



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:13 AM BST

PDB ID : 6KMA  
Title : Crystal structure of SucA with glycolaldehyde-1-13C from *Vibrio vulnificus*  
Authors : Seo, P.W.; Kim, J.S.  
Deposited on : 2019-07-31  
Resolution : 2.28 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

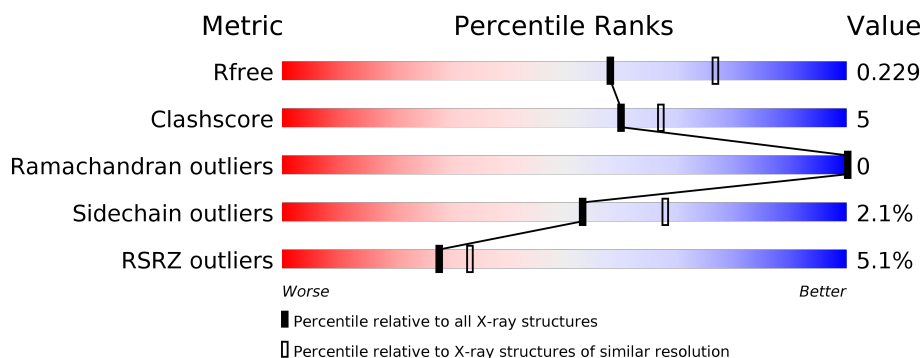
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	886	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	B	886	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• 6%</div> </div> </div>
1	C	886	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	D	886	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>

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
6	DW3	A	1005	-	-	X	-
6	DW3	B	1005	-	-	X	-
6	DW3	C	1005	-	-	X	-
6	DW3	D	1001	-	-	X	-
6	DW3	D	1005	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27925 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 Oxoglutarate dehydrogenase (Succinyl-transferring), E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6629	4174	1172	1245	38			
1	B	837	Total	C	N	O	S	0	0	0
			6612	4163	1168	1243	38			
1	C	839	Total	C	N	O	S	0	0	0
			6625	4171	1170	1246	38			
1	D	836	Total	C	N	O	S	0	0	0
			6598	4152	1166	1242	38			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	MET	-	initiating methionine	UNP A0A3Q0L1E1
A	57	GLY	-	expression tag	UNP A0A3Q0L1E1
A	58	SER	-	expression tag	UNP A0A3Q0L1E1
A	59	SER	-	expression tag	UNP A0A3Q0L1E1
A	60	HIS	-	expression tag	UNP A0A3Q0L1E1
A	61	HIS	-	expression tag	UNP A0A3Q0L1E1
A	62	HIS	-	expression tag	UNP A0A3Q0L1E1
A	63	HIS	-	expression tag	UNP A0A3Q0L1E1
A	64	HIS	-	expression tag	UNP A0A3Q0L1E1
A	65	HIS	-	expression tag	UNP A0A3Q0L1E1
A	66	ASP	-	expression tag	UNP A0A3Q0L1E1
A	67	TYR	-	expression tag	UNP A0A3Q0L1E1
A	68	ASP	-	expression tag	UNP A0A3Q0L1E1
A	69	ILE	-	expression tag	UNP A0A3Q0L1E1
A	70	PRO	-	expression tag	UNP A0A3Q0L1E1
A	71	THR	-	expression tag	UNP A0A3Q0L1E1
A	72	THR	-	expression tag	UNP A0A3Q0L1E1
A	73	GLU	-	expression tag	UNP A0A3Q0L1E1
A	74	ASN	-	expression tag	UNP A0A3Q0L1E1
A	75	LEU	-	expression tag	UNP A0A3Q0L1E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	TYR	-	expression tag	UNP A0A3Q0L1E1
A	77	PHE	-	expression tag	UNP A0A3Q0L1E1
A	78	GLN	-	expression tag	UNP A0A3Q0L1E1
A	79	GLY	-	expression tag	UNP A0A3Q0L1E1
A	80	GLY	-	expression tag	UNP A0A3Q0L1E1
A	81	GLY	-	expression tag	UNP A0A3Q0L1E1
A	82	GLY	-	expression tag	UNP A0A3Q0L1E1
A	83	GLY	-	expression tag	UNP A0A3Q0L1E1
A	84	GLY	-	expression tag	UNP A0A3Q0L1E1
B	56	MET	-	initiating methionine	UNP A0A3Q0L1E1
B	57	GLY	-	expression tag	UNP A0A3Q0L1E1
B	58	SER	-	expression tag	UNP A0A3Q0L1E1
B	59	SER	-	expression tag	UNP A0A3Q0L1E1
B	60	HIS	-	expression tag	UNP A0A3Q0L1E1
B	61	HIS	-	expression tag	UNP A0A3Q0L1E1
B	62	HIS	-	expression tag	UNP A0A3Q0L1E1
B	63	HIS	-	expression tag	UNP A0A3Q0L1E1
B	64	HIS	-	expression tag	UNP A0A3Q0L1E1
B	65	HIS	-	expression tag	UNP A0A3Q0L1E1
B	66	ASP	-	expression tag	UNP A0A3Q0L1E1
B	67	TYR	-	expression tag	UNP A0A3Q0L1E1
B	68	ASP	-	expression tag	UNP A0A3Q0L1E1
B	69	ILE	-	expression tag	UNP A0A3Q0L1E1
B	70	PRO	-	expression tag	UNP A0A3Q0L1E1
B	71	THR	-	expression tag	UNP A0A3Q0L1E1
B	72	THR	-	expression tag	UNP A0A3Q0L1E1
B	73	GLU	-	expression tag	UNP A0A3Q0L1E1
B	74	ASN	-	expression tag	UNP A0A3Q0L1E1
B	75	LEU	-	expression tag	UNP A0A3Q0L1E1
B	76	TYR	-	expression tag	UNP A0A3Q0L1E1
B	77	PHE	-	expression tag	UNP A0A3Q0L1E1
B	78	GLN	-	expression tag	UNP A0A3Q0L1E1
B	79	GLY	-	expression tag	UNP A0A3Q0L1E1
B	80	GLY	-	expression tag	UNP A0A3Q0L1E1
B	81	GLY	-	expression tag	UNP A0A3Q0L1E1
B	82	GLY	-	expression tag	UNP A0A3Q0L1E1
B	83	GLY	-	expression tag	UNP A0A3Q0L1E1
B	84	GLY	-	expression tag	UNP A0A3Q0L1E1
C	56	MET	-	initiating methionine	UNP A0A3Q0L1E1
C	57	GLY	-	expression tag	UNP A0A3Q0L1E1
C	58	SER	-	expression tag	UNP A0A3Q0L1E1
C	59	SER	-	expression tag	UNP A0A3Q0L1E1

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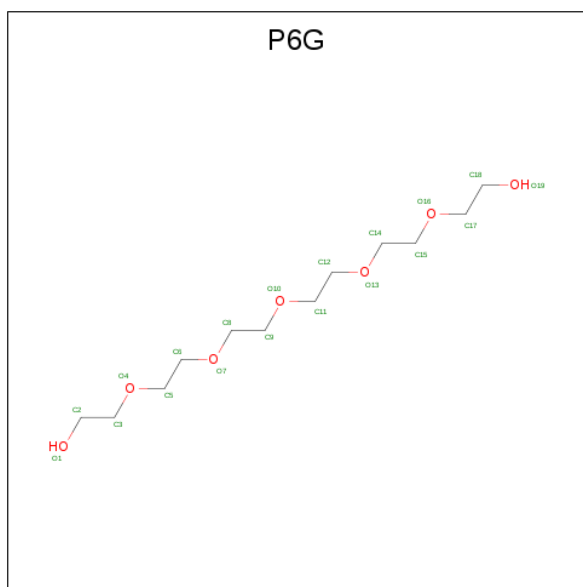
Chain	Residue	Modelled	Actual	Comment	Reference
C	60	HIS	-	expression tag	UNP A0A3Q0L1E1
C	61	HIS	-	expression tag	UNP A0A3Q0L1E1
C	62	HIS	-	expression tag	UNP A0A3Q0L1E1
C	63	HIS	-	expression tag	UNP A0A3Q0L1E1
C	64	HIS	-	expression tag	UNP A0A3Q0L1E1
C	65	HIS	-	expression tag	UNP A0A3Q0L1E1
C	66	ASP	-	expression tag	UNP A0A3Q0L1E1
C	67	TYR	-	expression tag	UNP A0A3Q0L1E1
C	68	ASP	-	expression tag	UNP A0A3Q0L1E1
C	69	ILE	-	expression tag	UNP A0A3Q0L1E1
C	70	PRO	-	expression tag	UNP A0A3Q0L1E1
C	71	THR	-	expression tag	UNP A0A3Q0L1E1
C	72	THR	-	expression tag	UNP A0A3Q0L1E1
C	73	GLU	-	expression tag	UNP A0A3Q0L1E1
C	74	ASN	-	expression tag	UNP A0A3Q0L1E1
C	75	LEU	-	expression tag	UNP A0A3Q0L1E1
C	76	TYR	-	expression tag	UNP A0A3Q0L1E1
C	77	PHE	-	expression tag	UNP A0A3Q0L1E1
C	78	GLN	-	expression tag	UNP A0A3Q0L1E1
C	79	GLY	-	expression tag	UNP A0A3Q0L1E1
C	80	GLY	-	expression tag	UNP A0A3Q0L1E1
C	81	GLY	-	expression tag	UNP A0A3Q0L1E1
C	82	GLY	-	expression tag	UNP A0A3Q0L1E1
C	83	GLY	-	expression tag	UNP A0A3Q0L1E1
C	84	GLY	-	expression tag	UNP A0A3Q0L1E1
D	56	MET	-	initiating methionine	UNP A0A3Q0L1E1
D	57	GLY	-	expression tag	UNP A0A3Q0L1E1
D	58	SER	-	expression tag	UNP A0A3Q0L1E1
D	59	SER	-	expression tag	UNP A0A3Q0L1E1
D	60	HIS	-	expression tag	UNP A0A3Q0L1E1
D	61	HIS	-	expression tag	UNP A0A3Q0L1E1
D	62	HIS	-	expression tag	UNP A0A3Q0L1E1
D	63	HIS	-	expression tag	UNP A0A3Q0L1E1
D	64	HIS	-	expression tag	UNP A0A3Q0L1E1
D	65	HIS	-	expression tag	UNP A0A3Q0L1E1
D	66	ASP	-	expression tag	UNP A0A3Q0L1E1
D	67	TYR	-	expression tag	UNP A0A3Q0L1E1
D	68	ASP	-	expression tag	UNP A0A3Q0L1E1
D	69	ILE	-	expression tag	UNP A0A3Q0L1E1
D	70	PRO	-	expression tag	UNP A0A3Q0L1E1
D	71	THR	-	expression tag	UNP A0A3Q0L1E1
D	72	THR	-	expression tag	UNP A0A3Q0L1E1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	73	GLU	-	expression tag	UNP A0A3Q0L1E1
D	74	ASN	-	expression tag	UNP A0A3Q0L1E1
D	75	LEU	-	expression tag	UNP A0A3Q0L1E1
D	76	TYR	-	expression tag	UNP A0A3Q0L1E1
D	77	PHE	-	expression tag	UNP A0A3Q0L1E1
D	78	GLN	-	expression tag	UNP A0A3Q0L1E1
D	79	GLY	-	expression tag	UNP A0A3Q0L1E1
D	80	GLY	-	expression tag	UNP A0A3Q0L1E1
D	81	GLY	-	expression tag	UNP A0A3Q0L1E1
D	82	GLY	-	expression tag	UNP A0A3Q0L1E1
D	83	GLY	-	expression tag	UNP A0A3Q0L1E1
D	84	GLY	-	expression tag	UNP A0A3Q0L1E1

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	12	7		
2	B	1	Total	C	O	0	0
			19	12	7		
2	C	1	Total	C	O	0	0
			19	12	7		
2	D	1	Total	C	O	0	0
			19	12	7		

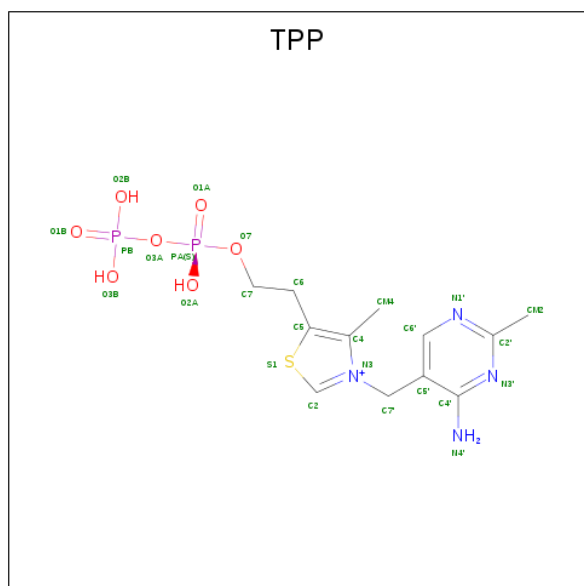
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

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

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by author).



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

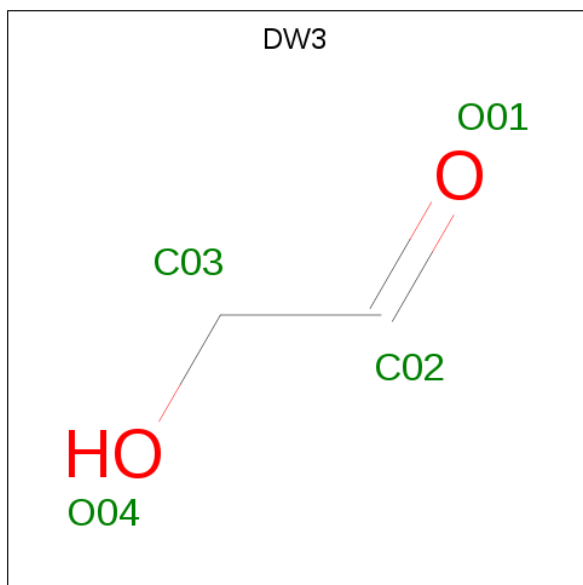
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is 2-oxidanylethanal (three-letter code: DW3) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



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

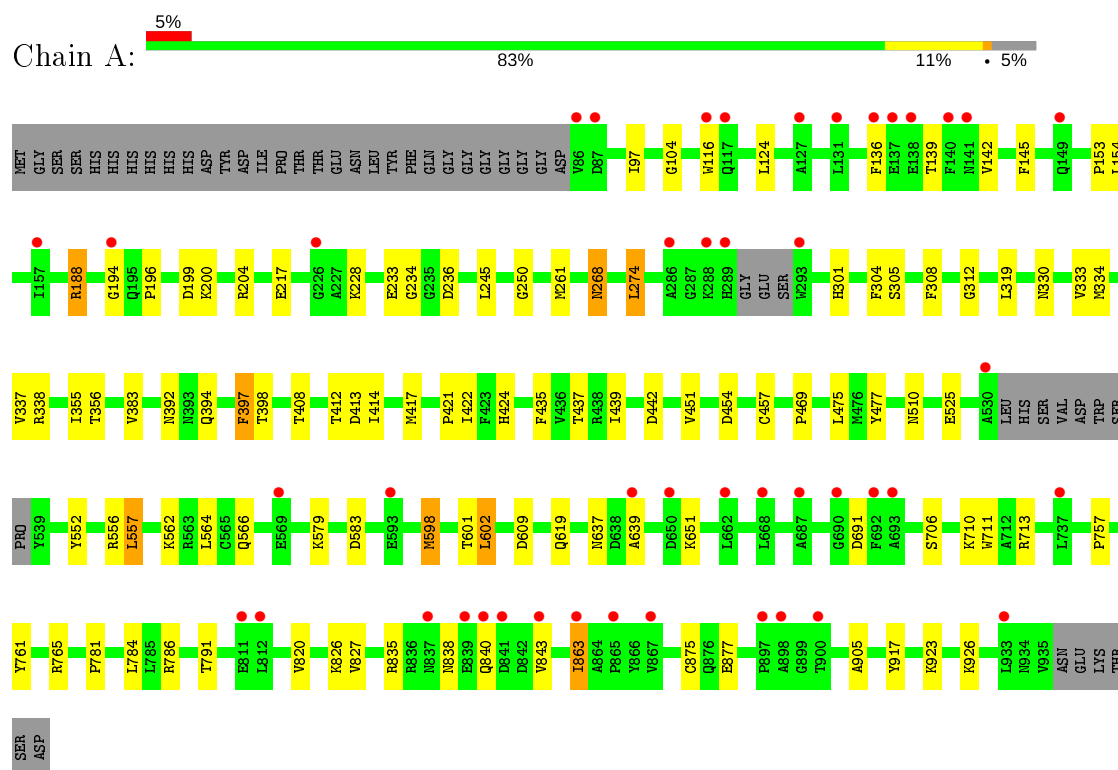
- Molecule 7 is water.

