



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:51 PM EDT

PDB ID : 3DR4  
Title : GDP-perosamine synthase K186A mutant from *Caulobacter crescentus* with bound sugar ligand  
Authors : Holden, H.M.; Cook, P.D.; Carney, A.E.  
Deposited on : 2008-07-10  
Resolution : 1.60 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 : 2.23.2  
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) : 2.23.2

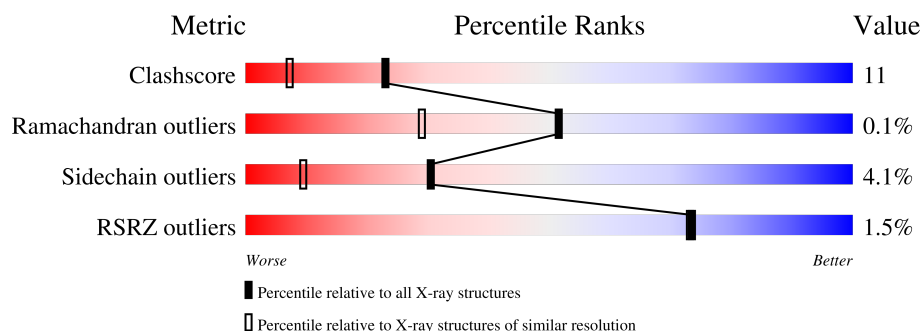
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	391	<div> <div>5%</div> <div>59% 28% 5% • 7%</div> </div>
1	B	391	<div> <div>72% 20% • 6%</div> </div>
1	C	391	<div> <div>78% 16% • 6%</div> </div>
1	D	391	<div> <div>77% 13% • 6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12778 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 Putative perosamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2792	1762	491	521	18			
1	B	366	Total	C	N	O	S	0	5	0
			2844	1796	501	529	18			
1	C	368	Total	C	N	O	S	0	2	0
			2840	1796	500	526	18			
1	D	367	Total	C	N	O	S	0	1	0
			2823	1784	497	524	18			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O85354
A	-18	GLY	-	expression tag	UNP O85354
A	-17	SER	-	expression tag	UNP O85354
A	-16	SER	-	expression tag	UNP O85354
A	-15	HIS	-	expression tag	UNP O85354
A	-14	HIS	-	expression tag	UNP O85354
A	-13	HIS	-	expression tag	UNP O85354
A	-12	HIS	-	expression tag	UNP O85354
A	-11	HIS	-	expression tag	UNP O85354
A	-10	HIS	-	expression tag	UNP O85354
A	-9	SER	-	expression tag	UNP O85354
A	-8	SER	-	expression tag	UNP O85354
A	-7	GLU	-	expression tag	UNP O85354
A	-6	ASN	-	expression tag	UNP O85354
A	-5	LEU	-	expression tag	UNP O85354
A	-4	TYR	-	expression tag	UNP O85354
A	-3	PHE	-	expression tag	UNP O85354
A	-2	GLN	-	expression tag	UNP O85354
A	-1	GLY	-	expression tag	UNP O85354
A	0	HIS	-	expression tag	UNP O85354
A	1	MET	-	expression tag	UNP O85354

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP O85354
A	3	ASP	-	expression tag	UNP O85354
A	4	LEU	-	expression tag	UNP O85354
A	5	PRO	-	expression tag	UNP O85354
A	6	ARG	-	expression tag	UNP O85354
A	7	ILE	-	expression tag	UNP O85354
A	8	SER	-	expression tag	UNP O85354
A	9	VAL	-	expression tag	UNP O85354
A	10	ALA	-	expression tag	UNP O85354
A	11	ALA	-	expression tag	UNP O85354
A	12	PRO	-	expression tag	UNP O85354
A	13	ARG	-	expression tag	UNP O85354
A	14	LEU	-	expression tag	UNP O85354
A	15	ASP	-	expression tag	UNP O85354
A	16	GLY	-	expression tag	UNP O85354
A	17	ASN	-	expression tag	UNP O85354
A	18	GLU	-	expression tag	UNP O85354
A	19	ARG	-	expression tag	UNP O85354
A	20	ASP	-	expression tag	UNP O85354
A	21	TYR	-	expression tag	UNP O85354
A	22	VAL	-	expression tag	UNP O85354
A	23	LEU	-	expression tag	UNP O85354
A	24	GLU	-	expression tag	UNP O85354
A	25	CYS	-	expression tag	UNP O85354
A	186	ALA	LYS	engineered mutation	UNP O85354
B	-19	MET	-	expression tag	UNP O85354
B	-18	GLY	-	expression tag	UNP O85354
B	-17	SER	-	expression tag	UNP O85354
B	-16	SER	-	expression tag	UNP O85354
B	-15	HIS	-	expression tag	UNP O85354
B	-14	HIS	-	expression tag	UNP O85354
B	-13	HIS	-	expression tag	UNP O85354
B	-12	HIS	-	expression tag	UNP O85354
B	-11	HIS	-	expression tag	UNP O85354
B	-10	HIS	-	expression tag	UNP O85354
B	-9	SER	-	expression tag	UNP O85354
B	-8	SER	-	expression tag	UNP O85354
B	-7	GLU	-	expression tag	UNP O85354
B	-6	ASN	-	expression tag	UNP O85354
B	-5	LEU	-	expression tag	UNP O85354
B	-4	TYR	-	expression tag	UNP O85354
B	-3	PHE	-	expression tag	UNP O85354

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP O85354
B	-1	GLY	-	expression tag	UNP O85354
B	0	HIS	-	expression tag	UNP O85354
B	1	MET	-	expression tag	UNP O85354
B	2	SER	-	expression tag	UNP O85354
B	3	ASP	-	expression tag	UNP O85354
B	4	LEU	-	expression tag	UNP O85354
B	5	PRO	-	expression tag	UNP O85354
B	6	ARG	-	expression tag	UNP O85354
B	7	ILE	-	expression tag	UNP O85354
B	8	SER	-	expression tag	UNP O85354
B	9	VAL	-	expression tag	UNP O85354
B	10	ALA	-	expression tag	UNP O85354
B	11	ALA	-	expression tag	UNP O85354
B	12	PRO	-	expression tag	UNP O85354
B	13	ARG	-	expression tag	UNP O85354
B	14	LEU	-	expression tag	UNP O85354
B	15	ASP	-	expression tag	UNP O85354
B	16	GLY	-	expression tag	UNP O85354
B	17	ASN	-	expression tag	UNP O85354
B	18	GLU	-	expression tag	UNP O85354
B	19	ARG	-	expression tag	UNP O85354
B	20	ASP	-	expression tag	UNP O85354
B	21	TYR	-	expression tag	UNP O85354
B	22	VAL	-	expression tag	UNP O85354
B	23	LEU	-	expression tag	UNP O85354
B	24	GLU	-	expression tag	UNP O85354
B	25	CYS	-	expression tag	UNP O85354
B	186	ALA	LYS	engineered mutation	UNP O85354
C	-19	MET	-	expression tag	UNP O85354
C	-18	GLY	-	expression tag	UNP O85354
C	-17	SER	-	expression tag	UNP O85354
C	-16	SER	-	expression tag	UNP O85354
C	-15	HIS	-	expression tag	UNP O85354
C	-14	HIS	-	expression tag	UNP O85354
C	-13	HIS	-	expression tag	UNP O85354
C	-12	HIS	-	expression tag	UNP O85354
C	-11	HIS	-	expression tag	UNP O85354
C	-10	HIS	-	expression tag	UNP O85354
C	-9	SER	-	expression tag	UNP O85354
C	-8	SER	-	expression tag	UNP O85354
C	-7	GLU	-	expression tag	UNP O85354

