/2/2/2
2	WGD	B	1001	-	-	0/6/18/18	0/2/2/2
2	WGD	A	1003	-	1/1/3/3	4/6/18/18	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	WGD	C4-N2-C8	4.64	121.07	113.59
2	A	1002	WGD	C4-N2-C8	4.47	120.79	113.59
2	A	1002	WGD	C7-C6-C5	-2.96	100.91	104.52
2	A	1003	WGD	C7-C6-C5	-2.63	101.31	104.52
2	A	1001	WGD	C4-N2-C5	2.48	116.41	113.11
2	A	1002	WGD	C5-N2-C8	2.46	109.73	105.35
2	B	1002	WGD	C4-N2-C8	2.33	117.34	113.59
2	B	1002	WGD	F1-C6-C5	2.03	111.33	108.41
2	A	1003	WGD	C5-N2-C8	2.01	108.94	105.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1002	WGD	C8
2	A	1003	WGD	C6
2	B	1002	WGD	C6

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	WGD	C3-C4-N2-C5
2	A	1003	WGD	C3-C4-N2-C5
2	A	1003	WGD	C3-C4-N2-C8
2	B	1002	WGD	C3-C4-N2-C8
3	A	1004	TPP	PA-O3A-PB-O2B
3	A	1004	TPP	PA-O3A-PB-O3B
2	A	1003	WGD	N1-C3-C4-N2
2	A	1002	WGD	C3-C4-N2-C8
2	A	1003	WGD	C10-C3-C4-N2
3	B	1003	TPP	PA-O3A-PB-O3B
3	A	1004	TPP	PA-O3A-PB-O1B

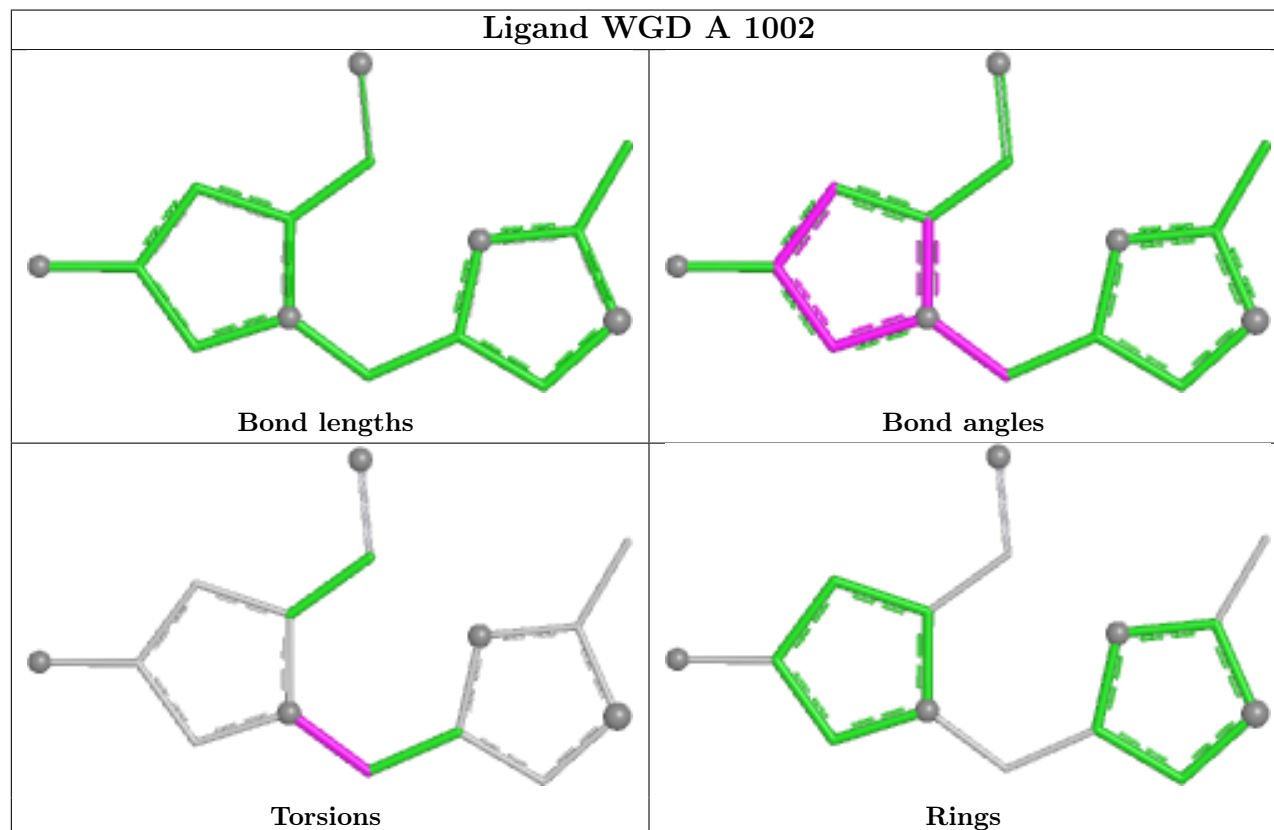
There are no ring outliers.