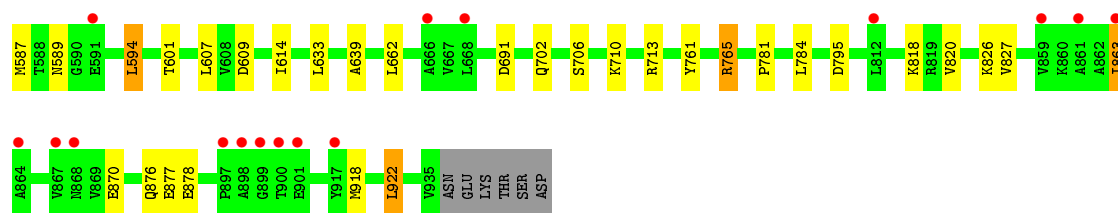
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	316	Total 316	O 316	0	0
7	B	323	Total 323	O 323	0	0
7	C	296	Total 296	O 296	0	0
7	D	308	Total 308	O 308	0	0

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

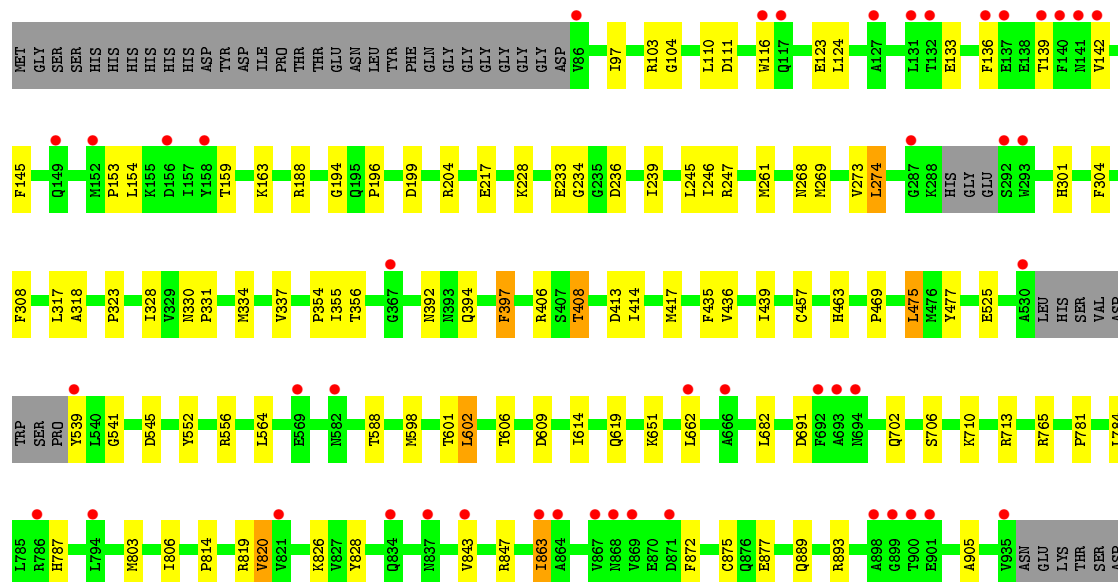
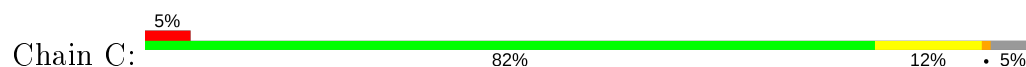
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Oxoglutarate dehydrogenase (Succinyl-transferring), E1 component

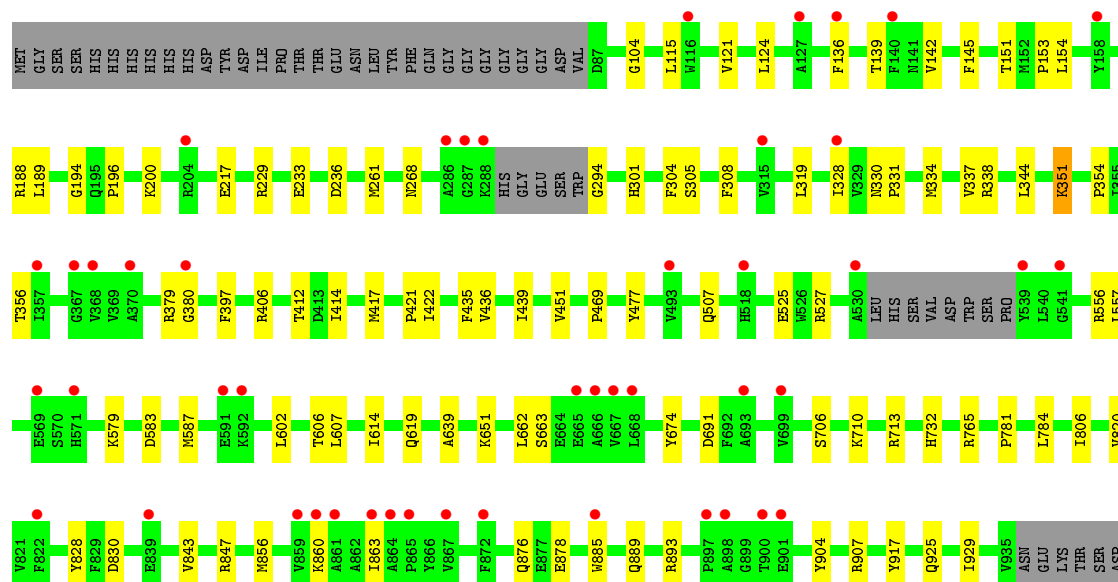
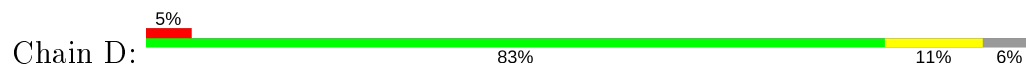




- Molecule 1: Oxoglutarate dehydrogenase (Succinyl-transferring), E1 component



- Molecule 1: Oxoglutarate dehydrogenase (Succinyl-transferring), E1 component



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.82Å 84.56Å 145.22Å 79.51° 88.47° 89.92°	Depositor
Resolution (Å)	47.65 – 2.28 47.65 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.65-2.28) 90.8 (47.65-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.200 , 0.230 0.200 , 0.229	Depositor DCC
$R_{free}$ test set	5900 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.083 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DW3, MG, CA, P6G, 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	0.32	1/6782 (0.0%)	0.45	0/9192
1	B	0.30	1/6764 (0.0%)	0.43	0/9167
1	C	0.29	0/6777	0.44	0/9185
1	D	0.30	1/6748 (0.0%)	0.45	0/9144
All	All	0.30	3/27071 (0.0%)	0.44	0/36688

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	917	TYR	CB-CG	-5.24	1.43	1.51
1	B	765	ARG	CZ-NH1	-5.06	1.26	1.33
1	D	917	TYR	CG-CD2	-5.02	1.32	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6629	0	6447	62	0
1	B	6612	0	6431	49	0
1	C	6625	0	6445	73	0
1	D	6598	0	6421	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	26	1	0
2	B	19	0	26	1	0
2	C	19	0	26	3	0
2	D	19	0	26	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	16	0	0
5	B	26	0	16	1	0
5	C	26	0	16	4	0
5	D	26	0	16	3	0
6	A	8	0	0	2	0
6	B	8	0	0	3	0
6	C	8	0	0	2	0
6	D	8	0	0	4	0
7	A	316	0	0	6	0
7	B	323	0	0	2	0
7	C	296	0	0	7	0
7	D	308	0	0	7	0
All	All	27925	0	25912	240	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 5.

All (240) 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:C:301:HIS:HE2	6:C:1005:DW3:C02	1.88	0.84
1:A:820:VAL:HG11	1:A:863:ILE:HD11	1.67	0.74
1:B:113:LEU:O	1:B:479:LYS:NZ	2.22	0.71
1:A:274:LEU:HD22	1:A:304:PHE:HB3	1.72	0.70
1:D:820:VAL:HG11	1:D:863:ILE:HD11	1.73	0.70
1:B:820:VAL:HG11	1:B:863:ILE:HD11	1.72	0.70
1:D:351:LYS:NZ	7:D:1107:HOH:O	2.27	0.68
1:D:527:ARG:NH1	7:D:1108:HOH:O	2.27	0.68
1:C:301:HIS:NE2	6:C:1005:DW3:C02	2.58	0.67
1:D:301:HIS:HE2	6:D:1005:DW3:C02	2.06	0.67
1:C:820:VAL:HG21	1:C:863:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:HIS:HE2	6:A:1005:DW3:C02	2.08	0.66
1:B:301:HIS:NE2	6:B:1005:DW3:C02	2.59	0.66
1:A:139:THR:HA	1:A:153:PRO:HA	1.77	0.66
1:C:408:THR:OG1	1:C:413:ASP:OD2	2.10	0.65
1:B:826:LYS:NZ	1:B:877:GLU:OE1	2.27	0.65
1:D:406:ARG:NH2	7:D:1111:HOH:O	2.30	0.65
1:A:781:PRO:HB2	1:A:784:LEU:HB2	1.78	0.65
1:C:139:THR:HA	1:C:153:PRO:HA	1.78	0.65
1:A:579:LYS:NZ	1:A:583:ASP:OD1	2.30	0.64
1:B:781:PRO:HB2	1:B:784:LEU:HB2	1.78	0.64
1:C:406:ARG:NH2	7:C:1107:HOH:O	2.30	0.64
1:C:111:ASP:HB2	1:C:116:TRP:CD2	2.34	0.63
1:D:308:PHE:CZ	1:D:525:GLU:HG3	2.34	0.63
1:C:781:PRO:HB2	1:C:784:LEU:HB2	1.80	0.62
1:C:116:TRP:NE1	1:C:394:GLN:OE1	2.33	0.62
5:C:1004:TPP:H2	6:D:1001:DW3:O01	2.00	0.62
1:A:116:TRP:NE1	1:A:394:GLN:OE1	2.32	0.62
1:C:713:ARG:NH2	2:C:1001:P6G:O10	2.33	0.62
1:D:294:GLY:N	7:D:1113:HOH:O	2.32	0.62
1:C:103:ARG:NH1	1:C:123:GLU:OE1	2.33	0.61
1:C:826:LYS:NZ	1:C:877:GLU:OE2	2.31	0.61
1:A:838:ASN:ND2	7:A:1110:HOH:O	2.33	0.61
1:C:228:LYS:NZ	7:C:1109:HOH:O	2.33	0.60
1:C:308:PHE:CZ	1:C:525:GLU:HG3	2.36	0.60
1:A:142:VAL:HB	1:A:145:PHE:HB3	1.83	0.60
1:B:337:VAL:HG23	1:B:383:VAL:HG11	1.83	0.60
1:D:781:PRO:HB2	1:D:784:LEU:HB2	1.82	0.60
1:A:826:LYS:NZ	1:A:877:GLU:OE2	2.32	0.60
1:D:856:MET:HG3	1:D:860:LYS:HE3	1.84	0.60
1:C:274:LEU:HD22	1:C:304:PHE:HB3	1.83	0.59
1:B:556:ARG:NH2	1:B:609:ASP:OD1	2.35	0.59
1:D:732:HIS:NE2	6:D:1001:DW3:C02	2.66	0.59
1:D:507:GLN:NE2	7:D:1122:HOH:O	2.36	0.58
1:D:139:THR:HA	1:D:153:PRO:HA	1.85	0.58
1:B:488:LYS:NZ	1:B:492:ASP:OD2	2.37	0.58
1:A:308:PHE:CZ	1:A:525:GLU:HG3	2.38	0.57
1:B:301:HIS:NE2	6:B:1005:DW3:O01	2.37	0.57
1:C:706:SER:HB2	1:C:710:LYS:HD3	1.86	0.57
1:C:889:GLN:NE2	1:D:889:GLN:HE22	2.02	0.57
1:A:408:THR:OG1	1:A:413:ASP:OD2	2.16	0.56
1:D:200:LYS:HD2	1:D:200:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:HIS:NE2	6:D:1005:DW3:O01	2.19	0.56
1:B:139:THR:HA	1:B:153:PRO:HA	1.86	0.56
1:C:318:ALA:HB1	2:C:1001:P6G:H112	1.88	0.56
1:B:706:SER:HB2	1:B:710:LYS:HD3	1.87	0.56
1:A:711:TRP:HB2	1:A:713:ARG:HG2	1.88	0.55
1:B:308:PHE:CZ	1:B:525:GLU:HG3	2.42	0.55
1:B:324:SER:HA	6:B:1005:DW3:O01	2.05	0.55
1:D:606:THR:OG1	1:D:765:ARG:HD2	2.06	0.55
1:D:337:VAL:HG21	1:D:354:PRO:HB3	1.88	0.55
1:B:918:MET:O	1:B:922:LEU:HD22	2.08	0.54
1:B:142:VAL:HB	1:B:145:PHE:HB3	1.89	0.54
1:C:159:THR:HG22	1:C:163:LYS:HD2	1.89	0.53
1:D:142:VAL:HB	1:D:145:PHE:HB3	1.90	0.53
1:A:217:GLU:HG2	1:A:233:GLU:HG3	1.89	0.52
1:C:142:VAL:HB	1:C:145:PHE:HB3	1.91	0.52
1:B:304:PHE:HA	2:B:1002:P6G:H151	1.90	0.52
1:D:828:TYR:CD1	1:D:847:ARG:HD2	2.44	0.52
1:C:806:ILE:HB	1:C:847:ARG:HB2	1.92	0.52
1:A:706:SER:HB2	1:A:710:LYS:HD3	1.91	0.52
1:B:136:PHE:HA	1:B:154:LEU:HB3	1.92	0.52
1:D:713:ARG:HH22	2:D:1002:P6G:H81	1.74	0.52
1:A:598:MET:O	1:A:602:LEU:HD22	2.10	0.51
1:A:637:ASN:O	1:B:475:LEU:HD11	2.10	0.51
1:C:475:LEU:HD22	1:D:639:ALA:HB2	1.92	0.51
5:C:1004:TPP:H6'	1:D:619:GLN:OE1	2.10	0.51
1:B:562:LYS:NZ	1:B:589:ASN:OD1	2.41	0.51
1:C:245:LEU:HD13	1:C:355:ILE:HD13	1.92	0.51
1:C:713:ARG:HH22	2:C:1001:P6G:H122	1.75	0.51
1:D:338:ARG:HH22	1:D:380:GLY:H	1.58	0.51
1:A:786:ARG:NH2	7:A:1108:HOH:O	2.31	0.51
1:A:104:GLY:HA2	1:A:124:LEU:HD21	1.92	0.50
1:B:261:MET:HG2	1:B:319:LEU:HD11	1.94	0.50
1:C:598:MET:O	1:C:602:LEU:HD22	2.12	0.50
1:A:835:ARG:HD2	1:A:843:VAL:HG23	1.94	0.50
1:A:333:VAL:O	1:A:337:VAL:HG13	2.11	0.49
1:C:556:ARG:NH2	1:C:609:ASP:OD1	2.45	0.49
1:D:706:SER:HB2	1:D:710:LYS:HD3	1.93	0.49
1:C:246:ILE:HD13	1:C:317:LEU:HD11	1.95	0.49
1:A:97:ILE:HD13	1:A:145:PHE:HB2	1.94	0.49
1:B:761:TYR:CZ	1:B:765:ARG:HD3	2.48	0.49
1:D:885:TRP:CH2	1:D:904:TYR:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:OD1	1:A:200:LYS:N	2.47	0.48
1:C:217:GLU:HG2	1:C:233:GLU:HG3	1.95	0.48
1:C:614:ILE:HG12	1:C:682:LEU:HB3	1.96	0.48
1:C:97:ILE:HD13	1:C:145:PHE:HB2	1.94	0.48
1:B:200:LYS:HG2	1:B:204:ARG:NH2	2.29	0.48
5:C:1004:TPP:HN42	5:C:1004:TPP:H2	1.79	0.47
1:B:351:LYS:HA	1:B:351:LYS:HD3	1.51	0.47
1:C:814:PRO:O	7:C:1101:HOH:O	2.20	0.47
1:A:557:LEU:CD1	1:A:602:LEU:HG	2.45	0.47
1:A:619:GLN:OE1	5:B:1004:TPP:H6 <sup>7</sup>	2.13	0.47
1:A:552:TYR:OH	1:A:609:ASP:OD2	2.32	0.47
1:C:435:PHE:CZ	1:C:439:ILE:HD11	2.50	0.47
1:C:392:ASN:ND2	7:C:1135:HOH:O	2.48	0.46
1:D:421:PRO:HG2	1:D:451:VAL:HG23	1.97	0.46
1:A:228:LYS:NZ	7:A:1133:HOH:O	2.49	0.46
1:A:926:LYS:HD3	1:A:926:LYS:HA	1.80	0.46
1:B:818:LYS:HE3	1:B:870:GLU:HG3	1.97	0.46
1:A:639:ALA:HB2	1:B:475:LEU:HD23	1.97	0.46
1:B:713:ARG:NH1	7:B:1133:HOH:O	2.46	0.46
1:C:525:GLU:OE2	7:C:1102:HOH:O	2.21	0.46
1:D:328:ILE:O	1:D:331:PRO:HD2	2.16	0.46
1:C:328:ILE:O	1:C:331:PRO:HD2	2.16	0.46
1:B:607:LEU:HB2	1:B:614:ILE:HD11	1.98	0.46
1:C:337:VAL:HG21	1:C:354:PRO:HB3	1.98	0.46
1:A:564:LEU:HD13	1:A:601:THR:HG22	1.98	0.46
1:A:827:VAL:HB	1:A:877:GLU:HG3	1.97	0.46
1:B:827:VAL:HB	1:B:877:GLU:HG3	1.98	0.45
1:D:435:PHE:CZ	1:D:439:ILE:HD11	2.51	0.45
1:D:261:MET:HG2	1:D:319:LEU:HD11	1.99	0.45
1:C:239:ILE:HD13	1:C:269:MET:HE2	1.98	0.45
1:C:261:MET:SD	1:C:269:MET:HG3	2.57	0.45
1:C:889:GLN:NE2	1:D:889:GLN:NE2	2.65	0.45
1:C:803:MET:HE3	1:C:806:ILE:HG12	1.99	0.45
1:C:828:TYR:CD1	1:C:847:ARG:HD2	2.52	0.45
1:C:564:LEU:HD13	1:C:601:THR:HG22	1.99	0.45
1:B:330:ASN:O	1:B:334:MET:HG2	2.17	0.44
1:C:713:ARG:NH2	7:C:1148:HOH:O	2.51	0.44
1:D:607:LEU:HB2	1:D:614:ILE:HD11	1.99	0.44
1:A:261:MET:HG2	1:A:319:LEU:HD11	1.99	0.44
1:A:392:ASN:ND2	7:A:1135:HOH:O	2.49	0.44
1:B:424:HIS:HA	1:B:454:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:GLN:HB2	1:D:878:GLU:OE2	2.18	0.44
1:C:889:GLN:OE1	1:C:893:ARG:NH2	2.44	0.44
1:C:397:PHE:HA	1:C:463:HIS:HB2	1.99	0.44
1:D:583:ASP:O	1:D:587:MET:HG3	2.17	0.44
1:A:424:HIS:HA	1:A:454:ASP:HB3	1.99	0.44
1:A:475:LEU:HD22	1:B:639:ALA:HB2	1.99	0.44
1:D:194:GLY:O	1:D:196:PRO:HD3	2.17	0.44
1:C:539:TYR:CZ	1:C:541:GLY:HA3	2.52	0.44
1:C:552:TYR:OH	1:C:609:ASP:OD2	2.35	0.44
1:A:136:PHE:HA	1:A:154:LEU:HB3	2.00	0.44
1:C:330:ASN:OD1	1:C:356:THR:HG21	2.18	0.44
1:C:606:THR:OG1	1:C:765:ARG:HD2	2.18	0.44
1:A:194:GLY:O	1:A:196:PRO:HD3	2.18	0.43
1:B:162:LYS:HB3	1:B:162:LYS:HE2	1.81	0.43
1:D:885:TRP:CZ2	1:D:904:TYR:HB2	2.54	0.43
1:A:761:TYR:CZ	1:A:765:ARG:HD3	2.53	0.43
1:A:840:GLN:HG2	1:A:843:VAL:HG22	1.99	0.43
1:A:330:ASN:OD1	1:A:356:THR:HG21	2.19	0.43
1:A:421:PRO:HG2	1:A:451:VAL:HG23	1.99	0.43
1:B:421:PRO:HG2	1:B:451:VAL:HG23	2.00	0.43
1:B:587:MET:HB3	1:B:594:LEU:CD2	2.48	0.43
1:C:337:VAL:HG11	1:C:354:PRO:HG3	2.00	0.43
1:C:875:CYS:HA	1:C:905:ALA:O	2.18	0.43
1:B:199:ASP:OD1	1:B:200:LYS:N	2.49	0.43
1:C:104:GLY:HA2	1:C:124:LEU:HD21	2.00	0.43
1:D:602:LEU:O	1:D:606:THR:HG23	2.18	0.43
1:A:338:ARG:HB2	1:A:383:VAL:HG12	2.00	0.43
1:C:133:GLU:OE1	1:C:133:GLU:N	2.51	0.43
1:C:414:ILE:O	1:C:417:MET:HG2	2.18	0.43
1:B:419:GLN:NE2	7:B:1145:HOH:O	2.51	0.43
1:C:110:LEU:HB2	1:C:116:TRP:HZ3	1.83	0.43
1:D:330:ASN:O	1:D:334:MET:HG2	2.19	0.43
1:A:305:SER:H	2:A:1001:P6G:H51	1.83	0.43
1:B:493:VAL:HG13	1:B:497:ARG:NH1	2.34	0.43
1:A:217:GLU:OE1	1:A:268:ASN:ND2	2.46	0.43
1:B:552:TYR:OH	1:B:609:ASP:OD2	2.36	0.43
1:D:104:GLY:HA2	1:D:124:LEU:HD21	2.00	0.43
1:D:579:LYS:NZ	1:D:583:ASP:OD1	2.52	0.43
1:A:651:LYS:NZ	7:A:1144:HOH:O	2.52	0.42
1:C:323:PRO:HG3	1:C:702:GLN:HB3	2.01	0.42
1:D:651:LYS:HD3	1:D:651:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:PRO:HB2	1:A:477:TYR:CE1	2.54	0.42
1:C:330:ASN:O	1:C:334:MET:HG2	2.19	0.42
1:B:234:GLY:O	1:B:457:CYS:HB2	2.18	0.42
1:D:217:GLU:HG3	1:D:229:ARG:HE	1.84	0.42
1:A:245:LEU:HD13	1:A:355:ILE:HD13	2.00	0.42
1:A:875:CYS:HA	1:A:905:ALA:O	2.19	0.42
1:A:556:ARG:NH2	1:A:609:ASP:OD1	2.53	0.42
1:A:562:LYS:O	1:A:566:GLN:HG3	2.20	0.42
1:B:564:LEU:HD13	1:B:601:THR:HG22	2.02	0.42
1:C:651:LYS:HA	1:C:651:LYS:HD3	1.84	0.42
5:D:1004:TPP:HN42	5:D:1004:TPP:H2	1.85	0.42
1:B:876:GLN:HB2	1:B:878:GLU:OE2	2.20	0.42
1:C:820:VAL:HG22	1:C:872:PHE:CD2	2.54	0.42
1:D:828:TYR:CG	1:D:847:ARG:HD2	2.55	0.42
1:B:328:ILE:O	1:B:331:PRO:HD2	2.20	0.42
1:C:136:PHE:HA	1:C:154:LEU:HB3	2.02	0.42
1:A:330:ASN:O	1:A:334:MET:HG2	2.19	0.42
1:D:379:ARG:O	7:D:1101:HOH:O	2.21	0.42
1:A:435:PHE:CZ	1:A:439:ILE:HD11	2.55	0.42
1:D:304:PHE:HA	2:D:1002:P6G:H152	2.02	0.42
1:C:784:LEU:HA	1:C:787:HIS:HB2	2.02	0.42
1:D:412:THR:HG21	1:D:422:ILE:HG21	2.02	0.42
1:A:412:THR:OG1	1:A:422:ILE:HG21	2.20	0.41
1:C:602:LEU:O	1:C:606:THR:HG23	2.19	0.41
1:C:619:GLN:OE1	5:D:1004:TPP:H6'	2.20	0.41
5:D:1004:TPP:HN42	5:D:1004:TPP:C2	2.33	0.41
1:D:907:ARG:NH1	1:D:925:GLN:OE1	2.54	0.41
1:B:581:TYR:CZ	1:B:633:LEU:HD21	2.55	0.41
1:C:110:LEU:HB2	1:C:116:TRP:CZ3	2.55	0.41
1:A:510:ASN:HB3	7:A:1408:HOH:O	2.20	0.41
1:B:217:GLU:HG2	1:B:233:GLU:HG3	2.01	0.41
1:B:554:LYS:HD2	1:B:795:ASP:OD1	2.19	0.41
1:C:194:GLY:O	1:C:196:PRO:HD3	2.20	0.41
1:A:234:GLY:O	1:A:457:CYS:HB2	2.21	0.41
1:C:234:GLY:O	1:C:457:CYS:HB2	2.21	0.41
1:A:250:GLY:O	1:A:312:GLY:HA3	2.21	0.41
1:C:247:ARG:HD3	7:C:1102:HOH:O	2.19	0.41
1:C:469:PRO:HB2	1:C:477:TYR:CE1	2.56	0.41
1:C:863:ILE:HA	1:C:863:ILE:HD12	1.90	0.41
1:D:414:ILE:O	1:D:417:MET:HG2	2.20	0.41
1:D:217:GLU:HG2	1:D:233:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:PHE:HB3	1:A:398:THR:H	1.73	0.41
1:D:330:ASN:OD1	1:D:356:THR:HG21	2.21	0.41
1:A:757:PRO:HG2	1:A:791:THR:HA	2.03	0.41
1:D:305:SER:H	2:D:1002:P6G:H151	1.85	0.41
1:B:323:PRO:HG3	1:B:702:GLN:HB3	2.03	0.41
1:D:136:PHE:HA	1:D:154:LEU:HB3	2.03	0.41
1:D:469:PRO:HB2	1:D:477:TYR:CE1	2.56	0.41
1:B:246:ILE:HD13	1:B:317:LEU:HD11	2.02	0.40
1:B:539:TYR:CZ	1:B:541:GLY:HA3	2.56	0.40
5:C:1004:TPP:HN42	5:C:1004:TPP:C2	2.34	0.40
1:C:269:MET:HE1	1:C:273:VAL:HG21	2.03	0.40
1:D:338:ARG:HG3	1:D:674:TYR:HE2	1.86	0.40
1:A:188:ARG:NH2	1:A:442:ASP:OD2	2.54	0.40
1:B:194:GLY:O	1:B:196:PRO:HD3	2.20	0.40
1:C:545:ASP:N	1:C:545:ASP:OD1	2.52	0.40
1:C:819:ARG:O	1:C:843:VAL:HA	2.22	0.40
1:C:828:TYR:CG	1:C:847:ARG:HD2	2.56	0.40
1:A:301:HIS:NE2	6:A:1005:DW3:O01	2.35	0.40
1:A:245:LEU:HG	1:A:437:THR:HG23	2.02	0.40
1:A:414:ILE:O	1:A:417:MET:HG2	2.21	0.40
1:D:188:ARG:NH1	7:D:1157:HOH:O	2.55	0.40
1:D:806:ILE:HB	1:D:847:ARG:HB2	2.03	0.40
1:D:889:GLN:O	1:D:893:ARG:HG3	2.21	0.40
1:D:830:ASP:HB3	1:D:929:ILE:CD1	2.52	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	833/886 (94%)	805 (97%)	28 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	831/886 (94%)	803 (97%)	28 (3%)	0	100	100
1	C	833/886 (94%)	805 (97%)	28 (3%)	0	100	100
1	D	830/886 (94%)	801 (96%)	29 (4%)	0	100	100
All	All	3327/3544 (94%)	3214 (97%)	113 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	706/745 (95%)	694 (98%)	12 (2%)	60	74
1	B	704/745 (94%)	690 (98%)	14 (2%)	55	70
1	C	706/745 (95%)	690 (98%)	16 (2%)	50	65
1	D	703/745 (94%)	687 (98%)	16 (2%)	50	65
All	All	2819/2980 (95%)	2761 (98%)	58 (2%)	53	68