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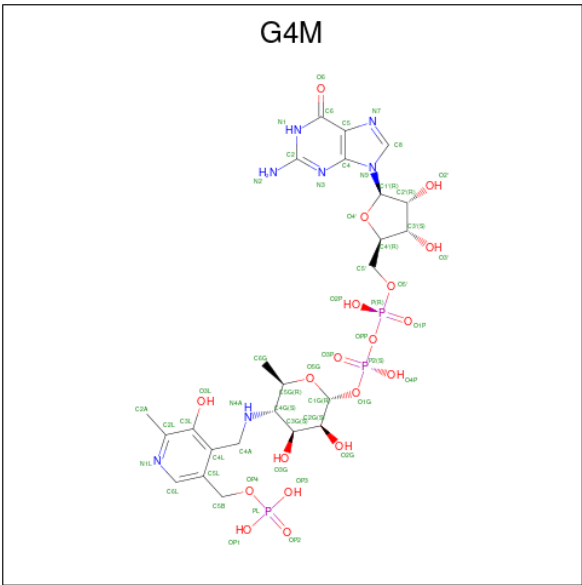
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C	-5	LEU	-	expression tag	UNP O85354
C	-4	TYR	-	expression tag	UNP O85354
C	-3	PHE	-	expression tag	UNP O85354
C	-2	GLN	-	expression tag	UNP O85354
C	-1	GLY	-	expression tag	UNP O85354
C	0	HIS	-	expression tag	UNP O85354
C	1	MET	-	expression tag	UNP O85354
C	2	SER	-	expression tag	UNP O85354
C	3	ASP	-	expression tag	UNP O85354
C	4	LEU	-	expression tag	UNP O85354
C	5	PRO	-	expression tag	UNP O85354
C	6	ARG	-	expression tag	UNP O85354
C	7	ILE	-	expression tag	UNP O85354
C	8	SER	-	expression tag	UNP O85354
C	9	VAL	-	expression tag	UNP O85354
C	10	ALA	-	expression tag	UNP O85354
C	11	ALA	-	expression tag	UNP O85354
C	12	PRO	-	expression tag	UNP O85354
C	13	ARG	-	expression tag	UNP O85354
C	14	LEU	-	expression tag	UNP O85354
C	15	ASP	-	expression tag	UNP O85354
C	16	GLY	-	expression tag	UNP O85354
C	17	ASN	-	expression tag	UNP O85354
C	18	GLU	-	expression tag	UNP O85354
C	19	ARG	-	expression tag	UNP O85354
C	20	ASP	-	expression tag	UNP O85354
C	21	TYR	-	expression tag	UNP O85354
C	22	VAL	-	expression tag	UNP O85354
C	23	LEU	-	expression tag	UNP O85354
C	24	GLU	-	expression tag	UNP O85354
C	25	CYS	-	expression tag	UNP O85354
C	186	ALA	LYS	engineered mutation	UNP O85354
D	-19	MET	-	expression tag	UNP O85354
D	-18	GLY	-	expression tag	UNP O85354
D	-17	SER	-	expression tag	UNP O85354
D	-16	SER	-	expression tag	UNP O85354
D	-15	HIS	-	expression tag	UNP O85354
D	-14	HIS	-	expression tag	UNP O85354
D	-13	HIS	-	expression tag	UNP O85354
D	-12	HIS	-	expression tag	UNP O85354
D	-11	HIS	-	expression tag	UNP O85354

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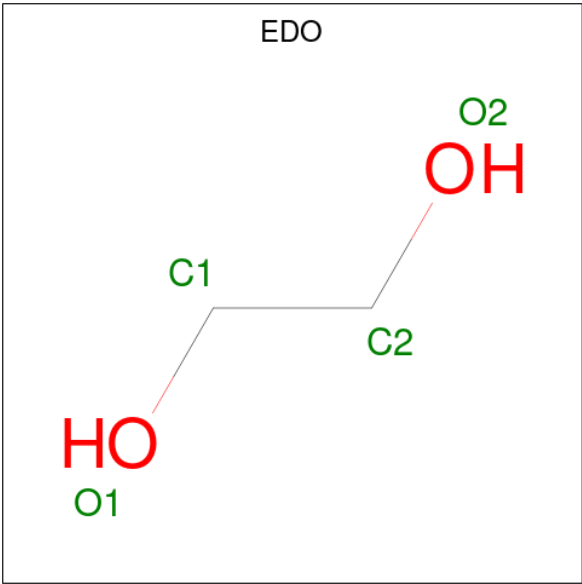
Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	expression tag	UNP O85354
D	-9	SER	-	expression tag	UNP O85354
D	-8	SER	-	expression tag	UNP O85354
D	-7	GLU	-	expression tag	UNP O85354
D	-6	ASN	-	expression tag	UNP O85354
D	-5	LEU	-	expression tag	UNP O85354
D	-4	TYR	-	expression tag	UNP O85354
D	-3	PHE	-	expression tag	UNP O85354
D	-2	GLN	-	expression tag	UNP O85354
D	-1	GLY	-	expression tag	UNP O85354
D	0	HIS	-	expression tag	UNP O85354
D	1	MET	-	expression tag	UNP O85354
D	2	SER	-	expression tag	UNP O85354
D	3	ASP	-	expression tag	UNP O85354
D	4	LEU	-	expression tag	UNP O85354
D	5	PRO	-	expression tag	UNP O85354
D	6	ARG	-	expression tag	UNP O85354
D	7	ILE	-	expression tag	UNP O85354
D	8	SER	-	expression tag	UNP O85354
D	9	VAL	-	expression tag	UNP O85354
D	10	ALA	-	expression tag	UNP O85354
D	11	ALA	-	expression tag	UNP O85354
D	12	PRO	-	expression tag	UNP O85354
D	13	ARG	-	expression tag	UNP O85354
D	14	LEU	-	expression tag	UNP O85354
D	15	ASP	-	expression tag	UNP O85354
D	16	GLY	-	expression tag	UNP O85354
D	17	ASN	-	expression tag	UNP O85354
D	18	GLU	-	expression tag	UNP O85354
D	19	ARG	-	expression tag	UNP O85354
D	20	ASP	-	expression tag	UNP O85354
D	21	TYR	-	expression tag	UNP O85354
D	22	VAL	-	expression tag	UNP O85354
D	23	LEU	-	expression tag	UNP O85354
D	24	GLU	-	expression tag	UNP O85354
D	25	CYS	-	expression tag	UNP O85354
D	186	ALA	LYS	engineered mutation	UNP O85354

- Molecule 2 is [(2R,3S,4R,5R)-5-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-3,4-dihydroxy tetrahydrofuran-2-yl]methyl (2R,3S,4S,5S,6R)-3,4-dihydroxy-5-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino]-6-methyltetrahydro-2H-pyran-2-yl dihydrogen diphosphate (three-letter code: G4M) (formula: C<sub>24</sub>H<sub>36</sub>N<sub>7</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	24	7	19	3		
2	B	1	Total	C	N	O	P	0	0
			53	24	7	19	3		
2	C	1	Total	C	N	O	P	0	0
			53	24	7	19	3		
2	D	1	Total	C	N	O	P	0	0
			53	24	7	19	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

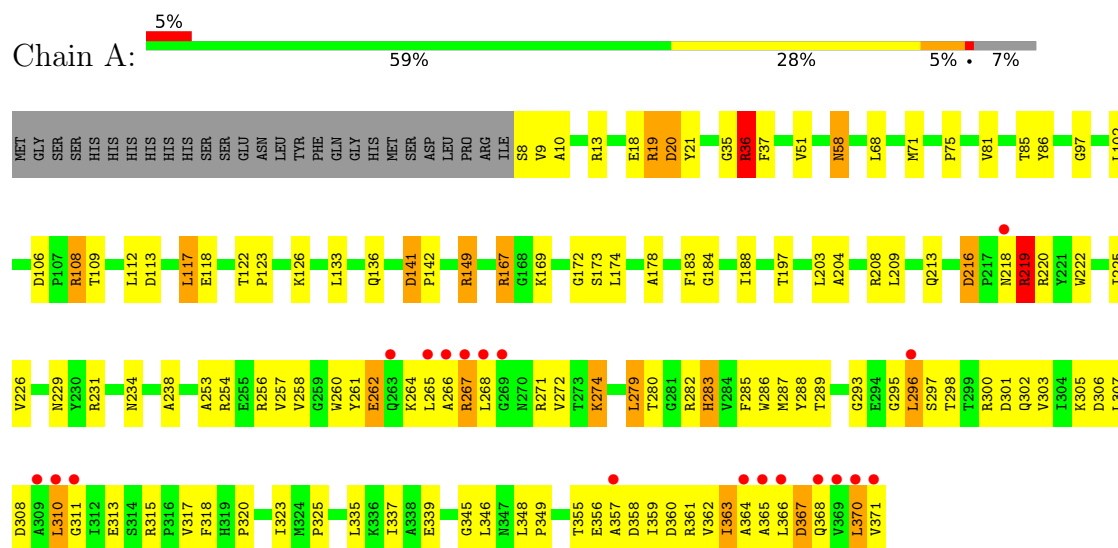
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total	O	0	0
			243	243		
4	B	290	Total	O	0	0
			290	290		
4	C	357	Total	O	0	0
			357	357		
4	D	369	Total	O	0	0
			369	369		