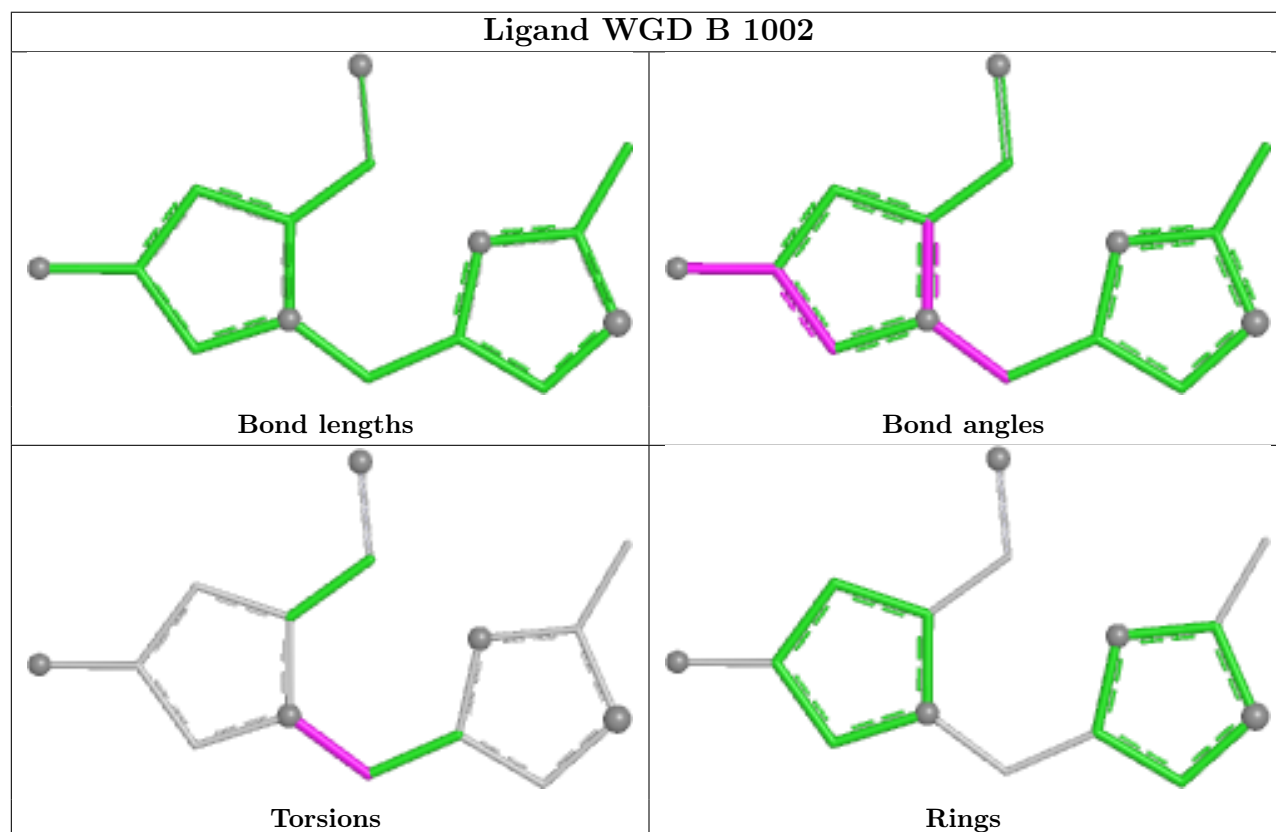
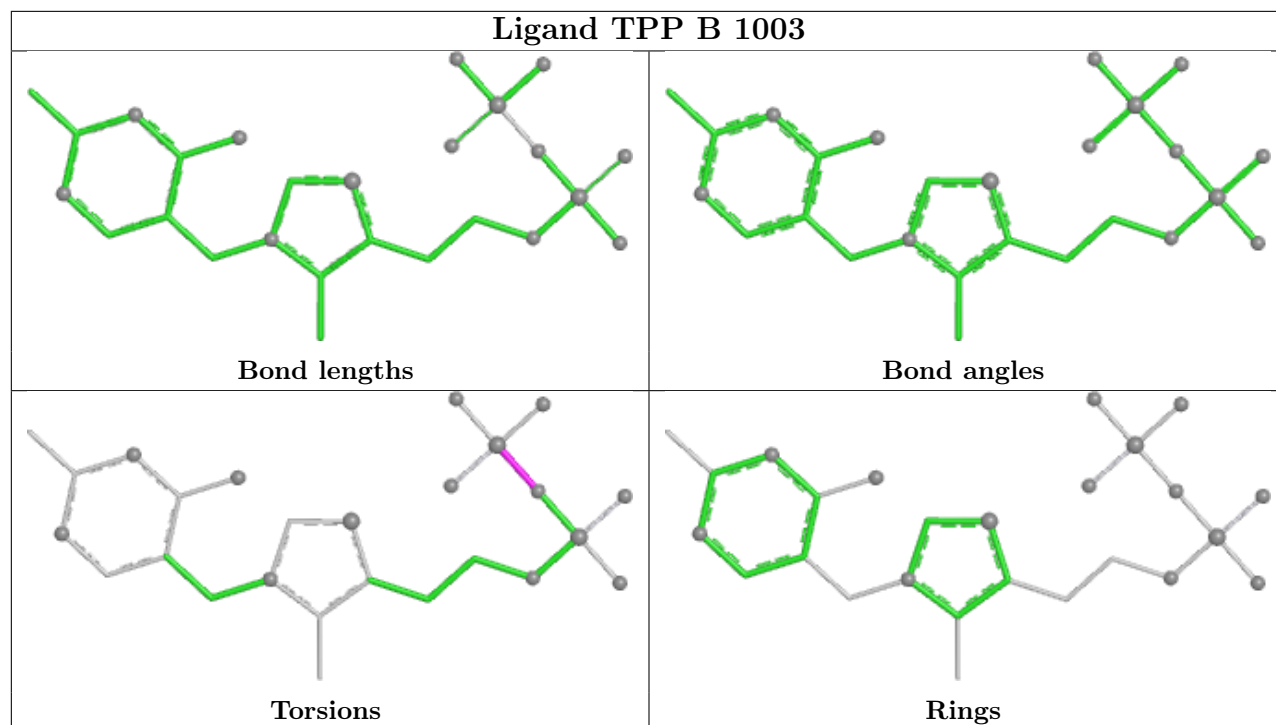
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	WGD	1	0
3	B	1003	TPP	3	0
3	A	1004	TPP	3	0
2	A	1001	WGD	1	0