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	204	ARG
1	A	236	ASP
1	A	268	ASN
1	A	274	LEU
1	A	397	PHE
1	A	557	LEU
1	A	598	MET
1	A	602	LEU
1	A	691	ASP
1	A	863	ILE
1	A	923	LYS
1	B	151	THR

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Mol	Chain	Res	Type
1	B	162	LYS
1	B	236	ASP
1	B	268	ASN
1	B	288	LYS
1	B	351	LYS
1	B	397	PHE
1	B	436	VAL
1	B	540	LEU
1	B	594	LEU
1	B	662	LEU
1	B	691	ASP
1	B	863	ILE
1	B	922	LEU
1	C	188	ARG
1	C	199	ASP
1	C	204	ARG
1	C	236	ASP
1	C	268	ASN
1	C	274	LEU
1	C	397	PHE
1	C	408	THR
1	C	436	VAL
1	C	475	LEU
1	C	588	THR
1	C	602	LEU
1	C	662	LEU
1	C	691	ASP
1	C	820	VAL
1	C	863	ILE
1	D	115	LEU
1	D	121	VAL
1	D	151	THR
1	D	189	LEU
1	D	236	ASP
1	D	268	ASN
1	D	344	LEU
1	D	351	LYS
1	D	397	PHE
1	D	436	VAL
1	D	556	ARG
1	D	557	LEU
1	D	662	LEU

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Mol	Chain	Res	Type
1	D	663	SER
1	D	691	ASP
1	D	843	VAL

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

Mol	Chain	Res	Type
1	D	889	GLN

### 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](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\# Z  > 2$
5	TPP	D	1004	4	22,27,27	1.64	5 (22%)	29,40,40	1.89	8 (27%)
2	P6G	A	1001	-	18,18,18	0.54	0	17,17,17	0.25	0
5	TPP	B	1004	4	22,27,27	1.63	5 (22%)	29,40,40	1.85	8 (27%)
5	TPP	A	1004	4	22,27,27	1.64	5 (22%)	29,40,40	1.85	8 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TPP	C	1004	4	22,27,27	1.69	5 (22%)	29,40,40	1.93	8 (27%)
6	DW3	D	1001	-	3,3,3	0.90	0	2,2,2	2.50	2 (100%)
6	DW3	B	1005	-	3,3,3	1.17	0	2,2,2	4.10	2 (100%)
6	DW3	D	1005	-	3,3,3	0.80	0	2,2,2	2.31	1 (50%)
6	DW3	B	1001	-	3,3,3	0.59	0	2,2,2	1.36	0
6	DW3	C	1006	-	3,3,3	0.78	0	2,2,2	1.78	1 (50%)
6	DW3	A	1006	-	3,3,3	0.57	0	2,2,2	1.29	0
6	DW3	A	1005	-	3,3,3	1.28	0	2,2,2	3.21	2 (100%)
6	DW3	C	1005	-	3,3,3	0.47	0	2,2,2	3.37	2 (100%)
2	P6G	B	1002	-	18,18,18	0.54	0	17,17,17	0.22	0
2	P6G	D	1002	-	18,18,18	0.54	0	17,17,17	0.25	0
2	P6G	C	1001	-	18,18,18	0.54	0	17,17,17	0.24	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
5	TPP	D	1004	4	-	1/16/17/17	0/2/2/2
2	P6G	A	1001	-	-	7/16/16/16	-
5	TPP	B	1004	4	-	4/16/17/17	0/2/2/2
5	TPP	A	1004	4	-	4/16/17/17	0/2/2/2
5	TPP	C	1004	4	-	0/16/17/17	0/2/2/2
6	DW3	D	1001	-	-	0/0/1/1	-
6	DW3	B	1005	-	-	0/0/1/1	-
6	DW3	D	1005	-	-	0/0/1/1	-
6	DW3	B	1001	-	-	0/0/1/1	-
6	DW3	C	1006	-	-	0/0/1/1	-
6	DW3	A	1006	-	-	0/0/1/1	-
6	DW3	A	1005	-	-	0/0/1/1	-
6	DW3	C	1005	-	-	0/0/1/1	-
2	P6G	B	1002	-	-	7/16/16/16	-
2	P6G	D	1002	-	-	8/16/16/16	-
2	P6G	C	1001	-	-	7/16/16/16	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1004	TPP	C4-N3	-4.92	1.35	1.39
5	A	1004	TPP	C4-N3	-4.71	1.35	1.39
5	D	1004	TPP	C4-N3	-4.63	1.35	1.39
5	B	1004	TPP	C4-N3	-4.54	1.35	1.39
5	D	1004	TPP	C2'-N1'	2.51	1.38	1.34
5	D	1004	TPP	C2'-N3'	2.51	1.38	1.34
5	C	1004	TPP	C2'-N3'	2.51	1.38	1.34
5	C	1004	TPP	C2'-N1'	2.50	1.38	1.34
5	B	1004	TPP	C2'-N1'	2.50	1.38	1.34
5	A	1004	TPP	C2'-N1'	2.49	1.38	1.34
5	A	1004	TPP	C2'-N3'	2.47	1.38	1.34
5	A	1004	TPP	C4'-N3'	2.45	1.38	1.35
5	C	1004	TPP	C4'-N3'	2.45	1.38	1.35
5	B	1004	TPP	C4'-N3'	2.45	1.38	1.35
5	B	1004	TPP	C2'-N3'	2.44	1.38	1.34
5	D	1004	TPP	C4'-N3'	2.44	1.38	1.35
5	B	1004	TPP	C7'-N3	-2.20	1.44	1.48
5	D	1004	TPP	C7'-N3	-2.18	1.44	1.48
5	C	1004	TPP	C7'-N3	-2.17	1.44	1.48
5	A	1004	TPP	C7'-N3	-2.12	1.44	1.48

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1004	TPP	C6-C5-C4	6.29	132.48	127.43
5	D	1004	TPP	C6-C5-C4	5.88	132.15	127.43
5	A	1004	TPP	C6-C5-C4	5.68	131.99	127.43
5	B	1004	TPP	C6-C5-C4	5.35	131.73	127.43
6	B	1005	DW3	O04-C03-C02	-4.47	100.79	110.79
6	C	1005	DW3	O01-C02-C03	-3.78	114.47	125.42
6	B	1005	DW3	O01-C02-C03	-3.70	114.72	125.42
6	A	1005	DW3	O04-C03-C02	-3.62	102.69	110.79
6	D	1005	DW3	O01-C02-C03	-3.26	115.99	125.42
5	C	1004	TPP	N1'-C2'-N3'	-3.24	119.96	125.54
5	D	1004	TPP	N1'-C2'-N3'	-3.21	120.01	125.54
5	A	1004	TPP	N1'-C2'-N3'	-3.21	120.02	125.54
5	B	1004	TPP	N1'-C2'-N3'	-3.17	120.09	125.54
5	C	1004	TPP	PA-O3A-PB	-2.99	122.56	132.83
6	D	1001	DW3	O01-C02-C03	-2.90	117.02	125.42
6	C	1005	DW3	O04-C03-C02	-2.90	104.30	110.79
5	D	1004	TPP	PA-O3A-PB	-2.80	123.21	132.83
5	B	1004	TPP	PA-O3A-PB	-2.79	123.25	132.83
5	B	1004	TPP	C6'-C5'-C4'	2.74	119.45	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1005	DW3	O01-C02-C03	-2.73	117.51	125.42
5	D	1004	TPP	C6'-C5'-C4'	2.71	119.40	115.72
5	C	1004	TPP	C6'-C5'-C4'	2.71	119.40	115.72
5	D	1004	TPP	CM2-C2'-N1'	2.66	120.06	117.14
5	A	1004	TPP	CM2-C2'-N1'	2.66	120.06	117.14
5	A	1004	TPP	C6'-C5'-C4'	2.66	119.34	115.72
5	A	1004	TPP	PA-O3A-PB	-2.64	123.78	132.83
5	B	1004	TPP	CM4-C4-N3	2.61	125.86	122.53
5	B	1004	TPP	CM2-C2'-N1'	2.58	119.98	117.14
5	C	1004	TPP	CM2-C2'-N1'	2.49	119.87	117.14
5	D	1004	TPP	C6'-N1'-C2'	2.46	120.15	115.96
5	C	1004	TPP	C6'-N1'-C2'	2.45	120.14	115.96
5	D	1004	TPP	CM4-C4-N3	2.44	125.64	122.53
5	B	1004	TPP	C6'-N1'-C2'	2.43	120.09	115.96
5	A	1004	TPP	C6'-N1'-C2'	2.42	120.08	115.96
6	C	1006	DW3	O04-C03-C02	2.29	115.92	110.79
5	A	1004	TPP	CM4-C4-N3	2.23	125.37	122.53
5	D	1004	TPP	C5'-C6'-N1'	-2.17	120.21	123.82
5	B	1004	TPP	C5'-C6'-N1'	-2.16	120.23	123.82
5	A	1004	TPP	C5'-C6'-N1'	-2.12	120.28	123.82
5	C	1004	TPP	C5'-C6'-N1'	-2.12	120.29	123.82
5	C	1004	TPP	CM4-C4-N3	2.12	125.23	122.53
6	D	1001	DW3	O04-C03-C02	-2.01	106.29	110.79