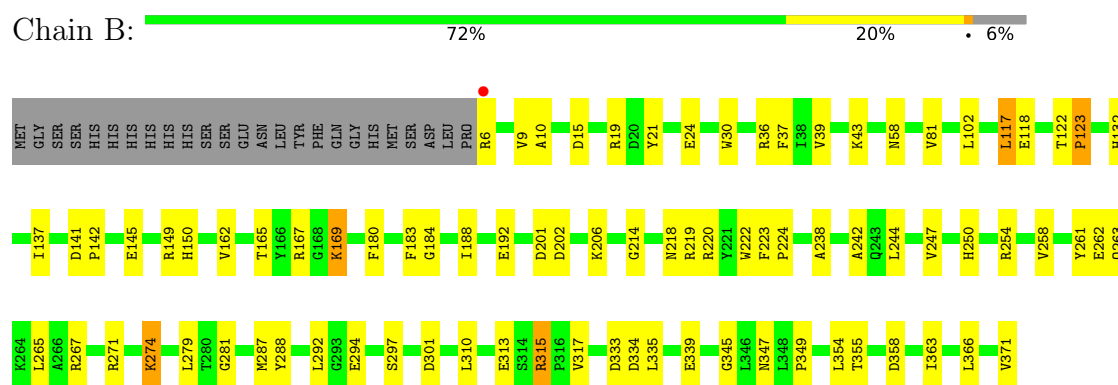
### 3 Residue-property plots

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.

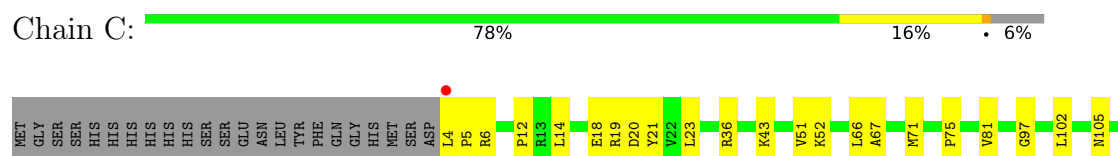
#### • Molecule 1: Putative perosamine synthetase

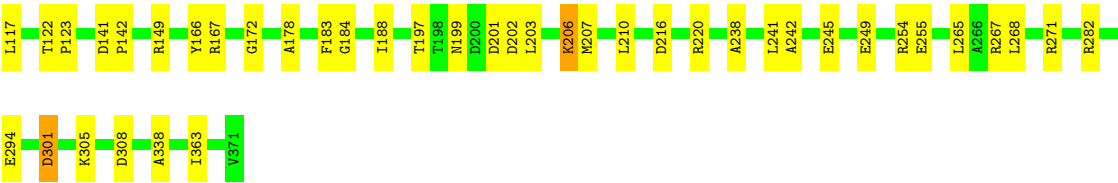


#### • Molecule 1: Putative perosamine synthetase

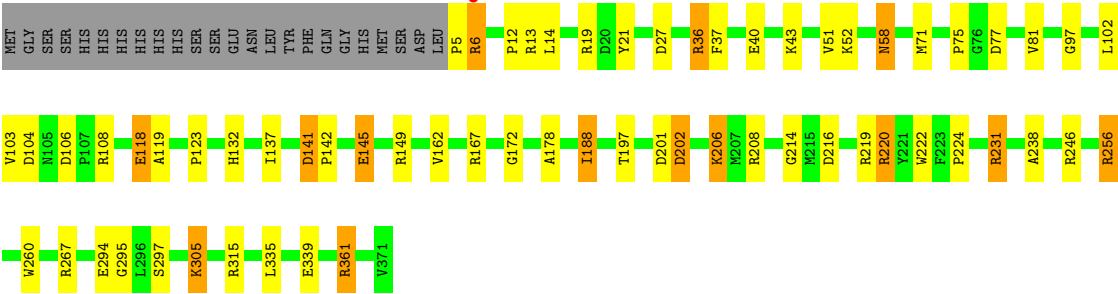


#### • Molecule 1: Putative perosamine synthetase





• Molecule 1: Putative perosamine synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.10Å 151.92Å 105.75Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	26.20 – 1.60 26.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.1 (26.20-1.60) 91.9 (26.20-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.166 , 0.238 0.168 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 92.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, G4M

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	0.73	0/2848	1.20	13/3872 (0.3%)
1	B	0.76	0/2912	1.19	14/3957 (0.4%)
1	C	0.77	0/2900	1.20	8/3942 (0.2%)
1	D	0.77	0/2883	1.22	19/3919 (0.5%)
All	All	0.76	0/11543	1.20	54/15690 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ARG	NE-CZ-NH2	14.03	127.32	120.30
1	C	271	ARG	NE-CZ-NH1	-13.97	113.31	120.30
1	A	36	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	D	13	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	246	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	D	27	ASP	CB-CG-OD1	8.07	125.56	118.30
1	D	361	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	C	220	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	19	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	113	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	167	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	174	LEU	CA-CB-CG	-6.74	99.80	115.30
1	D	71	MET	CG-SD-CE	-6.71	89.47	100.20
1	B	117	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	B	201	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	D	315	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	77	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	220	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	D	208	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	D	220	ARG	NE-CZ-NH1	6.15	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	310	LEU	CB-CG-CD2	-6.09	100.64	111.00
1	D	27	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	D	361	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	19	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	301	ASP	CB-CG-OD1	5.91	123.61	118.30
1	C	117	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	D	141	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	20	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	216	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	354	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	B	315	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	220	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	282	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	D	19	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	366	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	279	LEU	CB-CG-CD2	5.42	120.22	111.00
1	D	77	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	B	271	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	A	219	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	354	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	B	333	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	219	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	169	LYS	CD-CE-NZ	5.20	123.65	111.70
1	B	19	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	C	282	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	C	216	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	208	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	263	GLN	CB-CA-C	-5.12	100.16	110.40
1	B	301	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	167	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	202	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	226	VAL	CB-CA-C	-5.05	101.80	111.40
1	A	117	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2778	117	0
1	B	2844	0	2843	56	0
1	C	2840	0	2843	47	0
1	D	2823	0	2821	45	1
2	A	53	0	29	2	0
2	B	53	0	30	0	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
3	B	8	0	12	0	0
4	A	243	0	0	7	0
4	B	290	0	0	9	0
4	C	357	0	0	6	1
4	D	369	0	0	11	0
All	All	12778	0	11416	262	1

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 11.