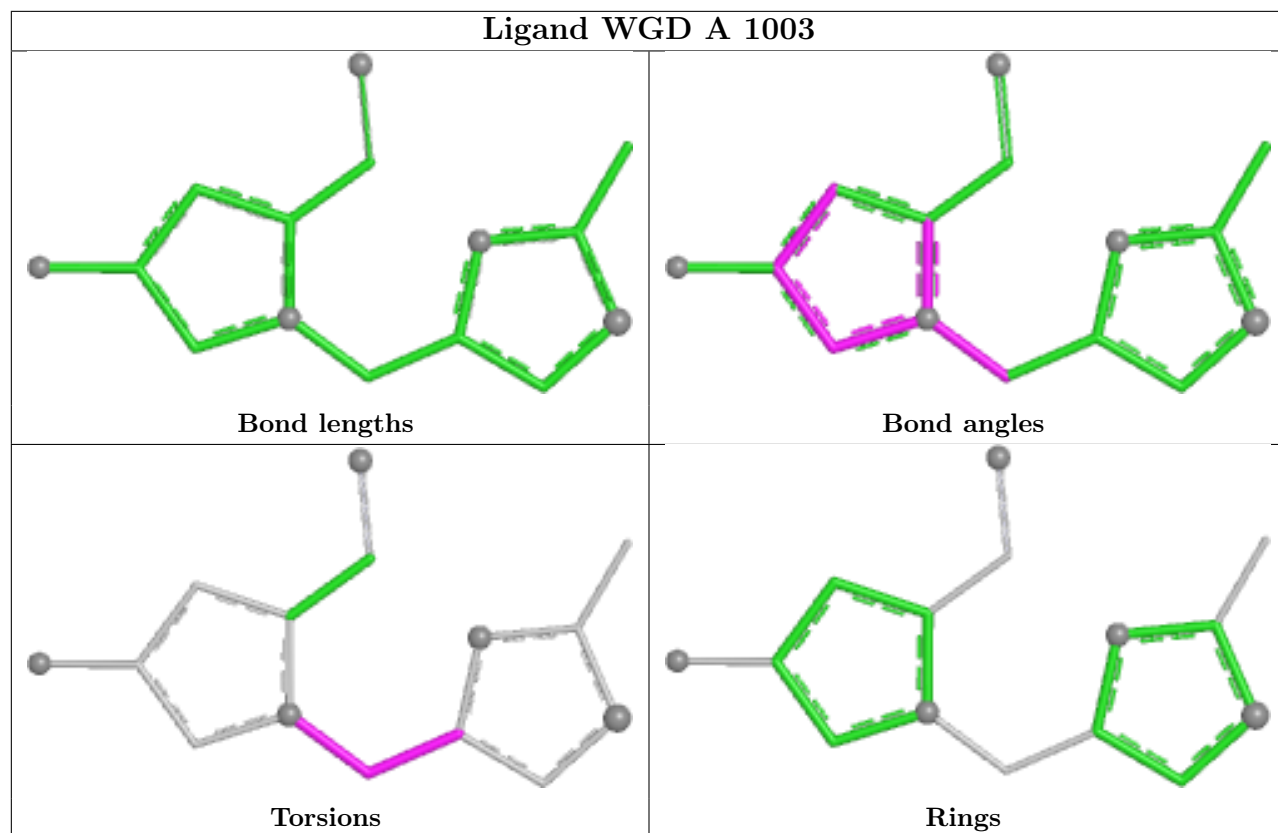
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