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1004	TPP	PA-O3A-PB-O2B
5	A	1004	TPP	PA-O3A-PB-O2B
2	D	1002	P6G	O13-C14-C15-O16
2	C	1001	P6G	O10-C11-C12-O13
2	A	1001	P6G	O13-C14-C15-O16
2	B	1002	P6G	O1-C2-C3-O4
2	D	1002	P6G	O1-C2-C3-O4
2	A	1001	P6G	O10-C11-C12-O13
2	D	1002	P6G	O7-C8-C9-O10
2	A	1001	P6G	O4-C5-C6-O7
2	B	1002	P6G	O7-C8-C9-O10
2	C	1001	P6G	O1-C2-C3-O4
2	A	1001	P6G	O16-C17-C18-O19
2	C	1001	P6G	O7-C8-C9-O10

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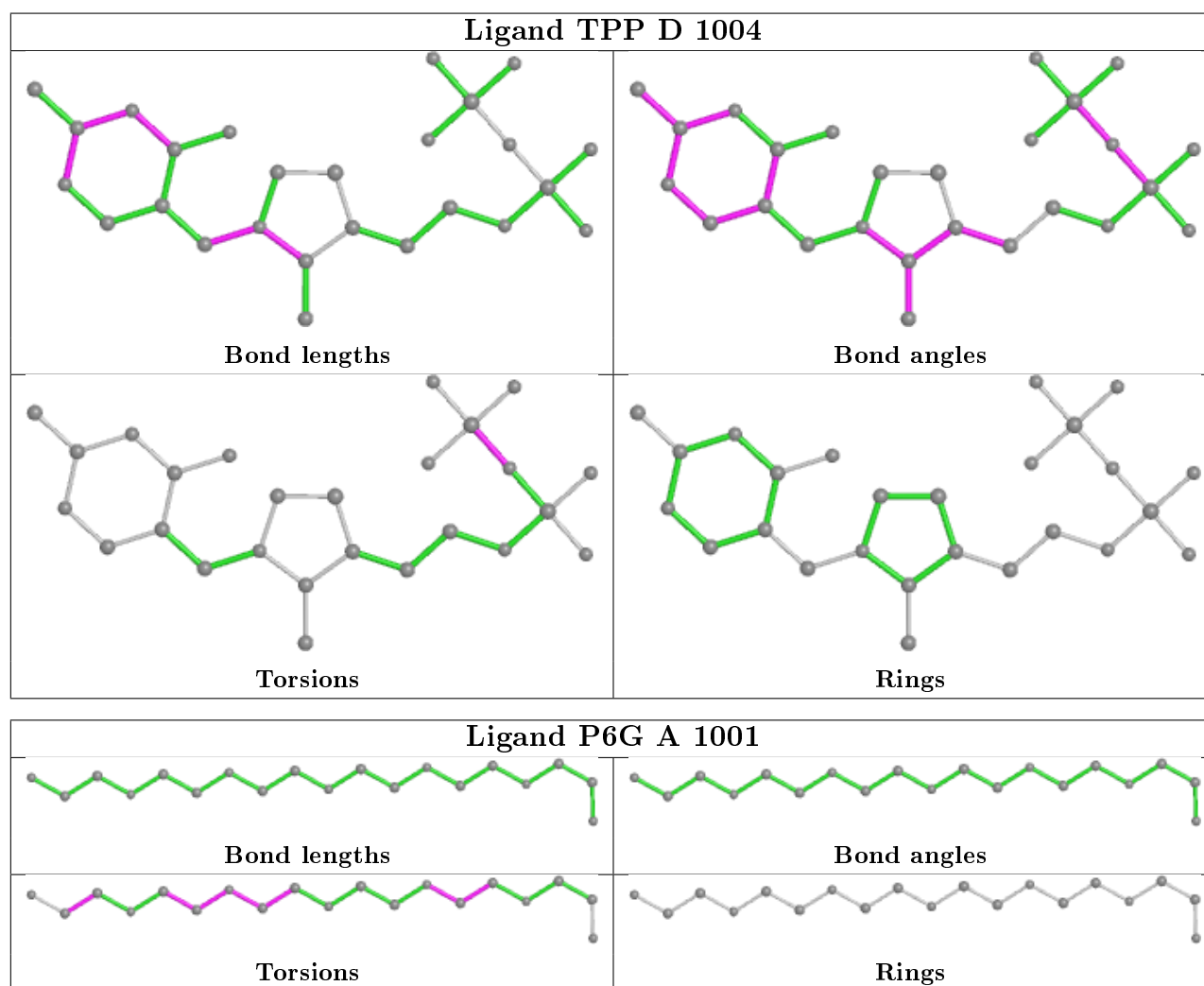
Mol	Chain	Res	Type	Atoms
2	B	1002	P6G	O10-C11-C12-O13
2	C	1001	P6G	C2-C3-O4-C5
2	C	1001	P6G	C12-C11-O10-C9
2	A	1001	P6G	C5-C6-O7-C8
2	B	1002	P6G	C8-C9-O10-C11
5	B	1004	TPP	PA-O3A-PB-O3B
2	D	1002	P6G	C5-C6-O7-C8
2	A	1001	P6G	C11-C12-O13-C14
2	B	1002	P6G	O13-C14-C15-O16
2	D	1002	P6G	C11-C12-O13-C14
2	C	1001	P6G	O16-C17-C18-O19
2	D	1002	P6G	C15-C14-O13-C12
2	B	1002	P6G	C5-C6-O7-C8
2	C	1001	P6G	C15-C14-O13-C12
5	A	1004	TPP	PA-O3A-PB-O1B
2	B	1002	P6G	C11-C12-O13-C14
2	A	1001	P6G	C15-C14-O13-C12
2	D	1002	P6G	O4-C5-C6-O7
5	B	1004	TPP	PA-O3A-PB-O1B
5	D	1004	TPP	PA-O3A-PB-O3B
5	A	1004	TPP	PA-O3A-PB-O3B
5	B	1004	TPP	C7-O7-PA-O1A
5	A	1004	TPP	C7-O7-PA-O1A
2	D	1002	P6G	O10-C11-C12-O13

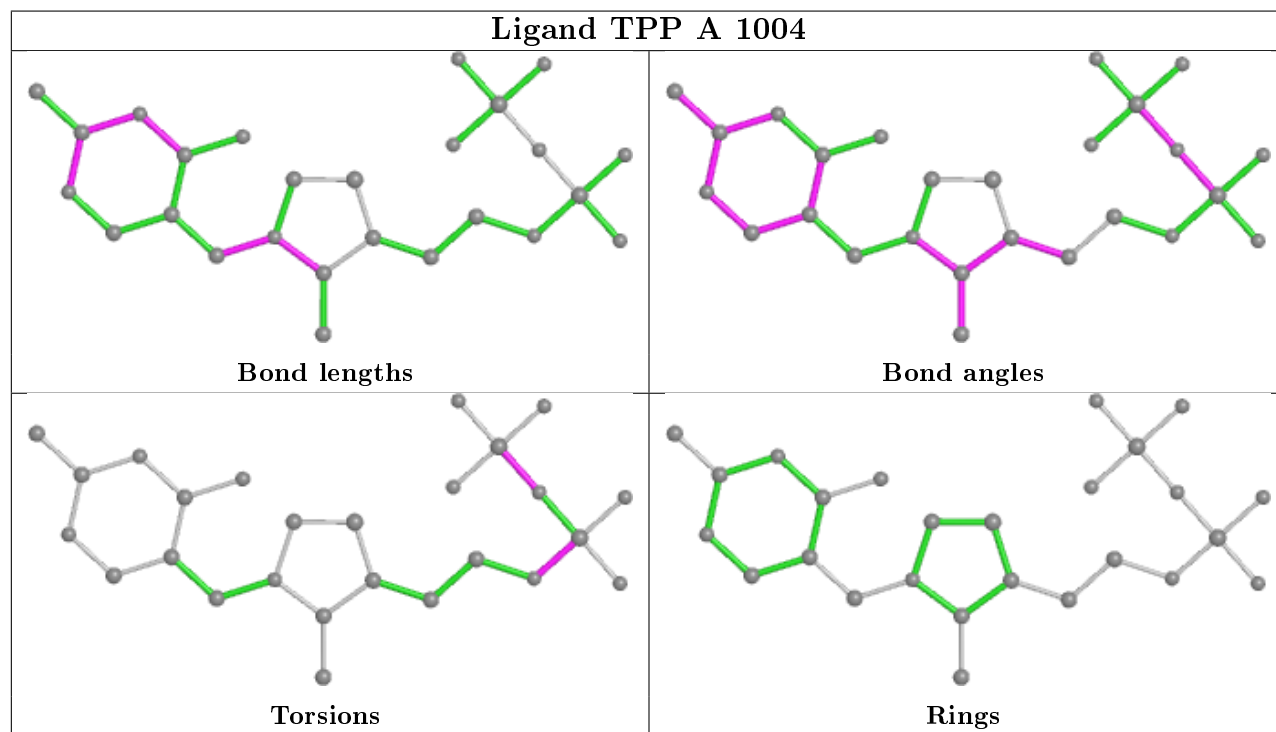
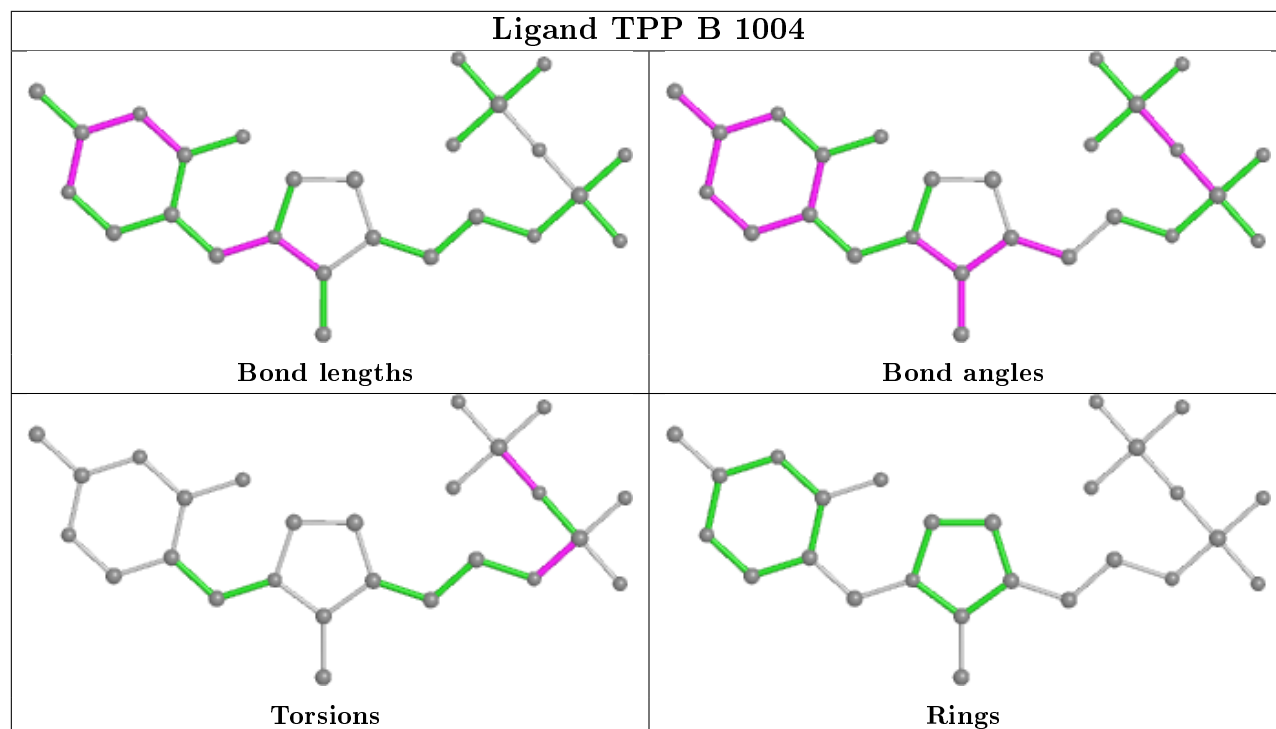
There are no ring outliers.

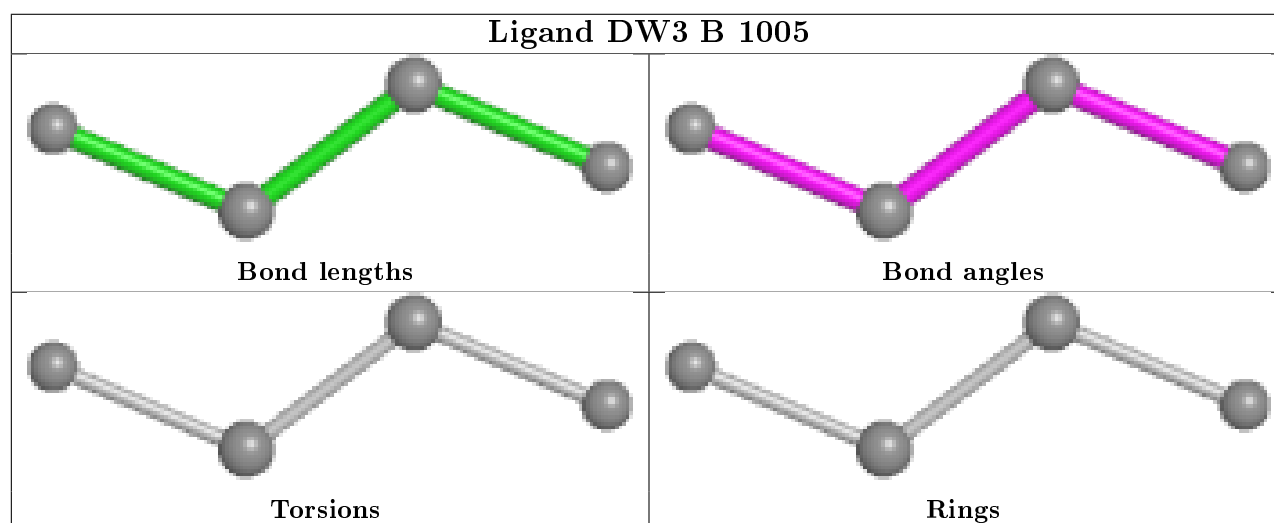
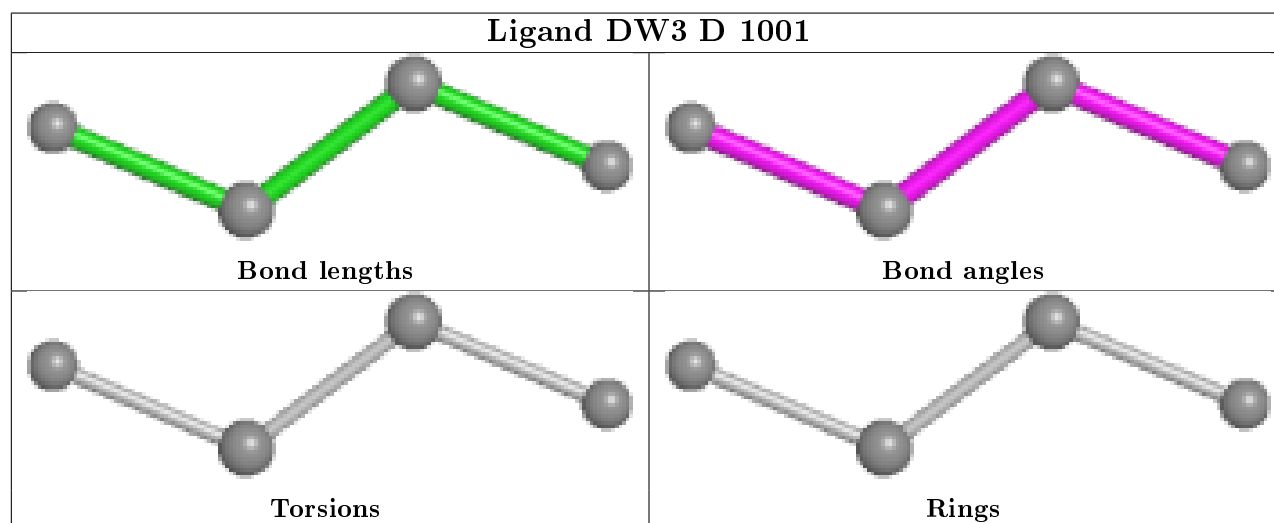
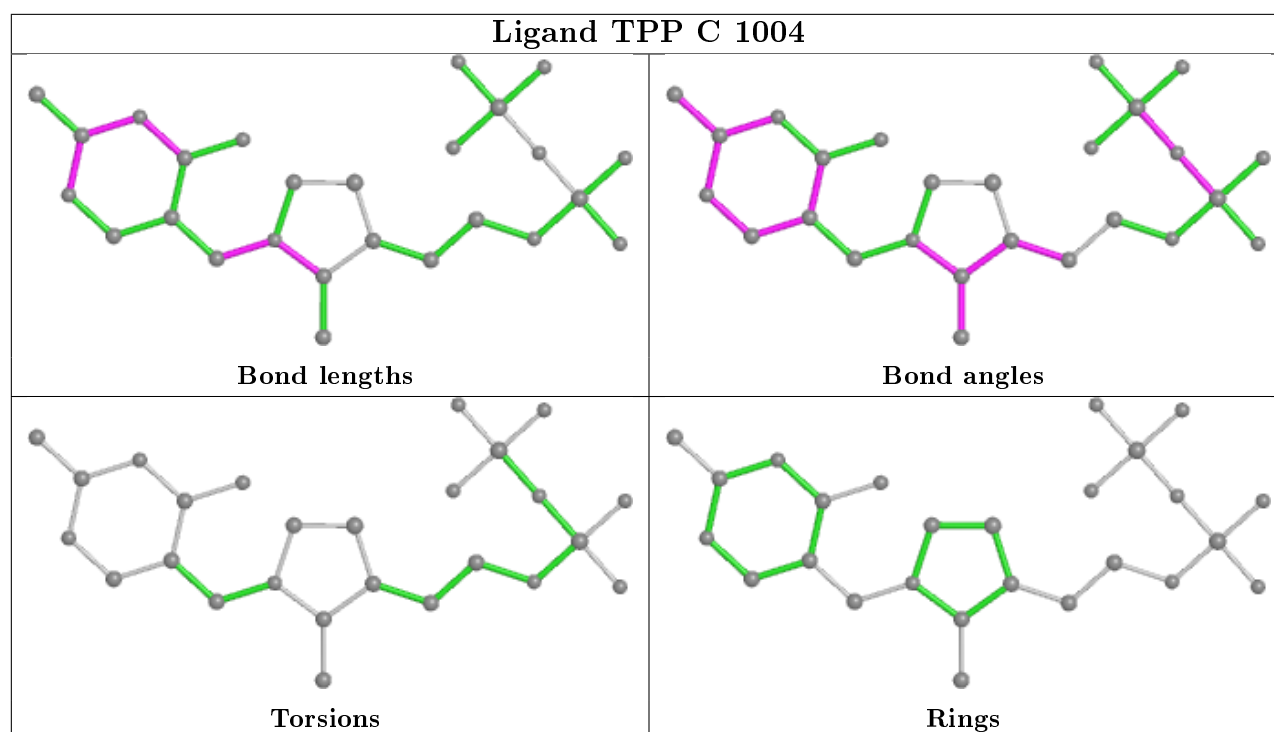
12 monomers are involved in 26 short contacts:

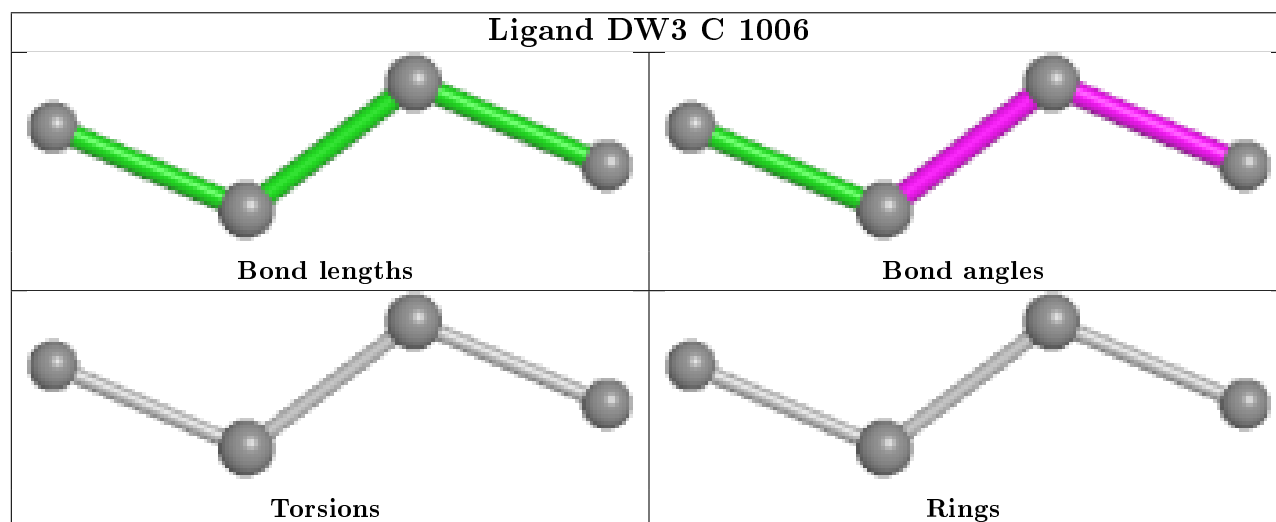
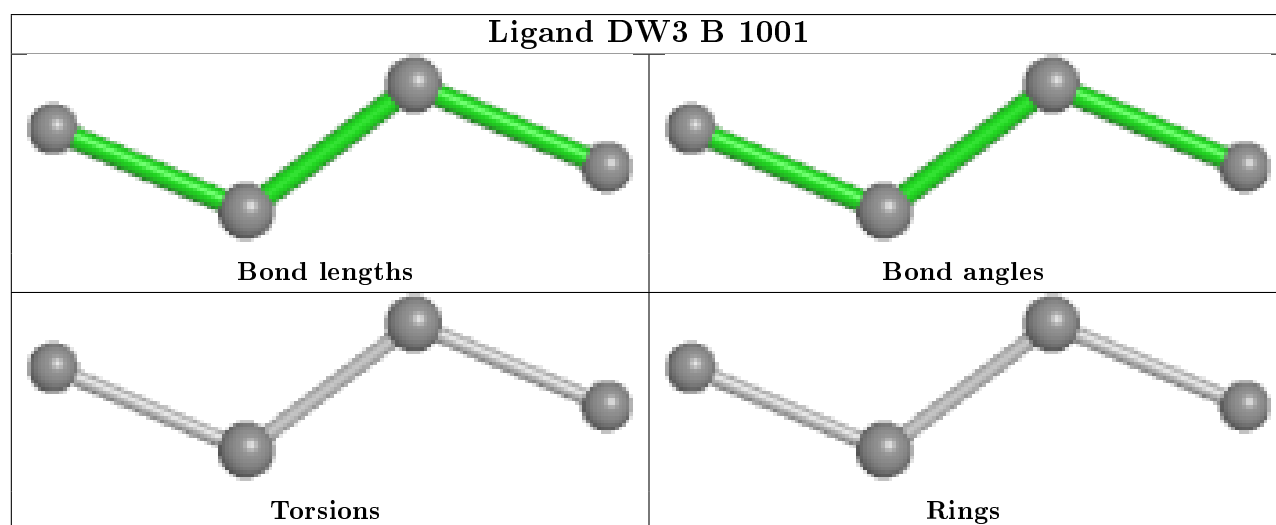
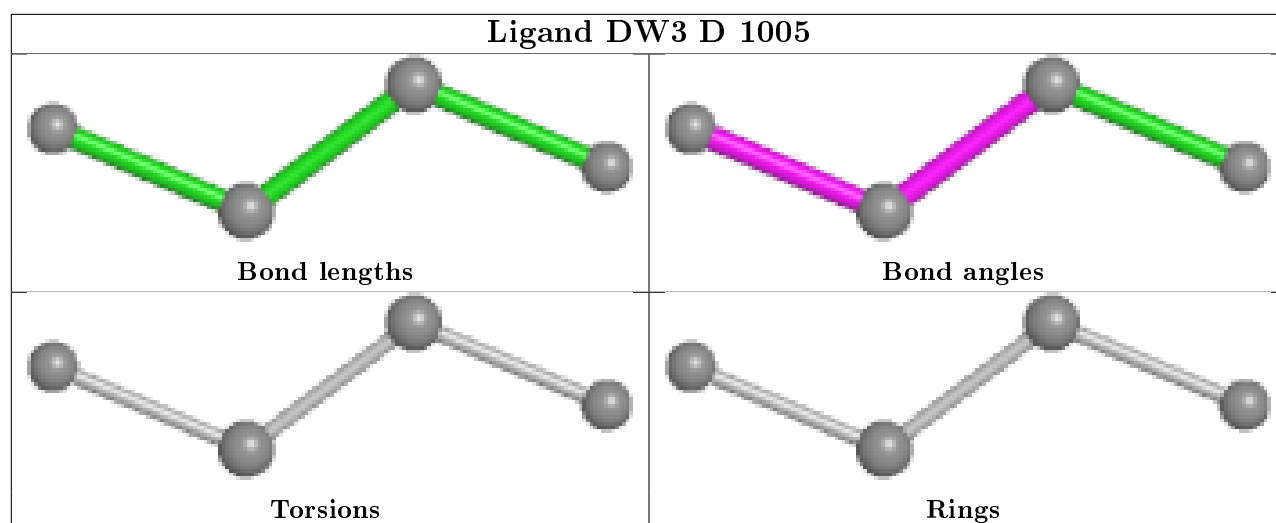
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1004	TPP	3	0
2	A	1001	P6G	1	0
5	B	1004	TPP	1	0
5	C	1004	TPP	4	0
6	D	1001	DW3	2	0
6	B	1005	DW3	3	0
6	D	1005	DW3	2	0
6	A	1005	DW3	2	0
6	C	1005	DW3	2	0
2	B	1002	P6G	1	0
2	D	1002	P6G	3	0
2	C	1001	P6G	3	0

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

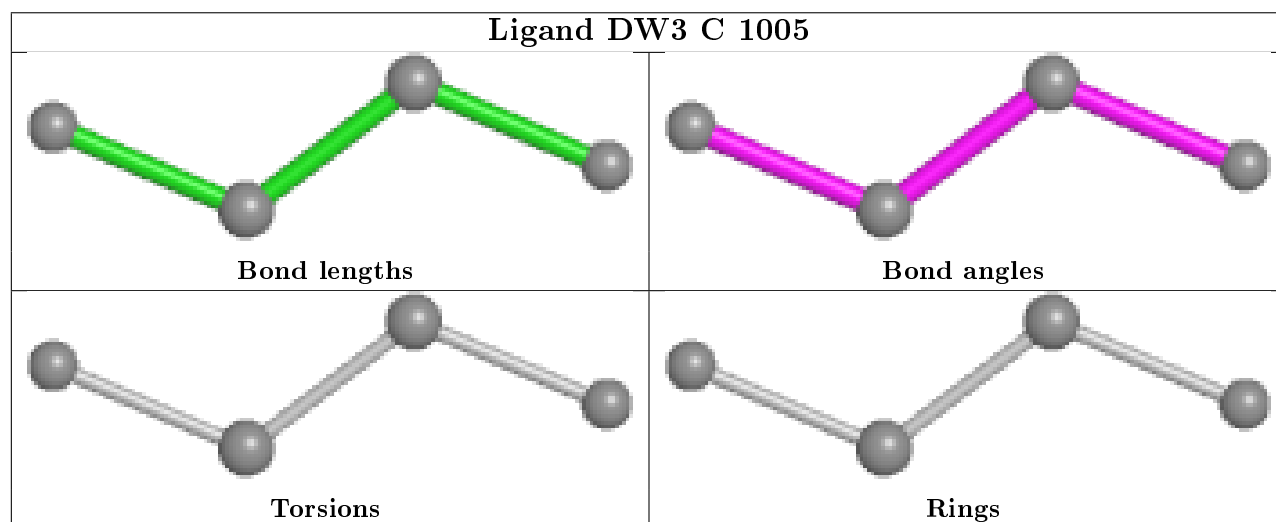
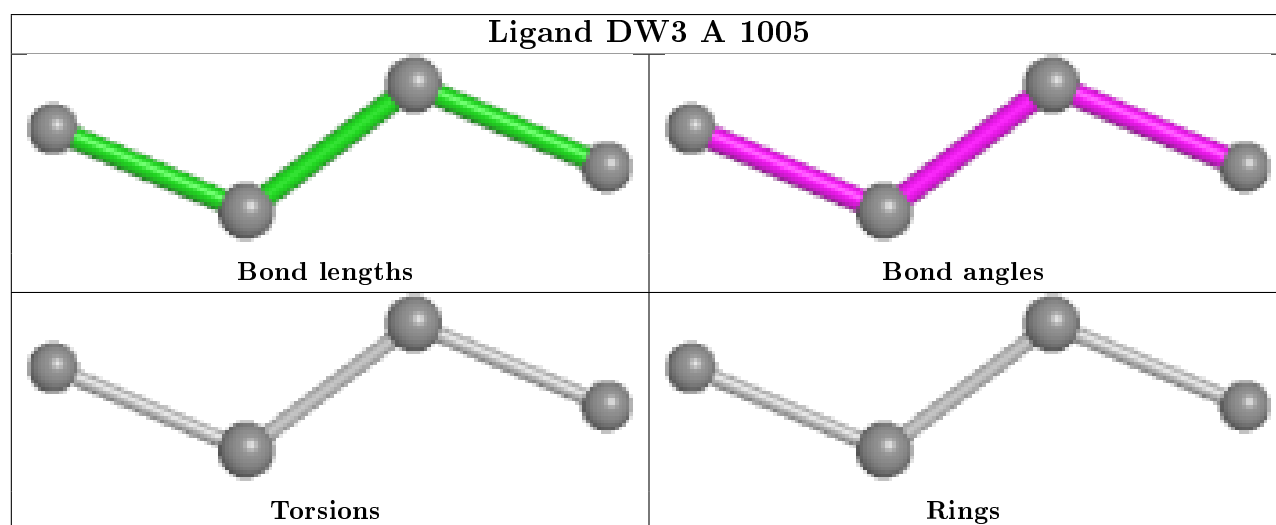
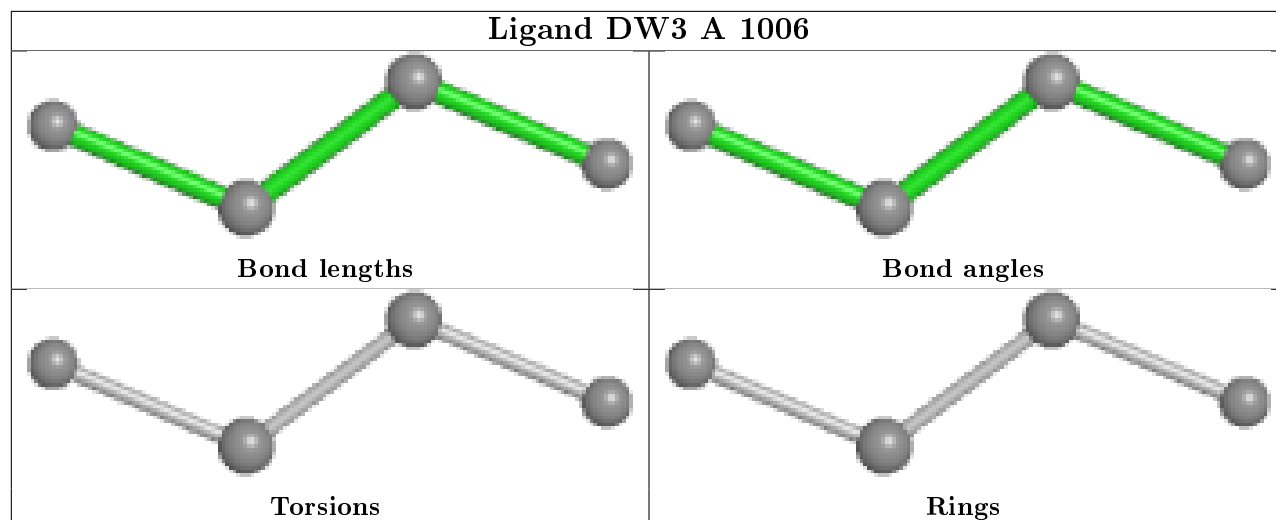