All (262) 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:355:THR:HG22	1:A:357:ALA:H	1.10	1.17
1:A:36:ARG:HH21	1:A:36:ARG:HG3	1.32	0.93
1:A:355:THR:O	1:A:358:ASP:HB2	1.72	0.90
1:C:188[A]:ILE:HD13	4:C:593:HOH:O	1.70	0.89
1:D:267:ARG:HB2	4:D:915:HOH:O	1.73	0.86
1:D:219:ARG:HG2	1:D:222:TRP:HB2	1.58	0.84
1:A:355:THR:HG22	1:A:357:ALA:N	1.93	0.83
1:C:249:GLU:OE1	1:C:249:GLU:N	2.13	0.81
1:C:4:LEU:HD12	1:C:5:PRO:HD2	1.63	0.80
1:B:202:ASP:O	1:B:206:LYS:HG3	1.82	0.78
1:C:4:LEU:HD12	1:C:5:PRO:CD	2.13	0.78
1:C:265:LEU:HD22	1:C:268:LEU:HD12	1.65	0.78
1:B:262:GLU:HG3	4:B:1524:HOH:O	1.81	0.78
1:A:106:ASP:OD1	1:A:108:ARG:HG3	1.87	0.75
1:B:355:THR:O	1:B:358:ASP:HB2	1.86	0.75
1:A:274:LYS:HE3	4:A:727:HOH:O	1.87	0.74
1:B:219:ARG:HB2	1:B:222:TRP:HB3	1.70	0.72
1:B:274:LYS:HD2	4:B:1524:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ASP:O	1:C:206:LYS:HG2	1.91	0.71
1:C:105:ASN:HD21	1:C:338:ALA:HA	1.56	0.70
1:A:169:LYS:NZ	1:A:173:SER:O	2.25	0.70
1:C:265:LEU:CD2	1:C:268:LEU:HD12	2.22	0.69
1:A:308:ASP:O	1:A:311:GLY:N	2.23	0.69
1:C:67:ALA:O	1:C:71:MET:HG3	1.92	0.69
1:C:301:ASP:O	1:C:305:LYS:HG3	1.93	0.68
1:B:313[B]:GLU:O	1:B:349:PRO:HG3	1.92	0.68
1:B:145[B]:GLU:OE1	1:B:149:ARG:NH2	2.27	0.67
1:A:266:ALA:O	1:A:267:ARG:C	2.29	0.67
1:A:359:ILE:O	1:A:362:VAL:HB	1.95	0.66
1:B:162[B]:VAL:HG11	1:B:188:ILE:HD12	1.77	0.66
1:C:6:ARG:NH2	1:C:308:ASP:OD1	2.27	0.66
1:A:335:LEU:O	1:A:339:GLU:HG3	1.95	0.66
1:A:141:ASP:N	1:A:142:PRO:HD2	2.12	0.65
1:A:219:ARG:HD3	4:B:1325:HOH:O	1.98	0.64
1:A:265:LEU:O	1:A:268:LEU:HB2	1.97	0.64
1:C:4:LEU:CD1	1:C:5:PRO:HD2	2.28	0.63
1:B:335:LEU:O	1:B:339:GLU:HG3	1.99	0.63
1:D:5:PRO:O	1:D:361:ARG:NH1	2.31	0.63
1:B:315:ARG:HB2	1:B:347:ASN:HD22	1.63	0.62
1:B:261:TYR:O	1:B:265:LEU:HB2	1.99	0.62
1:D:145:GLU:OE1	1:D:149:ARG:NH2	2.27	0.62
1:A:355:THR:N	1:A:358:ASP:OD2	2.27	0.61
1:B:297:SER:H	1:B:371:VAL:C	2.03	0.61
1:B:274:LYS:N	4:B:1529:HOH:O	2.26	0.61
1:D:256:ARG:NH2	1:D:260:TRP:CZ2	2.69	0.61
1:D:5:PRO:HD2	1:D:361:ARG:NH1	2.17	0.60
1:B:313[A]:GLU:O	1:B:349:PRO:HG3	2.00	0.60
1:A:219:ARG:HB3	1:A:222:TRP:HB3	1.82	0.60
1:A:36:ARG:HD2	1:A:37:PHE:N	2.17	0.59
1:A:36:ARG:HG3	1:A:36:ARG:NH2	2.12	0.59
1:C:52:LYS:HE2	1:C:201:ASP:OD1	2.03	0.59
1:B:169:LYS:HD3	4:B:1520:HOH:O	2.02	0.59
1:D:40:GLU:HA	1:D:43:LYS:HE2	1.85	0.59
1:D:118:GLU:OE1	1:D:149:ARG:NH1	2.36	0.59
1:B:118:GLU:OE2	1:B:150:HIS:NE2	2.33	0.58
1:C:265:LEU:CD2	1:C:363:ILE:HD13	2.33	0.58
1:B:267:ARG:O	1:B:267:ARG:HG3	2.01	0.58
1:C:21:TYR:HB3	1:C:238:ALA:HB1	1.86	0.58
1:A:268:LEU:HD11	1:A:366:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:TYR:HD2	1:A:348:LEU:HD12	1.68	0.57
1:A:254:ARG:HG3	4:A:684:HOH:O	2.03	0.57
1:A:264:LYS:NZ	1:A:360:ASP:OD1	2.38	0.57
1:D:206:LYS:NZ	4:D:791:HOH:O	2.37	0.57
1:A:122:THR:HB	1:A:123:PRO:CD	2.35	0.57
1:A:260:TRP:O	1:A:264:LYS:HG3	2.05	0.56
1:C:12:PRO:HA	4:C:655:HOH:O	2.04	0.56
1:A:8:SER:OG	1:A:10:ALA:O	2.22	0.56
1:A:264:LYS:HZ1	1:A:356:GLU:CG	2.19	0.56
1:A:122:THR:HB	1:A:123:PRO:HD2	1.88	0.56
1:A:258:VAL:HG12	4:A:679:HOH:O	2.05	0.56
1:A:36:ARG:HH21	1:A:36:ARG:CG	2.13	0.56
1:A:216:ASP:OD1	1:A:216:ASP:C	2.44	0.55
1:B:145[A]:GLU:OE2	4:B:1536:HOH:O	2.18	0.55
1:D:81:VAL:O	1:D:102:LEU:HA	2.06	0.55
1:D:36:ARG:HH21	1:D:36:ARG:HG3	1.72	0.55
1:A:167:ARG:HD3	1:A:280:THR:O	2.07	0.55
1:A:264:LYS:NZ	1:A:356:GLU:HG3	2.22	0.54
1:D:214:GLY:O	1:D:224:PRO:HD2	2.08	0.54
1:D:5:PRO:HD2	1:D:361:ARG:HH12	1.71	0.54
1:D:231:ARG:HD2	4:D:854:HOH:O	2.07	0.54
1:A:361:ARG:O	1:A:361:ARG:HG3	2.08	0.54
1:A:302:GLN:NE2	1:A:306:ASP:OD1	2.41	0.54
1:C:52:LYS:HB2	1:C:199:ASN:HA	1.90	0.54
1:A:231:ARG:NH2	1:B:192:GLU:OE2	2.38	0.54
1:A:21:TYR:HB3	1:A:238:ALA:HB1	1.89	0.53
1:B:118:GLU:OE1	1:B:149:ARG:NH1	2.33	0.53
1:C:203:LEU:HG	1:C:207:MET:CE	2.38	0.53
1:D:172:GLY:HA2	1:D:178:ALA:CB	2.38	0.53
1:D:267:ARG:NH1	4:D:856:HOH:O	2.42	0.53
1:C:141:ASP:N	1:C:142:PRO:HD2	2.24	0.53
1:A:315:ARG:CD	1:B:220:ARG:HD2	2.39	0.53
1:A:219:ARG:HD2	1:A:222:TRP:HB2	1.91	0.53
2:C:500:G4M:O4P	1:D:220:ARG:NH1	2.38	0.53
1:A:35:GLY:HA3	1:A:234:ASN:CG	2.29	0.52
1:A:36:ARG:CD	1:A:36:ARG:H	2.23	0.52
1:D:219:ARG:HG2	1:D:222:TRP:CB	2.34	0.52
1:A:172:GLY:HA2	1:A:178:ALA:CB	2.40	0.52
1:C:4:LEU:HD12	1:C:5:PRO:HD3	1.89	0.52
1:A:18:GLU:HB2	4:A:677:HOH:O	2.10	0.51
1:C:141:ASP:HB2	1:C:142:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLY:O	1:A:296:LEU:C	2.47	0.51
1:D:119:ALA:HB3	4:D:826:HOH:O	2.10	0.51
1:A:260:TRP:CZ3	1:A:356:GLU:N	2.79	0.51
1:D:36:ARG:HG3	1:D:36:ARG:NH2	2.26	0.51
1:A:118:GLU:CD	1:A:149:ARG:HH22	2.14	0.51
1:A:301:ASP:O	1:A:305:LYS:HG3	2.11	0.51
1:A:36:ARG:HD2	1:A:36:ARG:N	2.26	0.50
1:A:271:ARG:HD2	1:A:370:LEU:HB3	1.94	0.50
1:D:52:LYS:HE2	1:D:201:ASP:OD1	2.10	0.50
1:A:20:ASP:OD1	1:A:20:ASP:O	2.30	0.50
1:C:141:ASP:N	1:C:142:PRO:CD	2.74	0.50
1:A:253:ALA:O	1:A:257:VAL:HG23	2.12	0.49
1:B:317:VAL:HG21	1:B:345:GLY:HA3	1.94	0.49
1:C:105:ASN:HD21	1:C:338:ALA:CA	2.23	0.49
1:A:118:GLU:OE2	1:A:149:ARG:NH2	2.42	0.49
1:A:355:THR:H	1:A:358:ASP:CG	2.13	0.49
1:B:297:SER:N	1:B:371:VAL:OXT	2.41	0.49
1:A:149:ARG:HG2	1:A:149:ARG:HH21	1.77	0.49
1:C:203:LEU:HG	1:C:207:MET:HE3	1.95	0.48
1:A:257:VAL:HG13	1:A:359:ILE:HD11	1.94	0.48
1:A:303:VAL:O	1:A:307:LEU:HB2	2.13	0.48
1:A:310:LEU:HD22	1:A:365:ALA:HB2	1.95	0.48
1:A:313:GLU:OE2	4:A:715:HOH:O	2.20	0.48
1:A:264:LYS:HZ1	1:A:356:GLU:HG3	1.76	0.48
1:A:20:ASP:OD1	1:A:20:ASP:C	2.50	0.48
1:A:36:ARG:HD2	1:A:36:ARG:C	2.33	0.48
1:B:9:VAL:N	1:B:313[A]:GLU:HB3	2.28	0.48
1:A:213:GLN:NE2	1:A:229:ASN:HB2	2.29	0.48
1:B:183:PHE:CG	1:B:184:GLY:N	2.81	0.48
1:B:39:VAL:HG13	4:B:1477:HOH:O	2.14	0.48
1:C:206:LYS:NZ	1:C:206:LYS:HB3	2.29	0.48
1:A:9:VAL:N	1:A:313:GLU:OE1	2.27	0.48
1:A:302:GLN:HE21	1:A:306:ASP:CG	2.17	0.47