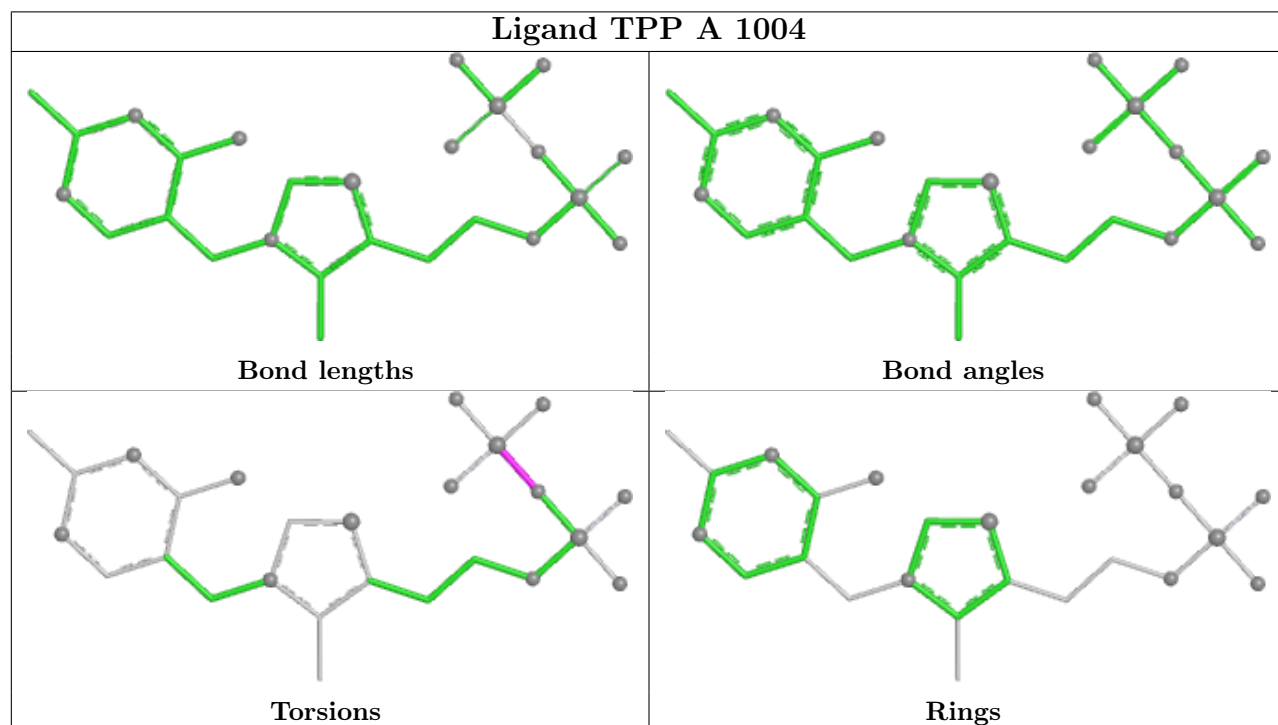




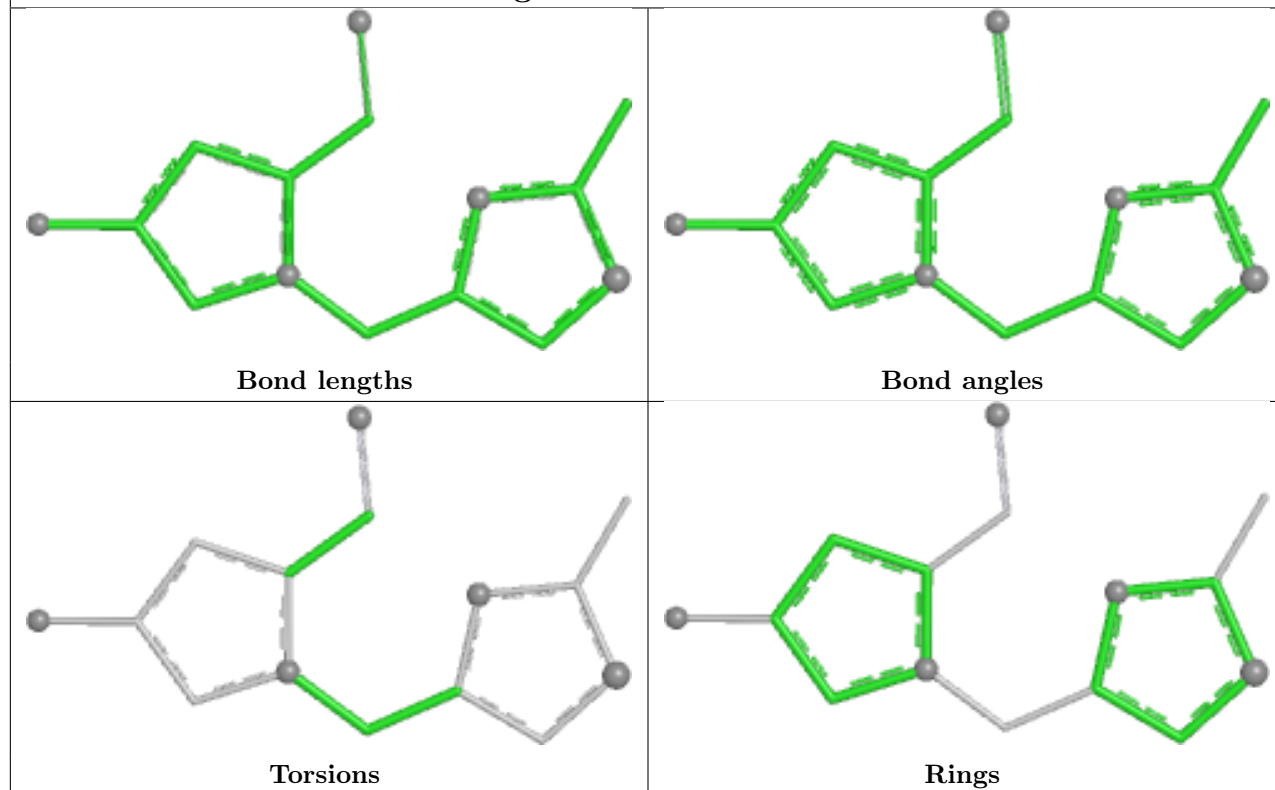
Ligand WGD A 1003



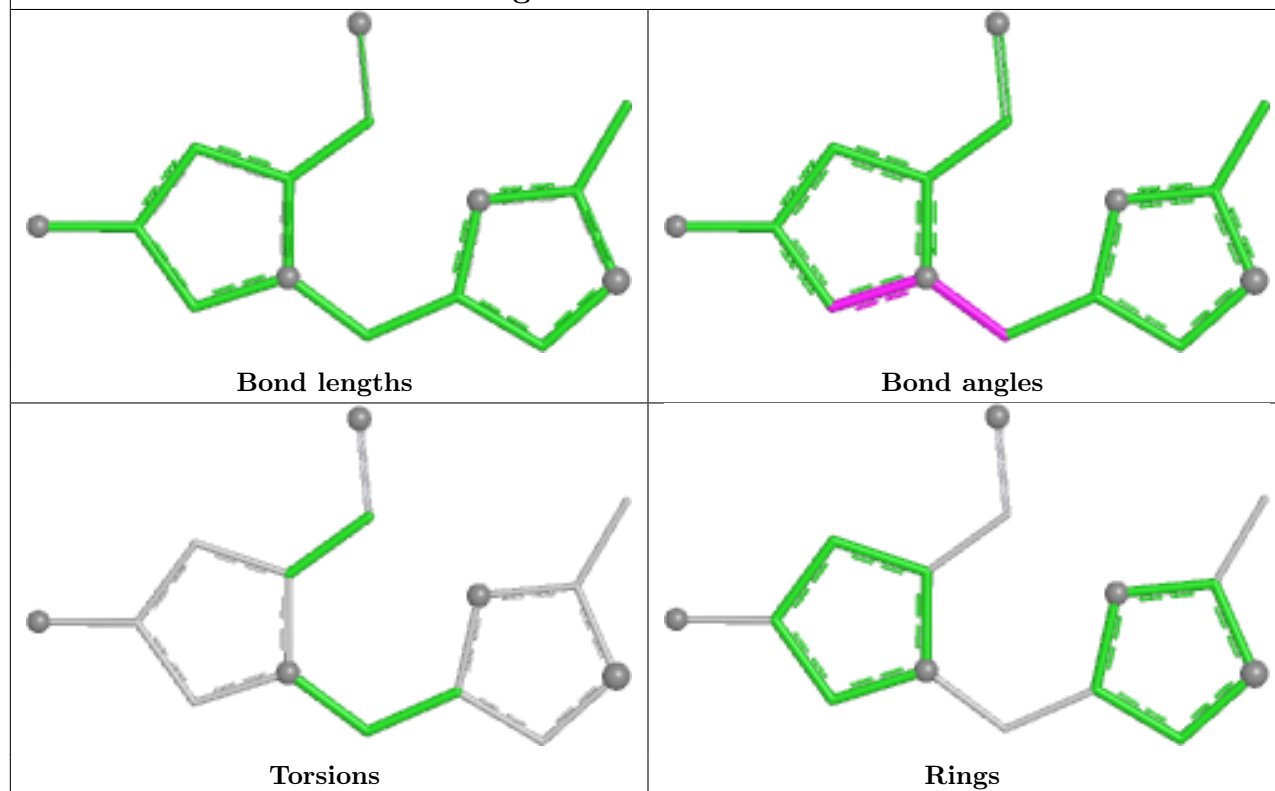
Ligand TPP A 1004



Ligand WGD B 1001



Ligand WGD A 1001



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, 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	867/898 (96%)	-0.11	39 (4%)	38	47	8, 19, 42, 58	5 (0%)
1	B	867/898 (96%)	0.12	72 (8%)	17	21	9, 23, 51, 72	2 (0%)
All	All	1734/1796 (96%)	0.00	111 (6%)	25	32	8, 20, 49, 72	7 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	7.6
1	A	83	LEU	6.9
1	A	505	LEU	6.1
1	B	98	GLY	5.8
1	A	503	LEU	5.7
1	B	101	HIS	5.7
1	A	81	ALA	5.5
1	A	104	GLY	4.9
1	B	102	THR	4.9
1	B	83	LEU	4.9
1	A	98	GLY	4.8
1	A	276	HIS	4.8
1	B	275	ALA	4.7
1	B	276	HIS	4.6
1	B	106	LEU	4.6
1	A	277	HIS	4.6
1	B	100	PHE	4.5
1	A	275	ALA	4.4
1	A	519	ILE	4.3
1	B	105	LEU	4.2
1	B	103	ALA	4.0
1	B	509	TRP	3.9
1	B	211	TYR	3.8
1	B	496	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	THR	3.8
1	B	85	ASN	3.7
1	A	105	LEU	3.6
1	A	504	ASN	3.6
1	B	81	ALA	3.6
1	A	110	LYS	3.5
1	B	473	THR	3.5
1	B	94	GLN	3.4
1	B	104	GLY	3.4
1	B	471	LEU	3.4
1	A	278	PRO	3.4
1	A	502	ALA	3.3
1	B	99	PRO	3.3
1	A	77	PHE	3.3
1	A	497[A]	HIS	3.2
1	B	508	HIS	3.2
1	B	273	PHE	3.2