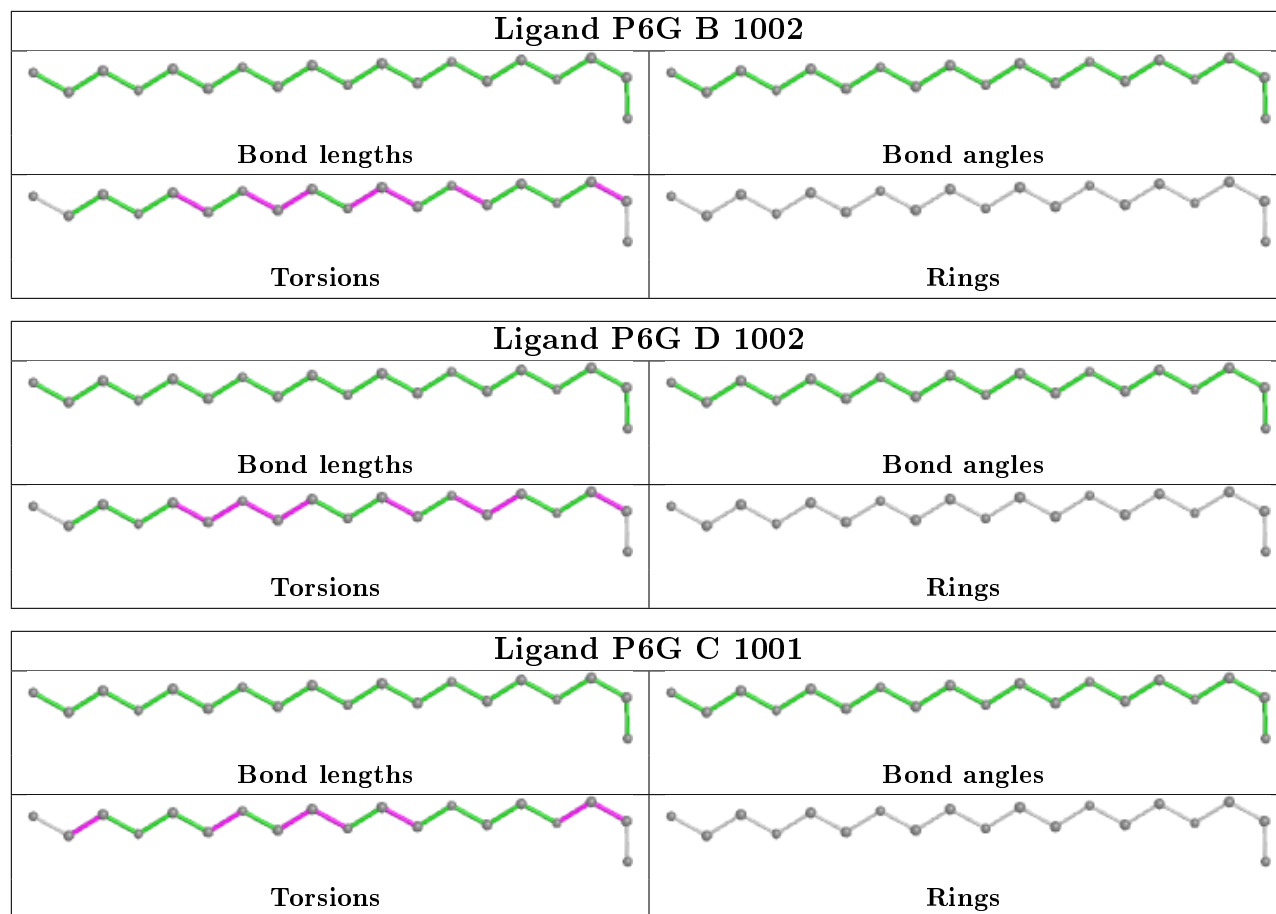












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	839/886 (94%)	0.34	45 (5%) 25 31	18, 33, 65, 100	0
1	B	837/886 (94%)	0.23	33 (3%) 39 44	19, 33, 58, 80	0
1	C	839/886 (94%)	0.33	46 (5%) 25 30	18, 33, 66, 87	0
1	D	836/886 (94%)	0.32	46 (5%) 25 30	21, 34, 61, 88	0
All	All	3351/3544 (94%)	0.30	170 (5%) 28 33	18, 33, 62, 100	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	VAL	5.5
1	B	899	GLY	5.5
1	A	811	GLU	5.1
1	A	293	TRP	4.9
1	A	812	LEU	4.4
1	D	867	VAL	4.4
1	B	864	ALA	4.3
1	B	901	GLU	4.2
1	D	530	ALA	3.9
1	D	897	PRO	3.9
1	B	530	ALA	3.8
1	C	116	TRP	3.8
1	A	289	HIS	3.8
1	B	117	GLN	3.8
1	A	86	VAL	3.7
1	B	861	ALA	3.6
1	D	287	GLY	3.6
1	C	901	GLU	3.6
1	C	293	TRP	3.6
1	A	288	LYS	3.5
1	A	87	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	900	THR	3.4
1	C	693	ALA	3.4
1	A	898	ALA	3.4
1	A	140	PHE	3.3
1	C	871	ASP	3.3
1	A	137	GLU	3.3
1	A	116	TRP	3.3
1	B	898	ALA	3.3
1	A	226	GLY	3.2
1	D	288	LYS	3.2
1	D	885	TRP	3.2
1	D	666	ALA	3.2
1	D	864	ALA	3.2
1	C	156	ASP	3.2
1	D	861	ALA	3.2
1	A	897	PRO	3.2
1	D	116	TRP	3.1
1	A	194	GLY	3.1
1	C	139	THR	3.1
1	C	867	VAL	3.1
1	D	315	VAL	3.1
1	C	899	GLY	3.1
1	C	136	PHE	3.1
1	C	898	ALA	3.1
1	C	869	VAL	3.0
1	D	863	ILE	3.0
1	D	571	HIS	3.0
1	C	137	GLU	3.0
1	C	582	ASN	3.0
1	B	668	LEU	2.9
1	C	158	TYR	2.9
1	C	132	THR	2.9
1	C	141	ASN	2.9
1	A	865	PRO	2.9
1	A	837	ASN	2.9
1	D	140	PHE	2.9
1	D	370	ALA	2.8
1	D	667	VAL	2.8
1	D	699	VAL	2.8
1	D	898	ALA	2.8
1	D	668	LEU	2.8
1	A	900	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	863	ILE	2.8
1	B	569	GLU	2.8
1	C	786	ARG	2.8
1	C	140	PHE	2.7
1	D	872	PHE	2.7
1	C	131	LEU	2.7
1	A	841	ASP	2.7
1	C	292	SER	2.7
1	A	692	PHE	2.7
1	D	839	GLU	2.7
1	B	293	TRP	2.7
1	A	662	LEU	2.7
1	A	843	VAL	2.7
1	A	569	GLU	2.6
1	C	539	TYR	2.6
1	B	867	VAL	2.6
1	C	843	VAL	2.6
1	D	286	ALA	2.6
1	A	136	PHE	2.6
1	C	287	GLY	2.6
1	D	569	GLU	2.6
1	C	117	GLN	2.6
1	C	794	LEU	2.5
1	D	539	TYR	2.5
1	D	665	GLU	2.5
1	C	864	ALA	2.5
1	A	157	ILE	2.5
1	D	901	GLU	2.5
1	C	837	ASN	2.5
1	B	286	ALA	2.5
1	C	569	GLU	2.5
1	A	863	ILE	2.5
1	B	897	PRO	2.5
1	B	116	TRP	2.5
1	D	592	LYS	2.5
1	B	666	ALA	2.5
1	D	518	HIS	2.5
1	C	692	PHE	2.4
1	B	868	ASN	2.4
1	C	662	LEU	2.4
1	A	933	LEU	2.4
1	D	380	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	519	GLY	2.4
1	C	367	GLY	2.4
1	C	935	VAL	2.4
1	D	900	THR	2.4
1	A	650	ASP	2.4
1	D	158	TYR	2.4
1	B	380	GLY	2.4
1	A	737	LEU	2.4
1	C	152	MET	2.3
1	A	839	GLU	2.3
1	B	863	ILE	2.3
1	A	131	LEU	2.3
1	B	370	ALA	2.3
1	B	127	ALA	2.3
1	D	859	VAL	2.3
1	D	328	ILE	2.3
1	A	639	ALA	2.3
1	C	142	VAL	2.3
1	A	141	ASN	2.3
1	A	117	GLN	2.3
1	B	363	ILE	2.3
1	B	812	LEU	2.2
1	B	859	VAL	2.2
1	B	287	GLY	2.2
1	B	900	THR	2.2
1	D	127	ALA	2.2
1	D	865	PRO	2.2
1	C	821	VAL	2.2
1	A	687	ALA	2.2
1	C	149	GLN	2.2
1	D	493	VAL	2.2
1	D	822	PHE	2.2
1	D	204	ARG	2.2
1	B	591	GLU	2.2
1	A	840	GLN	2.2
1	D	541	GLY	2.2
1	D	368	VAL	2.1
1	C	666	ALA	2.1
1	D	591	GLU	2.1
1	A	530	ALA	2.1
1	B	87	ASP	2.1
1	C	834	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	520	GLU	2.1
1	C	127	ALA	2.1
1	C	868	ASN	2.1
1	D	136	PHE	2.1
1	D	357	ILE	2.1
1	A	668	LEU	2.1
1	B	403	ARG	2.1
1	C	694	ASN	2.1
1	A	149	GLN	2.1
1	B	518	HIS	2.1
1	A	593	GLU	2.1
1	A	693	ALA	2.1
1	A	867	VAL	2.1
1	B	917	TYR	2.1
1	A	138	GLU	2.0
1	A	127	ALA	2.0
1	D	860	LYS	2.0
1	B	328	ILE	2.0
1	D	367	GLY	2.0
1	A	286	ALA	2.0
1	C	530	ALA	2.0
1	D	693	ALA	2.0
1	A	690	GLY	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

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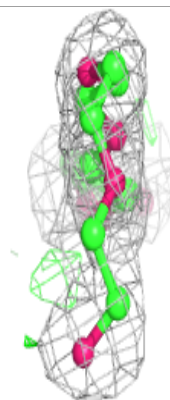
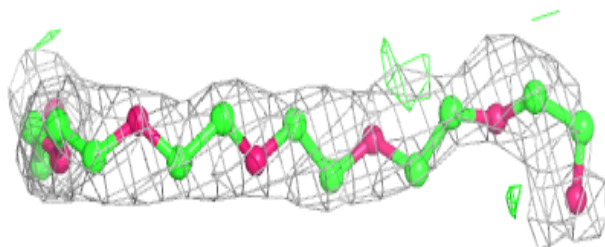
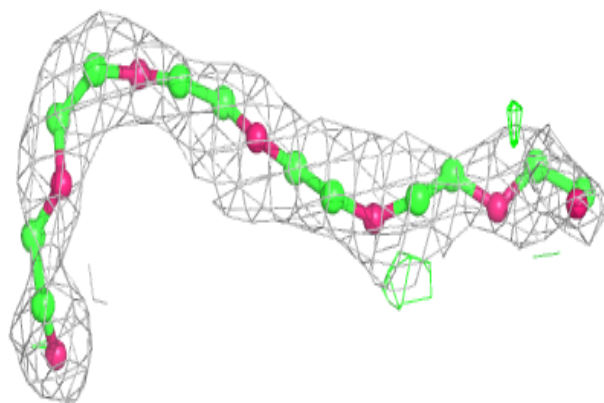
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	P6G	D	1002	19/19	0.73	0.23	51,59,68,68	0
2	P6G	C	1001	19/19	0.78	0.21	53,58,60,60	0
2	P6G	B	1002	19/19	0.84	0.18	42,49,59,59	0
2	P6G	A	1001	19/19	0.86	0.18	60,62,66,66	0
6	DW3	D	1001	4/4	0.89	0.28	61,61,62,62	0
6	DW3	A	1006	4/4	0.90	0.24	42,44,44,45	0
6	DW3	B	1001	4/4	0.91	0.20	56,57,57,58	0
6	DW3	D	1005	4/4	0.91	0.31	53,55,59,64	0
6	DW3	C	1005	4/4	0.92	0.21	54,54,54,54	0
6	DW3	C	1006	4/4	0.92	0.19	37,38,39,40	0
6	DW3	B	1005	4/4	0.94	0.36	52,53,55,58	0
4	MG	C	1003	1/1	0.95	0.21	22,22,22,22	0
6	DW3	A	1005	4/4	0.95	0.20	38,39,43,49	0
5	TPP	C	1004	26/26	0.97	0.14	18,25,30,31	0
4	MG	D	1003	1/1	0.97	0.23	20,20,20,20	0
4	MG	A	1003	1/1	0.98	0.20	19,19,19,19	0
5	TPP	B	1004	26/26	0.98	0.19	22,27,30,30	0
5	TPP	A	1004	26/26	0.98	0.13	22,24,27,28	0
4	MG	B	1003	1/1	0.98	0.21	21,21,21,21	0
3	CA	A	1002	1/1	0.98	0.22	41,41,41,41	0
5	TPP	D	1004	26/26	0.98	0.17	19,26,27,28	0
3	CA	C	1002	1/1	0.99	0.28	44,44,44,44	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.

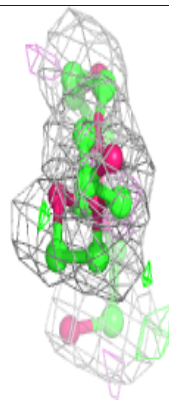
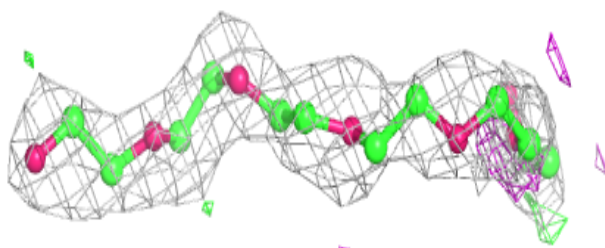
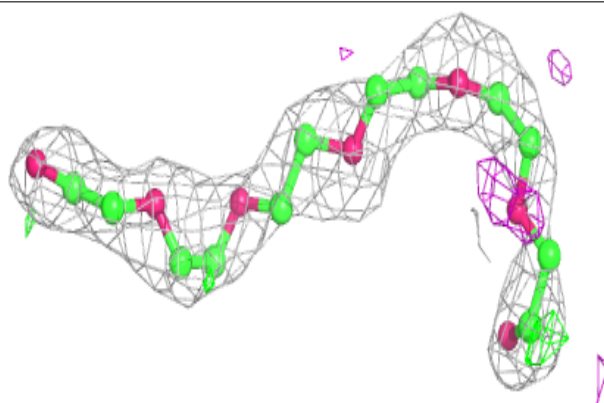


**Electron density around P6G D 1002:**

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

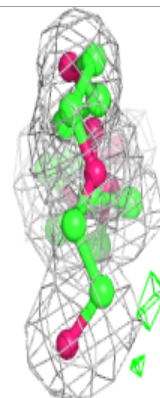
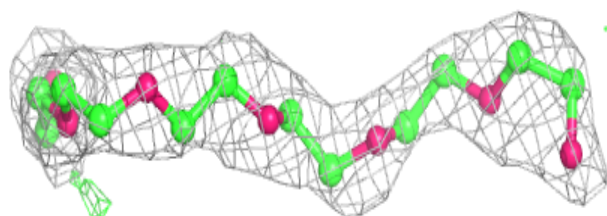
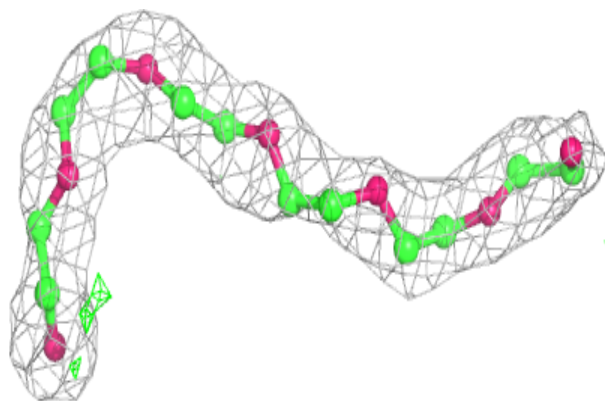
**Electron density around P6G C 1001:**

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

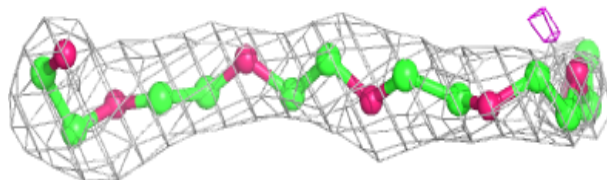
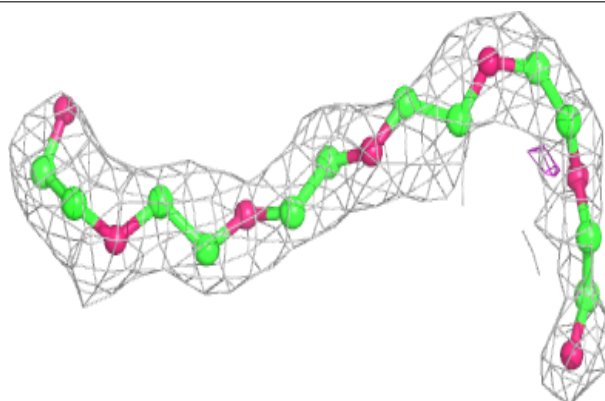


**Electron density around P6G B 1002:**

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

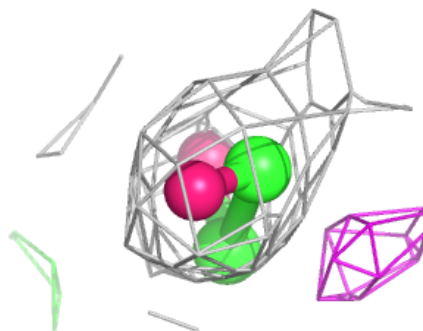
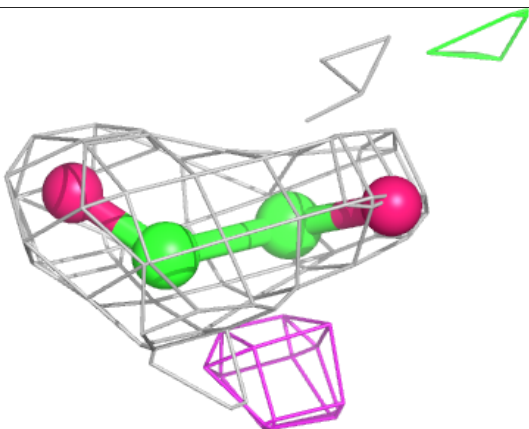
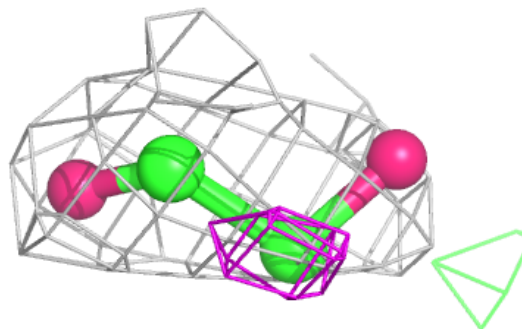
**Electron density around P6G A 1001:**