1:C:294:GLU:HG3	4:C:516:HOH:O	2.14	0.47
1:A:355:THR:HG22	1:A:356:GLU:N	2.29	0.47
1:C:75:PRO:HA	1:C:97:GLY:O	2.14	0.47
1:A:363:ILE:O	1:A:364:ALA:C	2.53	0.47
1:D:12:PRO:HD2	2:D:500:G4M:C2	2.45	0.47
1:C:81:VAL:O	1:C:102:LEU:HA	2.13	0.47
1:B:258:VAL:HG13	1:B:288:TYR:CD2	2.50	0.47
1:A:188:ILE:HD13	1:A:188:ILE:HG21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162[B]:VAL:HG22	1:B:180:PHE:CD2	2.50	0.46
1:B:254:ARG:O	1:B:258:VAL:HG23	2.15	0.46
1:B:292:LEU:HD23	1:B:292:LEU:N	2.30	0.46
1:C:4:LEU:HD12	1:C:4:LEU:HA	1.68	0.46
1:C:265:LEU:HD23	1:C:363:ILE:HD13	1.97	0.46
1:B:21:TYR:HB3	1:B:238:ALA:HB1	1.98	0.46
1:D:6:ARG:HG3	4:D:885:HOH:O	2.15	0.46
1:A:307:LEU:HA	1:A:307:LEU:HD23	1.48	0.46
1:A:325:PRO:HG2	1:B:224:PRO:HA	1.98	0.46
1:A:36:ARG:CD	1:A:36:ARG:N	2.78	0.46
1:B:162[B]:VAL:CG2	1:B:180:PHE:CD2	2.99	0.46
1:D:145:GLU:CD	1:D:149:ARG:HH22	2.17	0.46
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.71	0.46
1:A:265:LEU:O	1:A:268:LEU:N	2.49	0.45
1:A:272:VAL:CG1	1:A:370:LEU:HD21	2.46	0.45
1:A:359:ILE:O	1:A:362:VAL:N	2.47	0.45
1:C:122:THR:HB	1:C:123:PRO:CD	2.47	0.45
1:A:337:ILE:N	1:A:337:ILE:HD13	2.30	0.45
1:A:81:VAL:O	1:A:102:LEU:HA	2.16	0.45
1:D:162:VAL:HG11	1:D:188[B]:ILE:HG13	1.99	0.45
1:D:335:LEU:O	1:D:339:GLU:HG3	2.17	0.45
1:A:136:GLN:HB2	1:A:283:HIS:CD2	2.51	0.45
1:A:283:HIS:CE1	1:A:285:PHE:H	2.35	0.45
1:B:132:HIS:CE1	1:B:137:ILE:HG23	2.51	0.45
1:B:162[A]:VAL:HG21	1:B:188:ILE:HD12	1.98	0.45
1:D:6:ARG:NH1	4:D:774:HOH:O	2.49	0.45
1:D:202:ASP:HB3	4:D:815:HOH:O	2.15	0.45
1:A:300:ARG:NE	1:A:301:ASP:OD1	2.41	0.45
1:C:51:VAL:HG21	1:C:197:THR:HB	1.97	0.45
1:A:261:TYR:O	1:A:262:GLU:C	2.54	0.45
2:A:500:G4M:C2	1:B:30:TRP:CZ3	3.00	0.45
1:A:75:PRO:HA	1:A:97:GLY:O	2.16	0.45
1:C:172:GLY:HA2	1:C:178:ALA:CB	2.46	0.45
1:B:165:THR:O	1:B:281:GLY:HA3	2.17	0.44
1:D:305:LYS:HB2	1:D:305:LYS:HE2	1.67	0.44
1:A:271:ARG:NH1	1:A:367:ASP:HA	2.32	0.44
1:A:262:GLU:OE2	1:A:288:TYR:OH	2.29	0.44
1:A:306:ASP:O	1:A:307:LEU:C	2.55	0.44
1:C:265:LEU:HD21	1:C:363:ILE:HD13	1.99	0.44
1:A:371:VAL:O	1:A:371:VAL:HG23	2.16	0.44
1:D:141:ASP:CB	1:D:142:PRO:CD	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PHE:CG	1:A:184:GLY:N	2.85	0.44
1:A:368:GLN:HG2	1:A:368:GLN:O	2.17	0.44
1:C:265:LEU:CD2	1:C:363:ILE:CD1	2.96	0.44
1:D:103:VAL:HG22	1:D:104:ASP:N	2.33	0.43
1:A:204:ALA:O	1:A:208:ARG:HG3	2.18	0.43
1:A:317:VAL:CG2	1:A:345:GLY:HA3	2.48	0.43
1:B:141:ASP:N	1:B:142:PRO:HD2	2.34	0.43
1:A:219:ARG:HB3	1:A:222:TRP:CB	2.47	0.43
1:D:256:ARG:HH21	1:D:256:ARG:HG3	1.81	0.43
1:A:141:ASP:N	1:A:142:PRO:CD	2.80	0.43
1:A:368:GLN:O	1:A:368:GLN:CG	2.67	0.43
1:B:214:GLY:O	1:B:224:PRO:HD2	2.19	0.43
1:C:66:LEU:HD11	1:C:210:LEU:HB2	2.01	0.43
1:D:172:GLY:HA2	1:D:178:ALA:HB3	2.00	0.43
1:A:209:LEU:HG	1:A:225:ILE:HD11	1.99	0.43
1:A:298:THR:OG1	1:A:302:GLN:HB3	2.18	0.43
1:B:36:ARG:HG3	1:B:37:PHE:N	2.32	0.43
1:A:289:THR:HA	1:A:346:LEU:O	2.18	0.43
1:A:13:ARG:HG3	1:A:13:ARG:O	2.17	0.43
1:A:85:THR:OG1	1:A:86:TYR:N	2.51	0.43
1:B:334:ASP:HB2	4:B:1429:HOH:O	2.19	0.43
1:B:15:ASP:OD1	1:B:250:HIS:HE1	2.01	0.43
1:B:355:THR:H	1:B:358:ASP:HB2	1.83	0.43
1:A:58:ASN:N	1:A:58:ASN:HD22	2.16	0.42
1:A:271:ARG:HH12	1:A:367:ASP:HA	1.83	0.42
1:C:18:GLU:HG3	1:C:242:ALA:HB3	2.01	0.42
1:B:81:VAL:O	1:B:102:LEU:HA	2.18	0.42
1:B:223:PHE:HA	1:B:224:PRO:HD2	1.94	0.42
1:B:317:VAL:CG2	1:B:345:GLY:HA3	2.49	0.42
1:C:241:LEU:O	1:C:245:GLU:HG3	2.19	0.42
1:D:36:ARG:HG2	1:D:37:PHE:N	2.34	0.42
1:D:256:ARG:HH21	1:D:256:ARG:CG	2.31	0.42
1:A:19:ARG:NH2	4:A:685:HOH:O	2.29	0.42
1:A:112:LEU:HD21	1:A:117:LEU:HG	2.02	0.42
1:A:216:ASP:OD2	1:A:219:ARG:HB2	2.19	0.42
1:A:313:GLU:O	1:A:349:PRO:HG3	2.20	0.42
1:D:75:PRO:HA	1:D:97:GLY:O	2.19	0.42
1:C:305:LYS:HE3	4:C:517:HOH:O	2.20	0.42
1:D:36:ARG:HD3	4:D:691:HOH:O	2.18	0.42
1:D:132:HIS:CE1	1:D:137:ILE:HG23	2.55	0.42
1:D:58:ASN:H	1:D:58:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLY:HA3	4:D:634:HOH:O	2.19	0.42
1:A:19:ARG:HD3	4:A:685:HOH:O	2.19	0.42
1:A:133:LEU:HD22	1:A:318:PHE:HE2	1.83	0.41
1:C:265:LEU:HD23	1:C:363:ILE:CD1	2.50	0.41
1:A:320:PRO:O	1:A:323:ILE:HG12	2.20	0.41
2:A:500:G4M:N3	1:B:30:TRP:CZ3	2.88	0.41
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.69	0.41
1:A:106:ASP:HB3	1:A:109:THR:OG1	2.20	0.41
1:C:19:ARG:HD2	4:D:745:HOH:O	2.20	0.41
1:A:265:LEU:HD12	1:A:265:LEU:HA	1.42	0.41
1:C:122:THR:HB	1:C:123:PRO:HD2	2.02	0.41
1:C:166:TYR:O	1:C:167:ARG:C	2.59	0.41
1:C:183:PHE:CG	1:C:184:GLY:N	2.89	0.41
1:A:260:TRP:CE2	1:A:356:GLU:HB2	2.56	0.41
1:A:293:GLY:O	1:A:296:LEU:CD1	2.68	0.41
1:B:21:TYR:CD2	1:B:242:ALA:HB2	2.55	0.41
1:C:14:LEU:N	4:C:539:HOH:O	2.27	0.41
1:B:363:ILE:HD13	1:B:363:ILE:HA	1.85	0.41
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.98	0.41
1:A:58:ASN:HD22	1:A:58:ASN:H	1.69	0.41
1:B:10:ALA:HB2	1:B:287:MET:CE	2.51	0.41
1:B:117:LEU:HA	1:B:117:LEU:HD23	1.93	0.41
1:B:122:THR:HB	1:B:123:PRO:HD2	2.03	0.41
1:B:162[B]:VAL:HG23	1:B:180:PHE:HD2	1.85	0.41
1:A:167:ARG:CZ	1:A:280:THR:HA	2.51	0.40
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.82	0.40
1:D:21:TYR:HB3	1:D:238:ALA:HB1	2.02	0.40
1:A:286:TRP:O	1:A:287:MET:HE2	2.20	0.40
4:C:634:HOH:O	1:D:14:LEU:CB	2.68	0.40
1:D:51:VAL:HG21	1:D:197:THR:HB	2.04	0.40
1:D:106:ASP:OD2	1:D:108:ARG:N	2.40	0.40
1:A:355:THR:HB	1:A:358:ASP:H	1.86	0.40
1:B:244:LEU:O	1:B:247:VAL:HG12	2.22	0.40
1:B:262:GLU:CG	4:B:1524:HOH:O	2.52	0.40
1:A:68:LEU:HD23	1:A:71:MET:CE	2.52	0.40
1:A:293:GLY:O	1:A:296:LEU:HD12	2.22	0.40
1:A:51:VAL:HG21	1:A:197:THR:HB	2.04	0.40
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.69	0.40
1:D:149:ARG:HH21	1:D:149:ARG:HD3	1.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ARG:NH2	4:C:785:HOH:O[2_557]	2.14	0.06