1	B	500	PRO	3.1
1	A	855	HIS	3.1
1	A	106	LEU	3.1
1	A	211	TYR	3.1
1	B	498	TYR	3.1
1	A	80	GLN	3.0
1	B	107	ASN	3.0
1	B	97	GLN	3.0
1	A	102	THR	2.9
1	A	79	GLY	2.9
1	A	78	THR	2.9
1	B	477	VAL	2.9
1	B	96	LEU	2.9
1	B	49	ARG	2.8
1	A	103	ALA	2.8
1	B	93	VAL	2.8
1	B	317	ASN	2.8
1	B	497	HIS	2.8
1	B	501	PRO	2.8
1	B	511	GLY	2.8
1	B	797	VAL	2.7
1	B	82	LEU	2.7
1	A	494	ASN	2.7
1	B	826	LYS	2.7
1	A	109	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	466	LEU	2.6
1	B	551	LEU	2.6
1	B	368	LEU	2.6
1	B	111	GLU	2.5
1	B	77	PHE	2.5
1	B	254	ASN	2.4
1	B	512	LEU	2.4
1	B	856	VAL	2.4
1	A	84	GLU	2.4
1	A	101	HIS	2.4
1	B	110	LYS	2.4
1	B	277	HIS	2.4
1	B	316	ASP	2.3
1	B	108	MET	2.3
1	B	472	MET	2.3
1	A	97	GLN	2.3
1	B	824	GLY	2.3
1	B	157	THR	2.3
1	B	495	MET	2.3
1	B	625	PRO	2.3
1	A	94	GLN	2.3
1	A	274	GLY	2.3
1	B	470	GLY	2.3
1	B	113	ALA	2.2
1	B	468	ALA	2.2
1	B	114	SER	2.2
1	A	107	ASN	2.2
1	B	80	GLN	2.2
1	B	467	ILE	2.2
1	A	854	LYS	2.1
1	B	475	GLU	2.1
1	B	499	ARG	2.1
1	A	856	VAL	2.1
1	B	52	VAL	2.1
1	B	552	LEU	2.1
1	B	510	GLN	2.1
1	A	501	PRO	2.1
1	B	120	VAL	2.1
1	B	78	THR	2.1
1	B	50	PRO	2.1
1	B	469	GLY	2.0
1	A	517	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	507	ALA	2.0
1	A	100	PHE	2.0
1	B	463	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