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



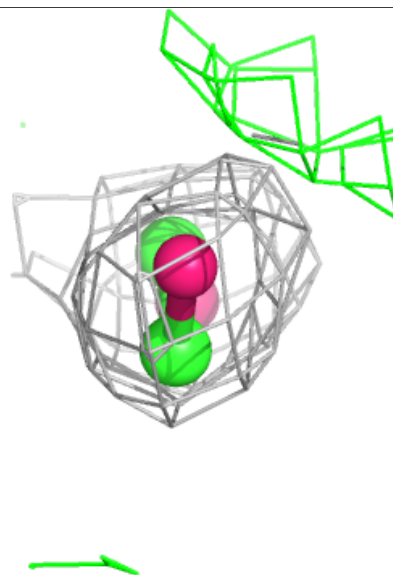
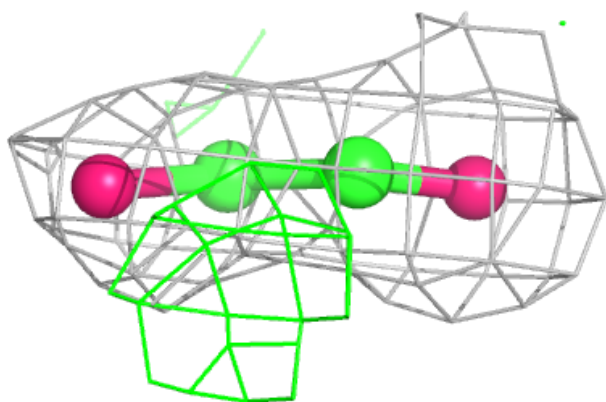
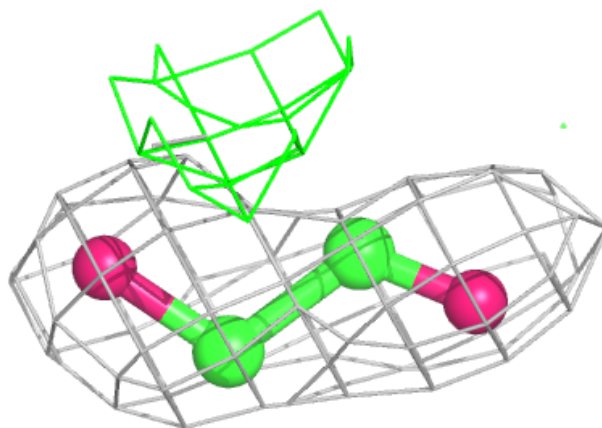
**Electron density around DW3 D 1001:**

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



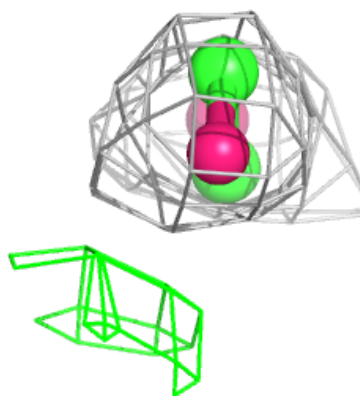
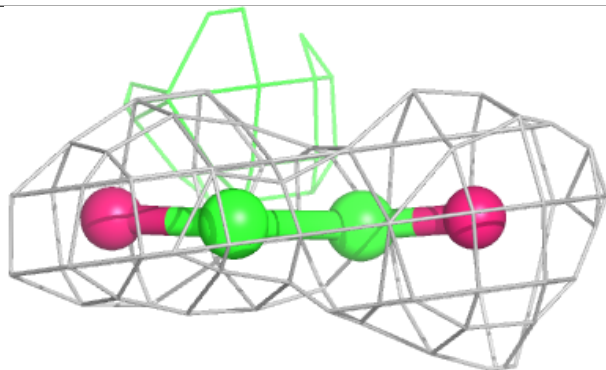
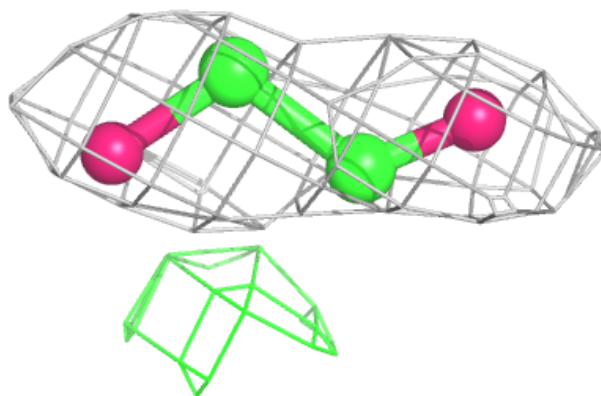
**Electron density around DW3 A 1006:**

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



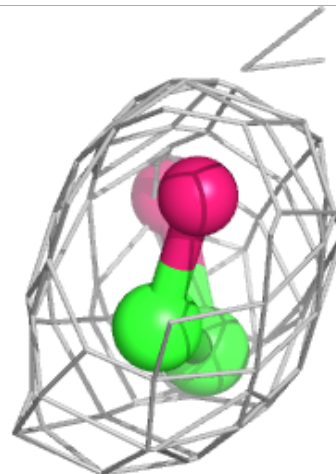
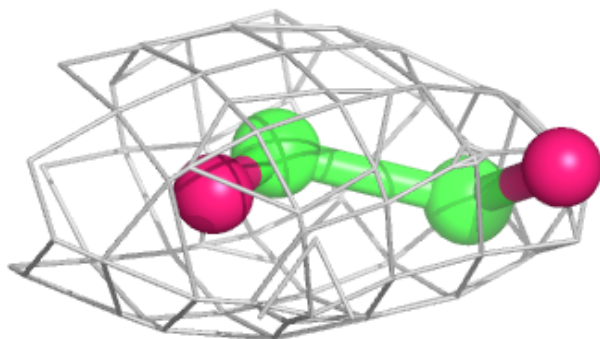
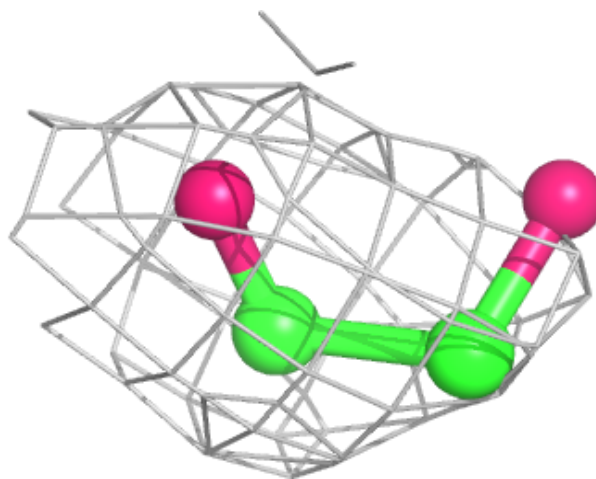
**Electron density around DW3 B 1001:**

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



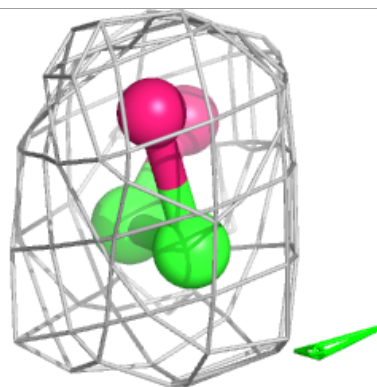
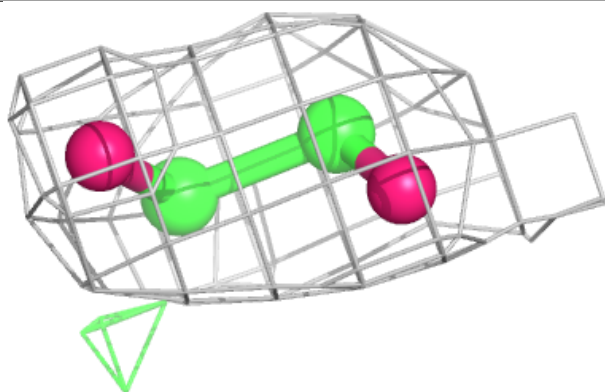
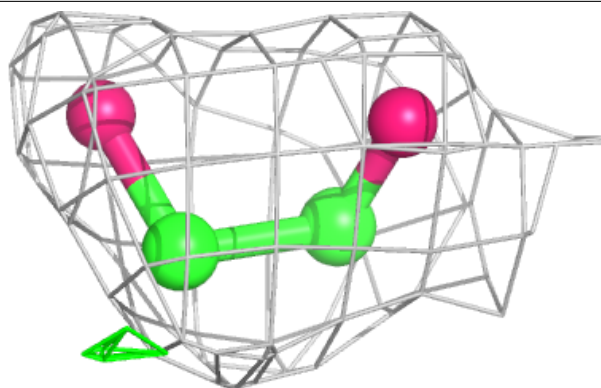
**Electron density around DW3 D 1005:**

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



**Electron density around DW3 C 1005:**

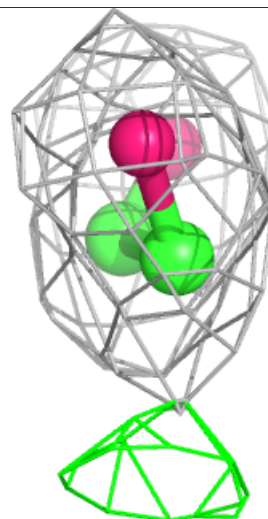
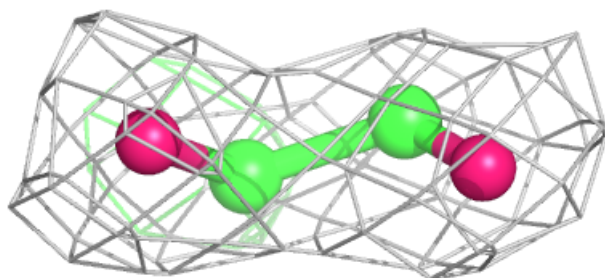
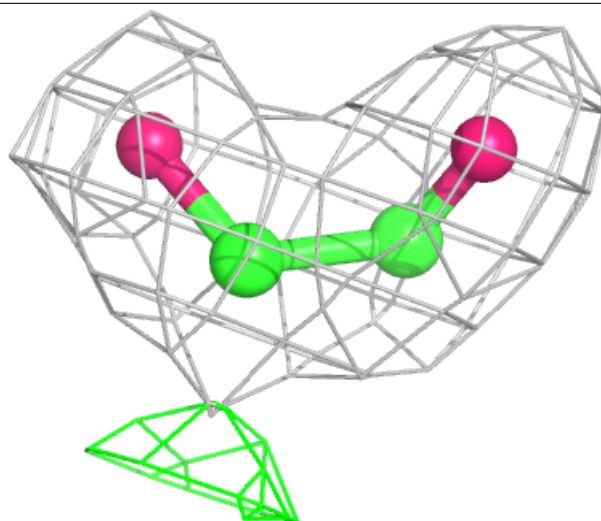
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DW3 C 1006:**

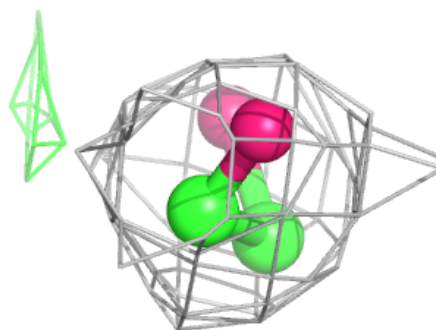
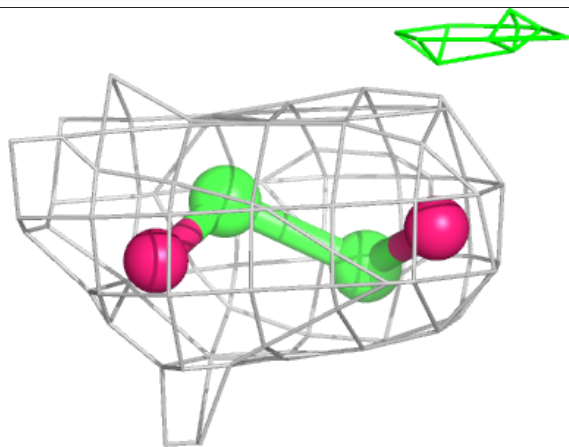
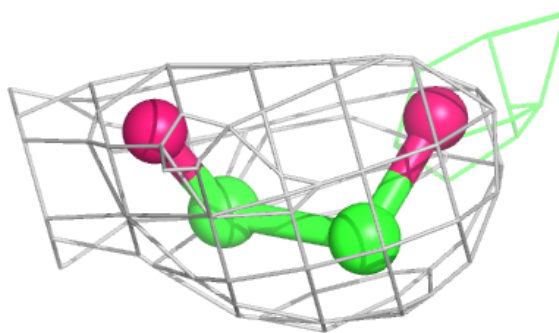
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





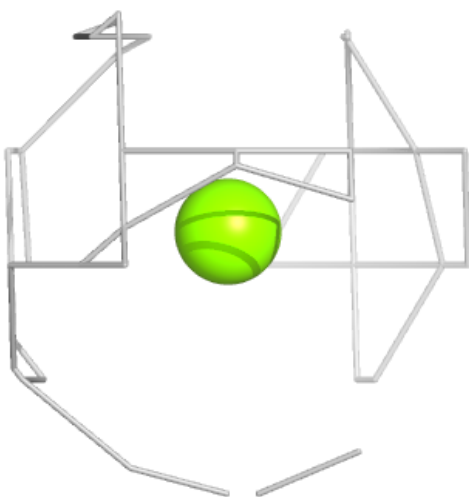
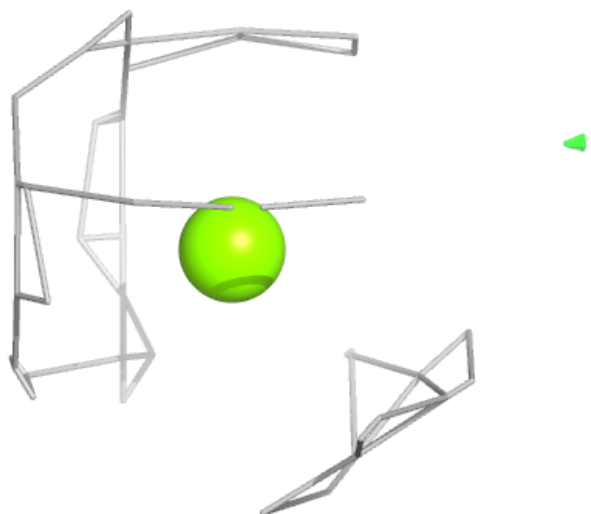
**Electron density around DW3 B 1005:**

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

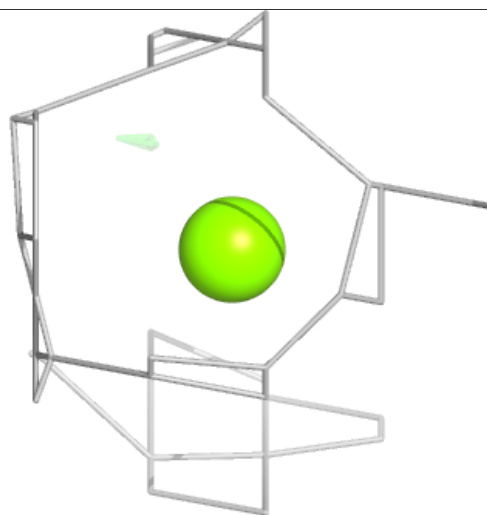


**Electron density around MG C 1003:**

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

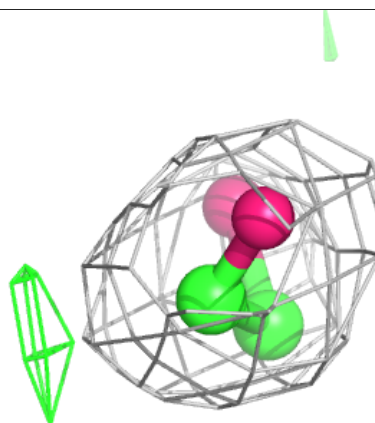
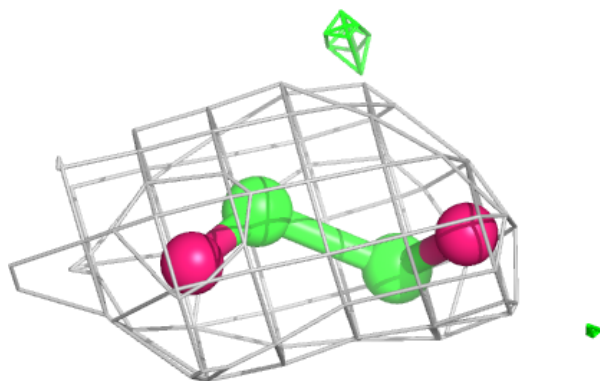
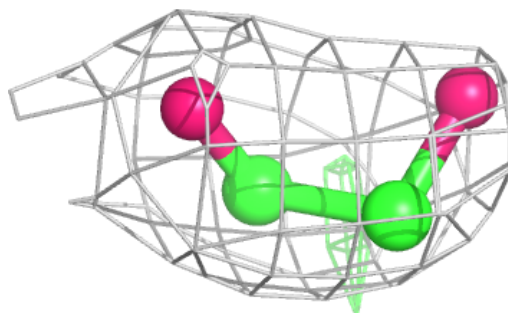