## 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	362/391 (93%)	338 (93%)	23 (6%)	1 (0%)	41	21
1	B	369/391 (94%)	361 (98%)	8 (2%)	0	100	100
1	C	368/391 (94%)	362 (98%)	6 (2%)	0	100	100
1	D	366/391 (94%)	360 (98%)	6 (2%)	0	100	100
All	All	1465/1564 (94%)	1421 (97%)	43 (3%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/318 (92%)	272 (93%)	21 (7%)	14	2
1	B	300/318 (94%)	292 (97%)	8 (3%)	44	20
1	C	299/318 (94%)	290 (97%)	9 (3%)	41	16
1	D	297/318 (93%)	284 (96%)	13 (4%)	28	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1189/1272 (94%)	1138 (96%)	51 (4%)	30 9

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	58	ASN
1	A	108	ARG
1	A	126	LYS
1	A	141	ASP
1	A	149	ARG
1	A	167	ARG
1	A	216	ASP
1	A	218	ASN
1	A	219	ARG
1	A	256	ARG
1	A	262	GLU
1	A	267	ARG
1	A	274	LYS
1	A	279	LEU
1	A	283	HIS
1	A	297	SER
1	A	310	LEU
1	A	363	ILE
1	A	367	ASP
1	A	370	LEU
1	B	6	ARG
1	B	24	GLU
1	B	58	ASN
1	B	123	PRO
1	B	218	ASN
1	B	274	LYS
1	B	279	LEU
1	B	294	GLU
1	C	20	ASP
1	C	36	ARG
1	C	43[A]	LYS
1	C	43[B]	LYS
1	C	149	ARG
1	C	206	LYS
1	C	254	ARG
1	C	255	GLU

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Mol	Chain	Res	Type
1	C	267	ARG
1	D	6	ARG
1	D	36	ARG
1	D	58	ASN
1	D	118	GLU
1	D	123	PRO
1	D	145	GLU
1	D	188[A]	ILE
1	D	188[B]	ILE
1	D	206	LYS
1	D	256	ARG
1	D	294	GLU
1	D	297	SER
1	D	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	250	HIS
1	A	263	GLN
1	A	302	GLN
1	B	58	ASN
1	B	263	GLN
1	B	347	ASN
1	C	91	ASN
1	C	105	ASN
1	C	347	ASN
1	D	58	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	G4M	C	500	-	49,57,57	1.89	9 (18%)	66,88,88	1.90	10 (15%)
2	G4M	A	500	-	49,57,57	1.89	6 (12%)	66,88,88	2.07	13 (19%)
3	EDO	B	1260	-	3,3,3	0.45	0	2,2,2	0.06	0
2	G4M	D	500	-	49,57,57	1.81	8 (16%)	66,88,88	1.99	14 (21%)
3	EDO	B	1261	-	3,3,3	0.38	0	2,2,2	0.70	0
2	G4M	B	500	-	49,57,57	1.86	8 (16%)	66,88,88	1.88	14 (21%)