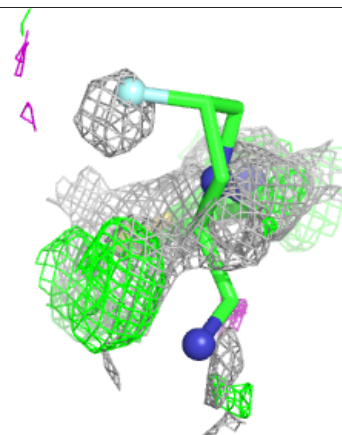
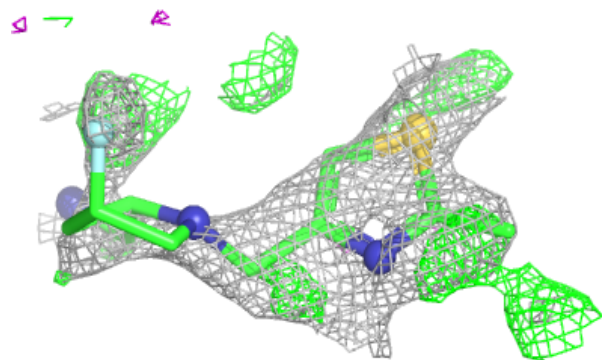
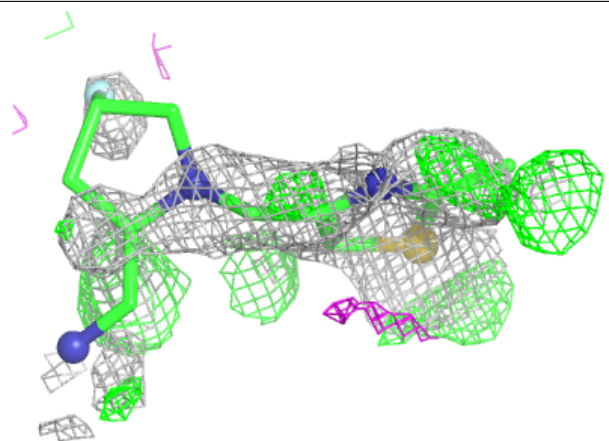
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	WGD	A	1002	15/15	0.78	0.37	56,56,56,57	15
2	WGD	B	1002	15/15	0.79	0.38	33,35,37,38	15
2	WGD	B	1001	15/15	0.82	0.20	30,32,33,33	15
2	WGD	A	1003	15/15	0.82	0.22	34,35,37,38	15
2	WGD	A	1001	15/15	0.90	0.12	16,17,18,19	15
3	TPP	B	1003	26/26	0.98	0.05	12,14,15,16	0
4	MG	A	1005	1/1	0.98	0.02	13,13,13,13	0
3	TPP	A	1004	26/26	0.99	0.04	10,12,13,14	0
4	MG	B	1004	1/1	0.99	0.02	15,15,15,15	0
4	MG	B	1005	1/1	0.99	0.01	10,10,10,10	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.

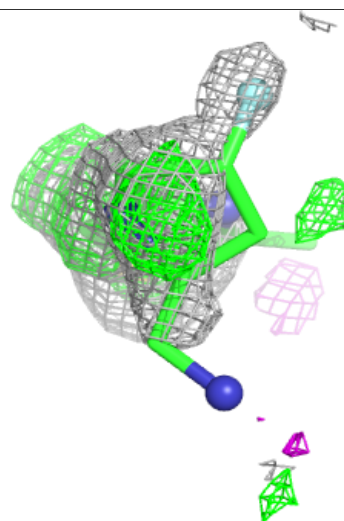
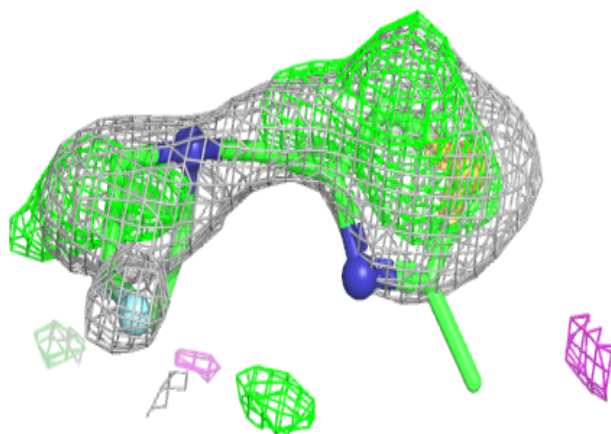
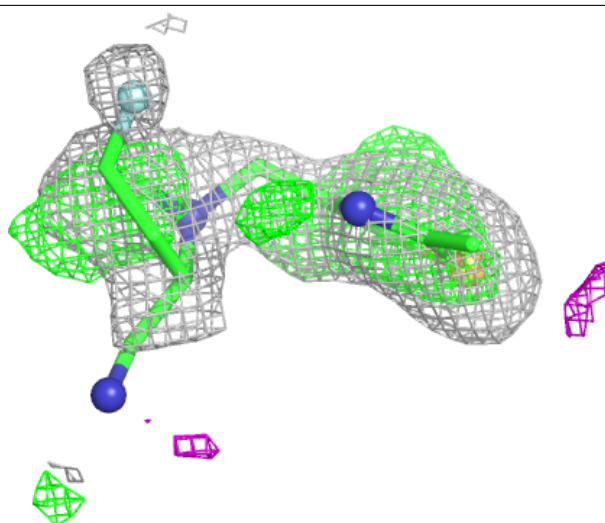
Electron density around WGD A 1002:

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



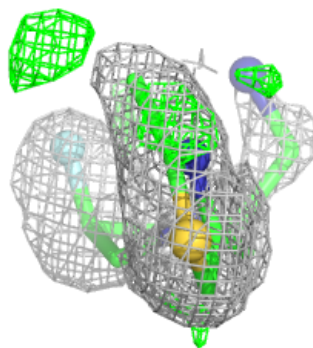
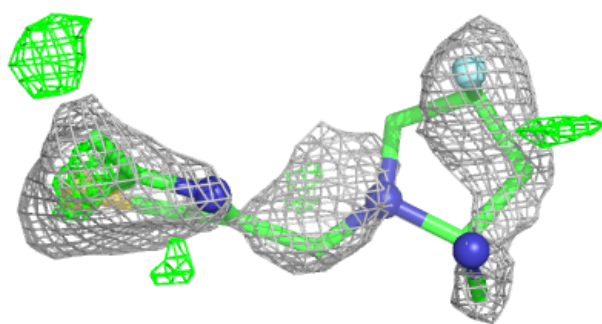
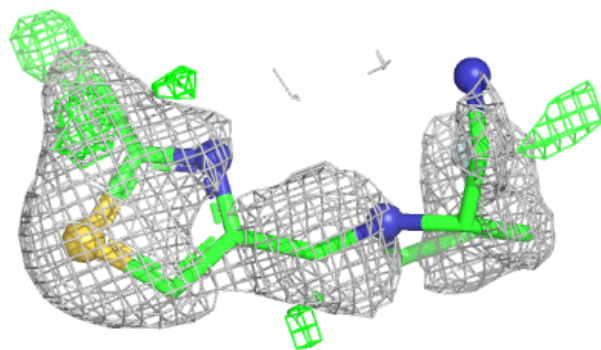
Electron density around WGD B 1002:

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



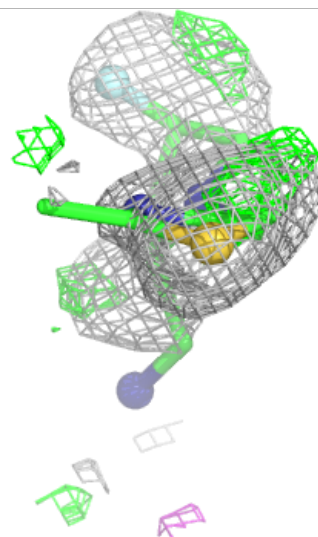
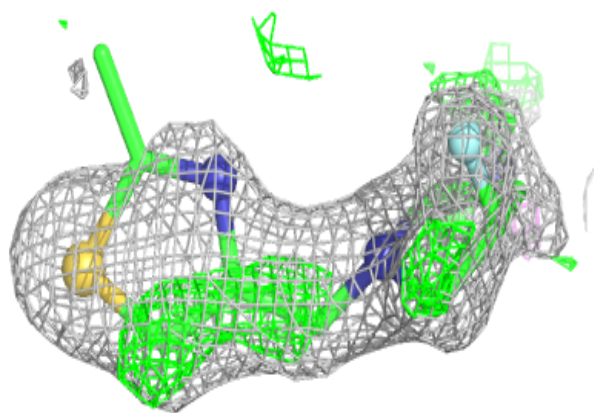
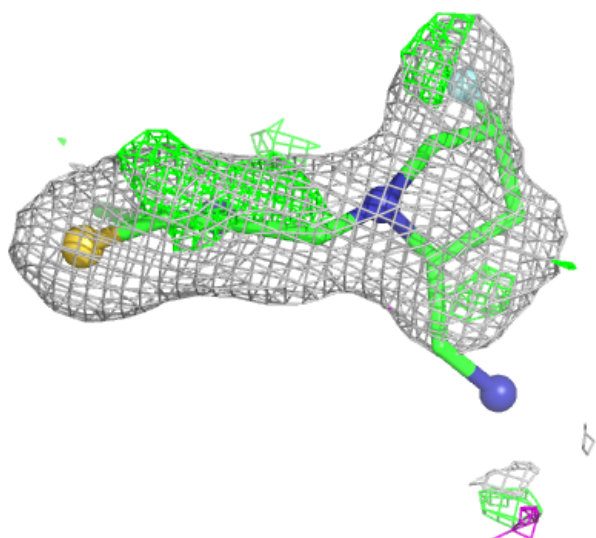
Electron density around WGD B 1001:

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



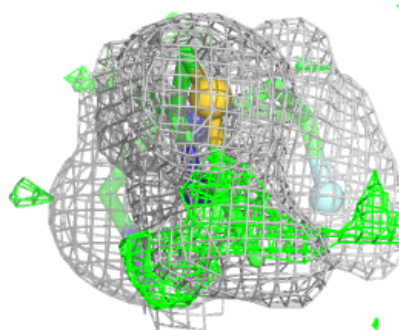
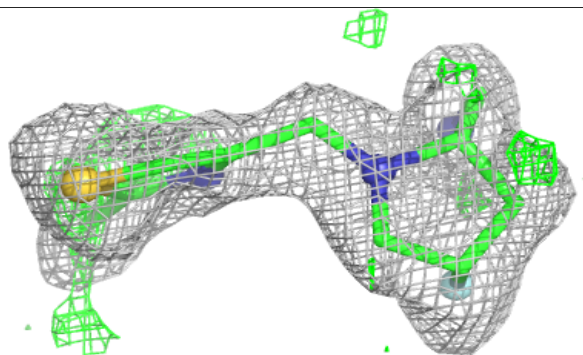
Electron density around WGD A 1003:

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

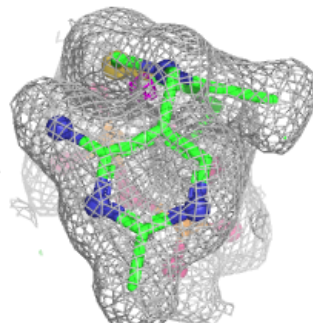
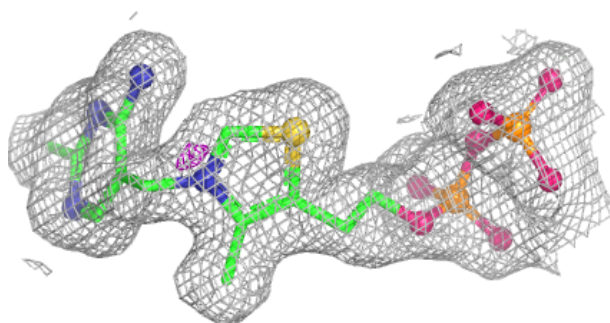
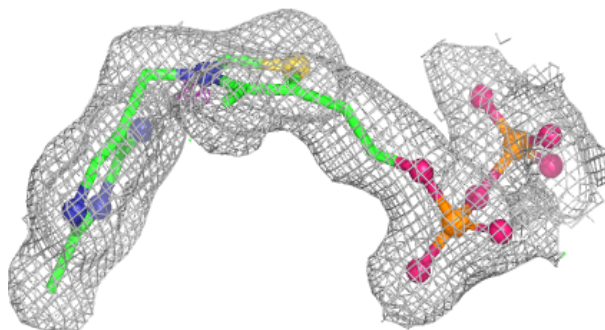


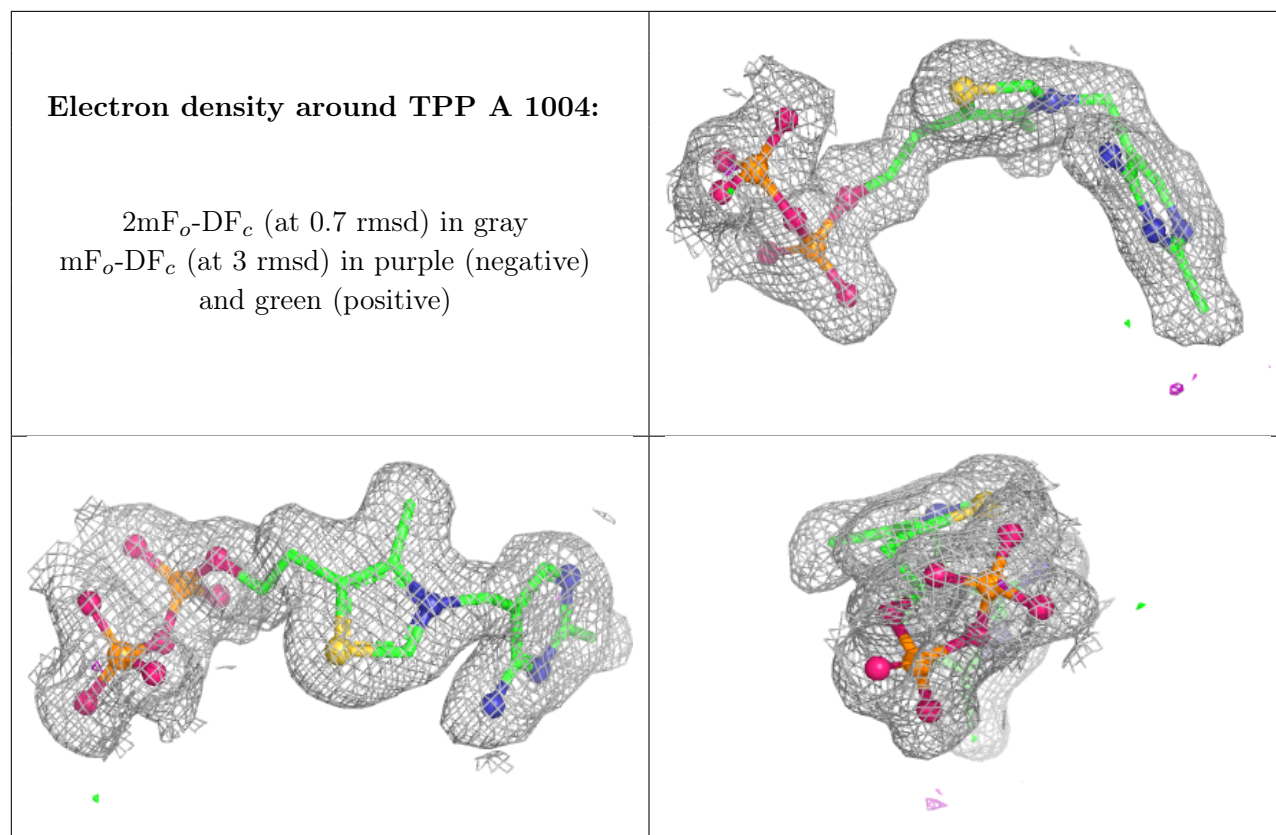
Electron density around WGD A 1001:

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

**Electron density around TPP B 1003:**

$2mF_o-DF_c$ (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.