4

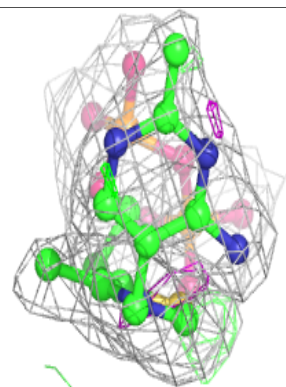
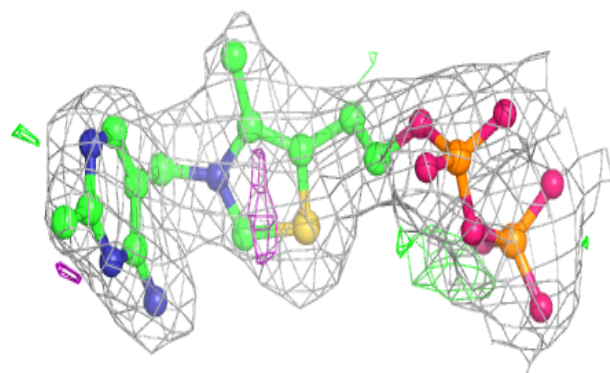
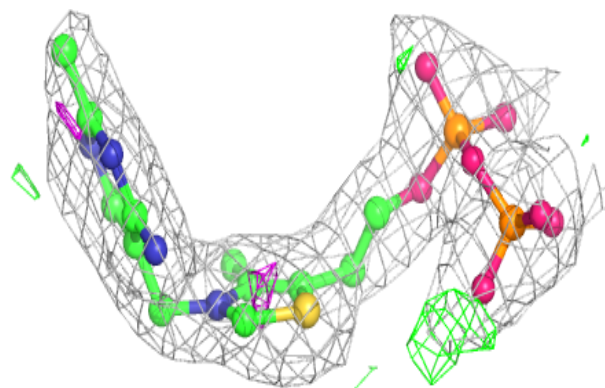


**Electron density around DW3 A 1005:**

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

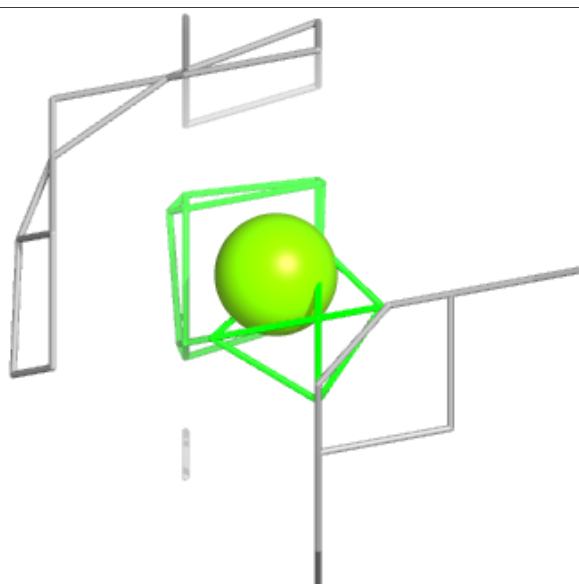
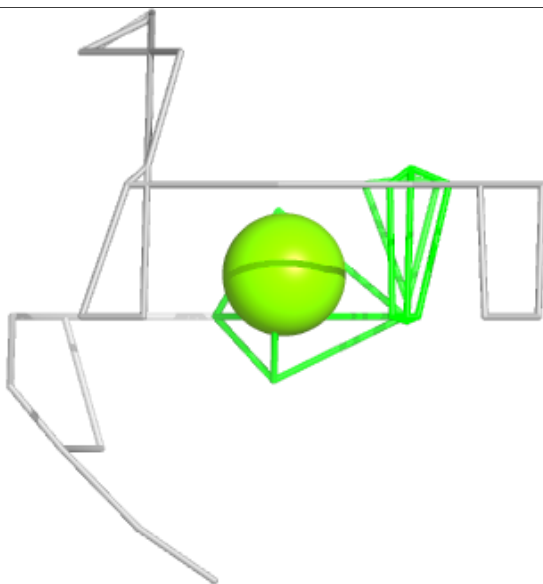
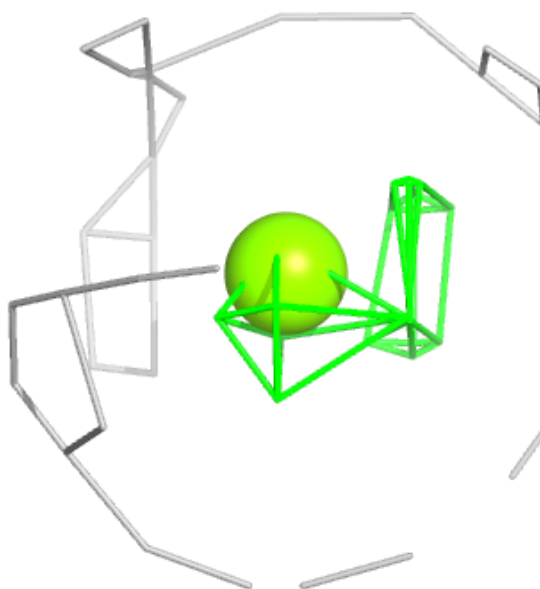
**Electron density around TPP C 1004:**

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



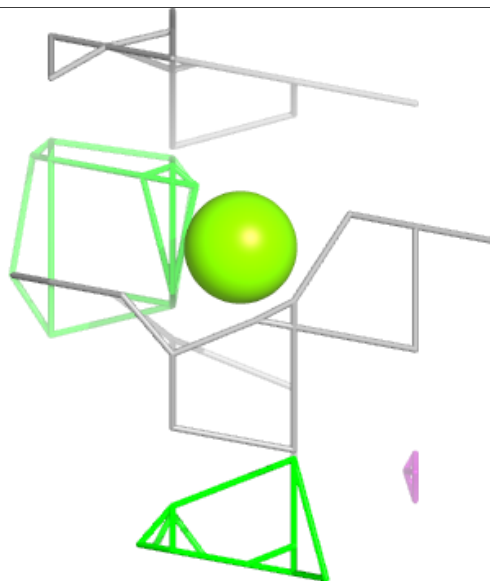
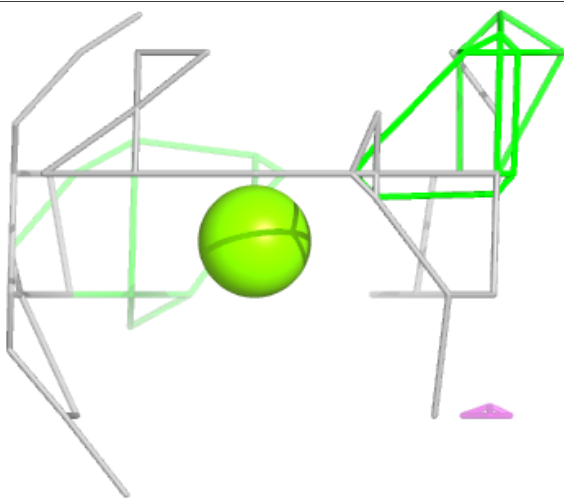
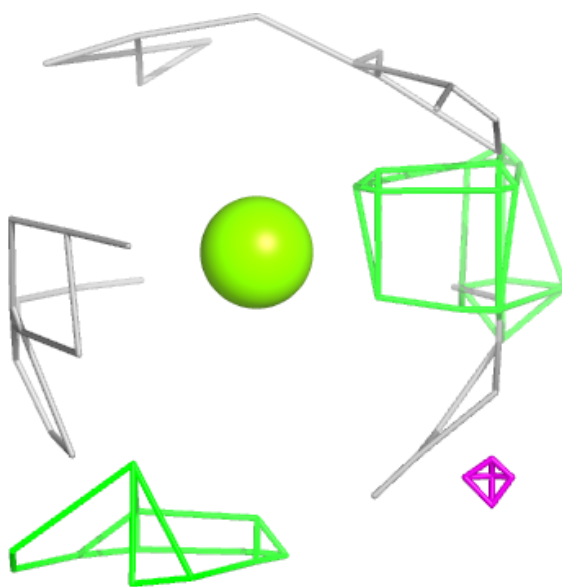
**Electron density around MG D 1003:**

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



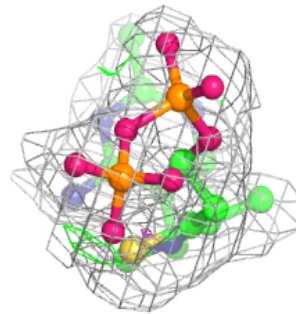
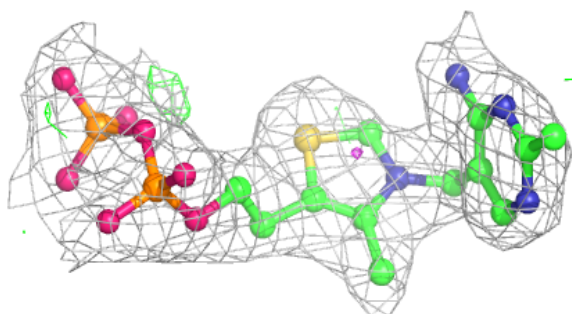
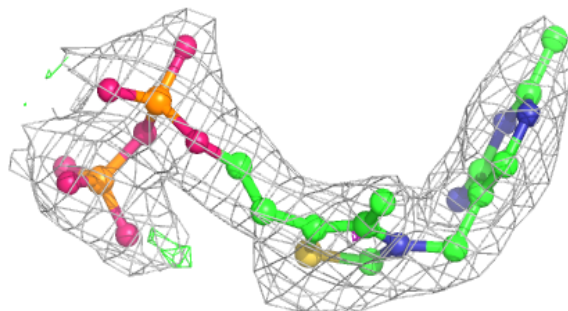
**Electron density around MG A 1003:**

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

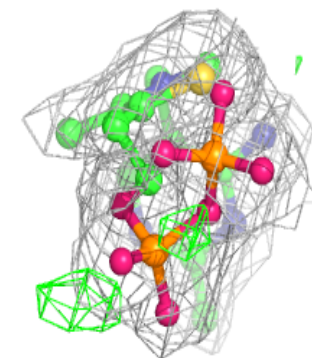
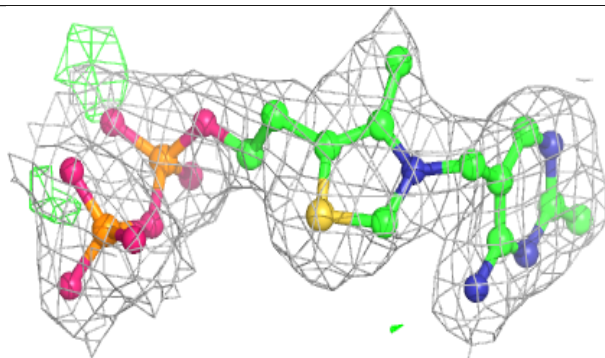
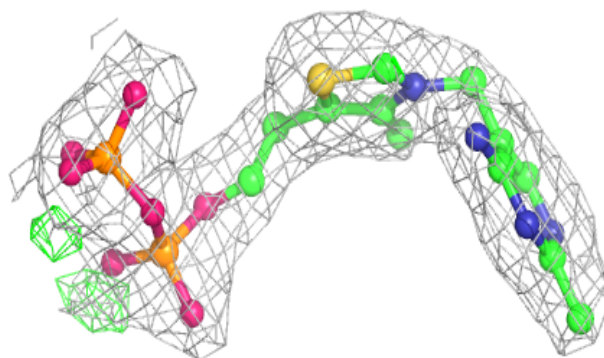


**Electron density around TPP B 1004:**

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

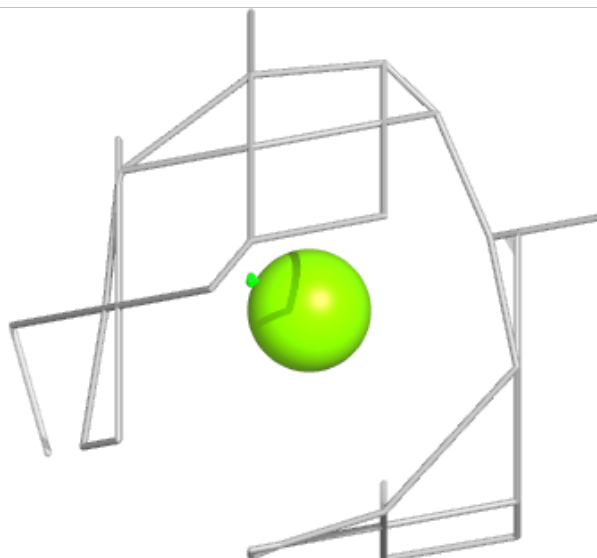
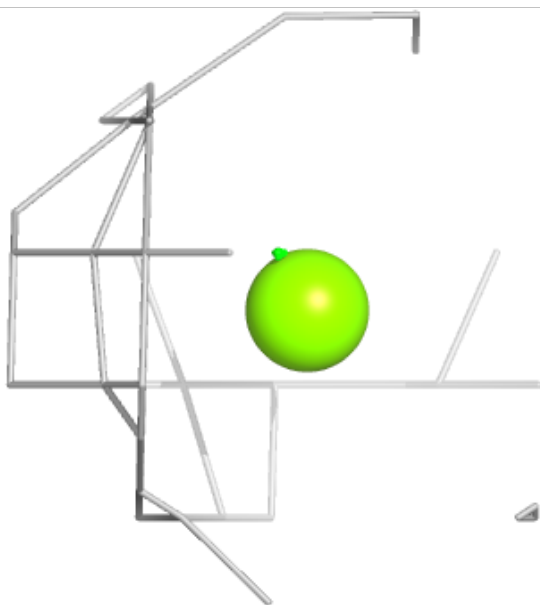
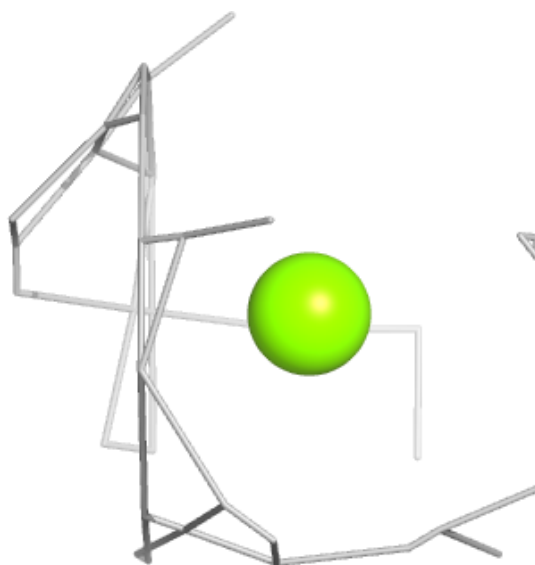
**Electron density around TPP A 1004:**

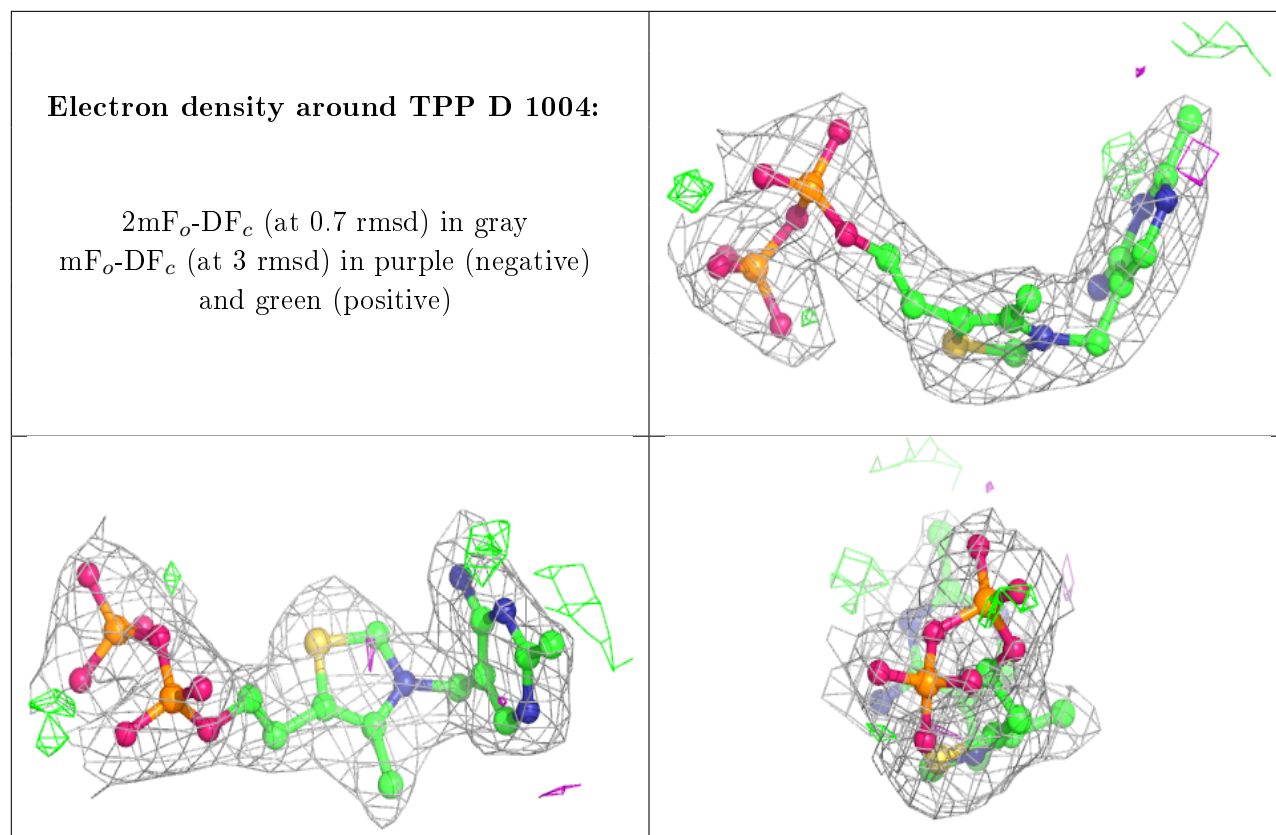
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG 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.