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	G4M	C	500	-	-	4/28/68/68	0/5/5/5
2	G4M	A	500	-	-	4/28/68/68	0/5/5/5
3	EDO	B	1260	-	-	0/1/1/1	-
2	G4M	D	500	-	-	4/28/68/68	0/5/5/5
3	EDO	B	1261	-	-	1/1/1/1	-
2	G4M	B	500	-	-	5/28/68/68	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	G4M	C4A-N4A	-7.80	1.23	1.46
2	B	500	G4M	C4A-N4A	-7.79	1.23	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	G4M	C4A-N4A	-7.46	1.24	1.46
2	D	500	G4M	C4A-N4A	-7.20	1.25	1.46
2	C	500	G4M	O3L-C3L	-5.61	1.23	1.37
2	A	500	G4M	O3L-C3L	-5.51	1.24	1.37
2	B	500	G4M	O3L-C3L	-5.14	1.25	1.37
2	A	500	G4M	C4A-C4L	-5.13	1.45	1.51
2	D	500	G4M	O3L-C3L	-4.67	1.26	1.37
2	D	500	G4M	C4A-C4L	-4.16	1.46	1.51
2	C	500	G4M	C3L-C2L	-3.98	1.36	1.40
2	B	500	G4M	C4A-C4L	-3.75	1.47	1.51
2	B	500	G4M	PL-OP3	-3.37	1.41	1.54
2	C	500	G4M	C2'-C1'	-3.31	1.48	1.53
2	B	500	G4M	C2'-C1'	-3.00	1.49	1.53
2	A	500	G4M	PL-OP3	-2.96	1.43	1.54
2	C	500	G4M	PL-OP3	-2.76	1.44	1.54
2	D	500	G4M	P-O1P	-2.67	1.41	1.50
2	D	500	G4M	PL-OP3	-2.67	1.44	1.54
2	B	500	G4M	PL-OP1	-2.66	1.44	1.54
2	C	500	G4M	C4A-C4L	-2.43	1.48	1.51
2	B	500	G4M	PL-OP2	-2.34	1.43	1.50
2	B	500	G4M	C3L-C2L	-2.34	1.38	1.40
2	C	500	G4M	O5G-C5G	-2.33	1.39	1.44
2	D	500	G4M	P2-O1G	-2.32	1.54	1.60
2	A	500	G4M	O5G-C5G	-2.27	1.39	1.44
2	D	500	G4M	P2-O4P	-2.11	1.45	1.55
2	A	500	G4M	C5L-C4L	-2.11	1.37	1.40
2	C	500	G4M	C6L-N1L	-2.10	1.30	1.34
2	C	500	G4M	P2-O4P	-2.08	1.45	1.55
2	D	500	G4M	O5G-C5G	-2.01	1.40	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	G4M	C4A-N4A-C4G	6.86	127.11	114.04
2	D	500	G4M	C4A-N4A-C4G	6.82	127.04	114.04
2	A	500	G4M	C4A-N4A-C4G	6.64	126.69	114.04
2	B	500	G4M	C4A-N4A-C4G	6.07	125.61	114.04
2	A	500	G4M	N3-C2-N1	-5.30	120.16	127.22
2	D	500	G4M	C2-N3-C4	5.24	121.34	115.36
2	D	500	G4M	N3-C2-N1	-5.13	120.38	127.22
2	A	500	G4M	C1G-C2G-C3G	5.11	120.64	110.00
2	A	500	G4M	C2-N3-C4	4.76	120.79	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	G4M	C2-N3-C4	4.74	120.77	115.36
2	B	500	G4M	N3-C2-N1	-4.61	121.07	127.22
2	C	500	G4M	C5-C6-N1	-4.40	117.41	123.43
2	C	500	G4M	C2-N3-C4	4.36	120.34	115.36
2	D	500	G4M	C5-C6-N1	-4.18	117.71	123.43
2	D	500	G4M	C6-N1-C2	4.13	122.49	115.93
2	B	500	G4M	C1G-C2G-C3G	4.12	118.57	110.00
2	C	500	G4M	N3-C2-N1	-4.08	121.78	127.22
2	A	500	G4M	O2G-C2G-C3G	4.06	119.74	110.35
2	C	500	G4M	OP4-C5B-C5L	4.01	116.99	109.35
2	C	500	G4M	C1G-C2G-C3G	4.00	118.33	110.00
2	C	500	G4M	C6-N1-C2	4.00	122.29	115.93
2	A	500	G4M	C5-C6-N1	-3.98	117.98	123.43
2	A	500	G4M	C6-N1-C2	3.91	122.15	115.93
2	B	500	G4M	P-OPP-P2	-3.89	119.49	132.83
2	A	500	G4M	C4L-C4A-N4A	3.86	122.42	111.78
2	B	500	G4M	C5-C6-N1	-3.73	118.33	123.43
2	A	500	G4M	OP4-C5B-C5L	3.67	116.35	109.35
2	D	500	G4M	OP4-C5B-C5L	3.53	116.07	109.35
2	D	500	G4M	C4L-C4A-N4A	3.50	121.41	111.78
2	B	500	G4M	OP4-C5B-C5L	3.49	116.01	109.35
2	B	500	G4M	C6-N1-C2	3.26	121.11	115.93
2	C	500	G4M	C4L-C4A-N4A	3.20	120.60	111.78
2	B	500	G4M	C4L-C4A-N4A	3.11	120.34	111.78
2	D	500	G4M	O5G-C5G-C4G	-3.05	104.23	110.10
2	D	500	G4M	C4-C5-N7	-3.03	106.24	109.40
2	D	500	G4M	C1G-C2G-C3G	2.88	115.99	110.00
2	B	500	G4M	O5'-P-O1P	2.72	119.69	109.07
2	A	500	G4M	P-OPP-P2	-2.69	123.61	132.83
2	C	500	G4M	C4-C5-N7	-2.68	106.61	109.40
2	D	500	G4M	C4A-C4L-C5L	2.52	122.52	119.71
2	B	500	G4M	O5G-C5G-C6G	2.49	112.09	106.70
2	B	500	G4M	C2G-C3G-C4G	2.47	113.96	110.34
2	A	500	G4M	C5'-C4'-C3'	-2.44	106.05	115.18
2	D	500	G4M	O1G-C1G-C2G	-2.41	103.97	108.38
2	D	500	G4M	P-OPP-P2	-2.39	124.61	132.83
2	C	500	G4M	P-OPP-P2	-2.39	124.62	132.83
2	B	500	G4M	OP4-PL-OP2	-2.39	99.78	106.47
2	A	500	G4M	N2-C2-N1	2.33	120.87	117.25
2	B	500	G4M	C4-C5-N7	-2.32	106.98	109.40
2	D	500	G4M	OP4-PL-OP2	-2.17	100.39	106.47
2	A	500	G4M	C4-C5-N7	-2.17	107.14	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

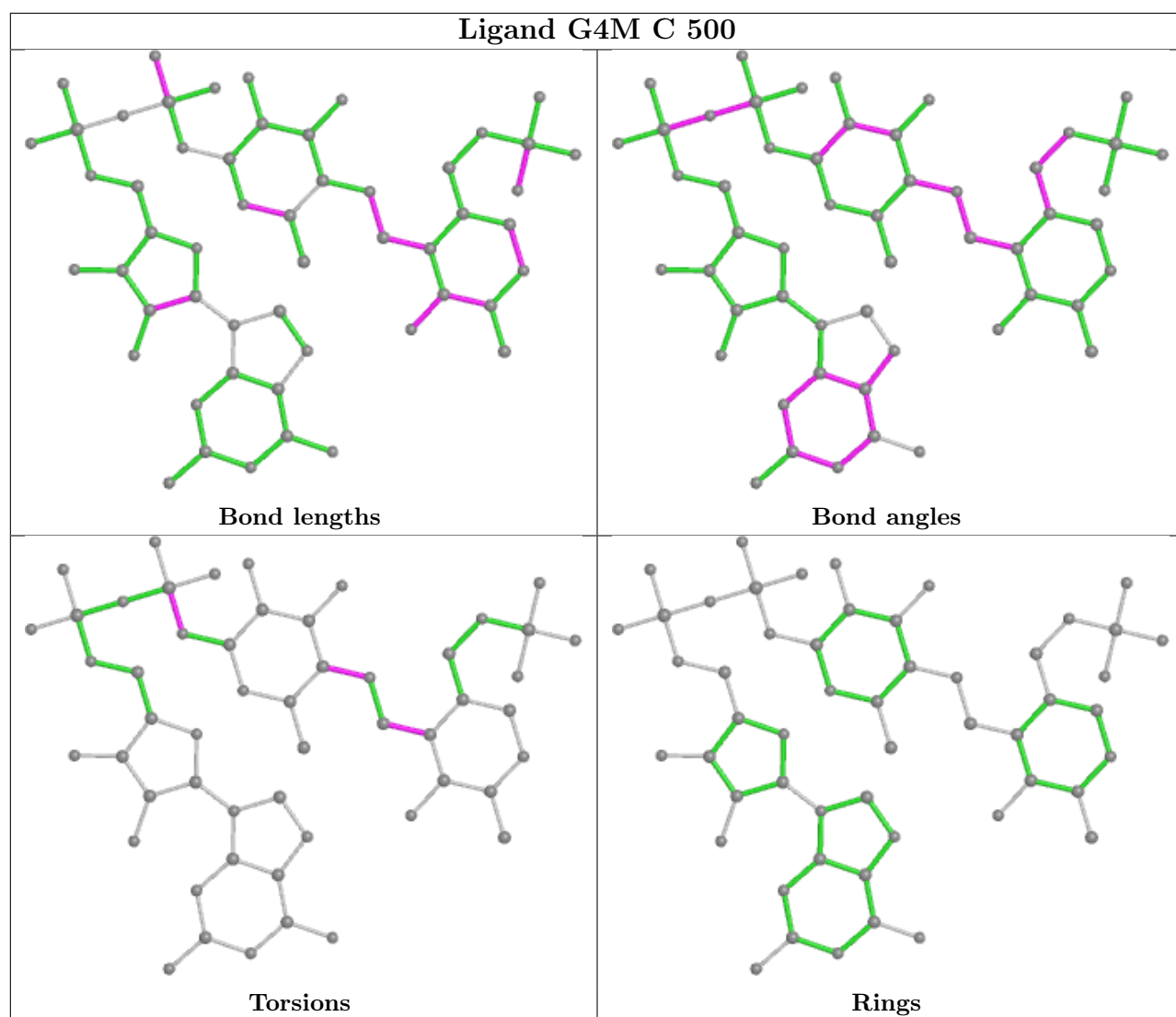
Mol	Chain	Res	Type	Atoms
2	A	500	G4M	N4A-C4A-C4L-C5L
2	A	500	G4M	C3G-C4G-N4A-C4A
2	B	500	G4M	N4A-C4A-C4L-C5L
2	B	500	G4M	C3G-C4G-N4A-C4A
2	C	500	G4M	N4A-C4A-C4L-C5L
2	C	500	G4M	N4A-C4A-C4L-C3L
2	C	500	G4M	C3G-C4G-N4A-C4A
2	D	500	G4M	N4A-C4A-C4L-C5L
2	D	500	G4M	N4A-C4A-C4L-C3L
2	D	500	G4M	C3G-C4G-N4A-C4A
2	B	500	G4M	N4A-C4A-C4L-C3L
3	B	1261	EDO	O1-C1-C2-O2
2	D	500	G4M	C1G-O1G-P2-OPP
2	A	500	G4M	N4A-C4A-C4L-C3L
2	A	500	G4M	C1G-O1G-P2-OPP
2	B	500	G4M	P2-OPP-P-O1P
2	B	500	G4M	C1G-O1G-P2-OPP
2	C	500	G4M	C1G-O1G-P2-OPP

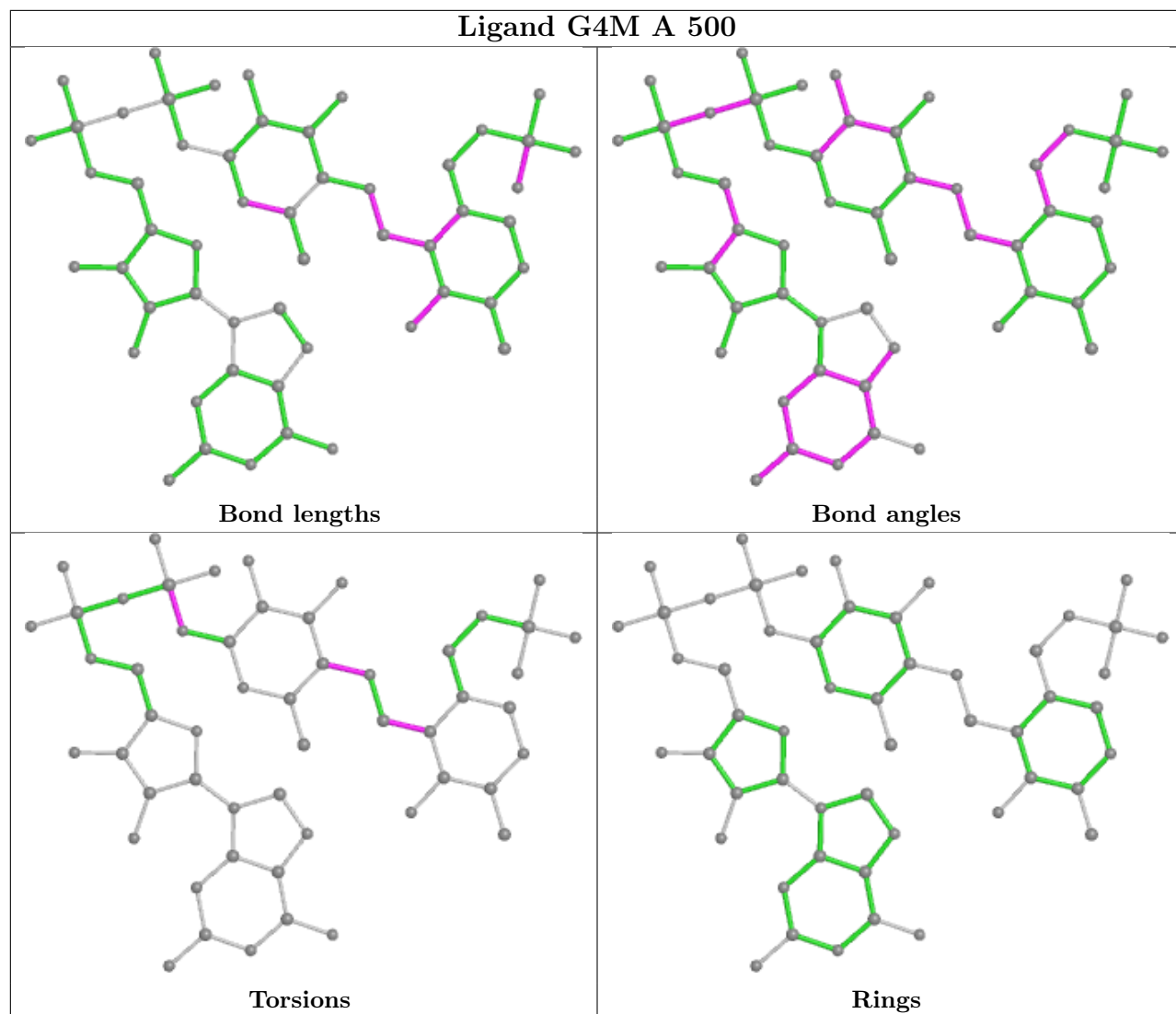
There are no ring outliers.

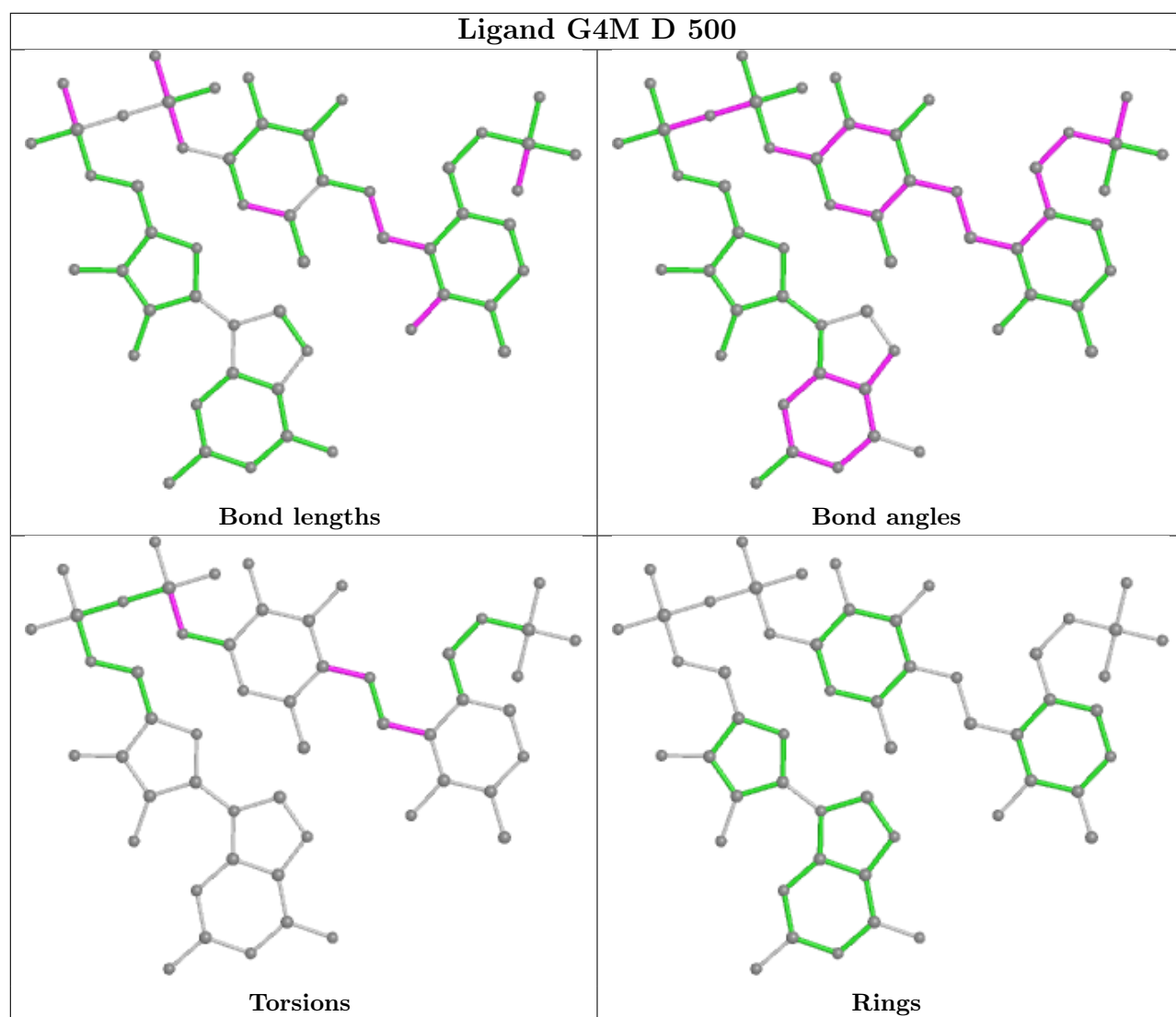
3 monomers are involved in 4 short contacts:

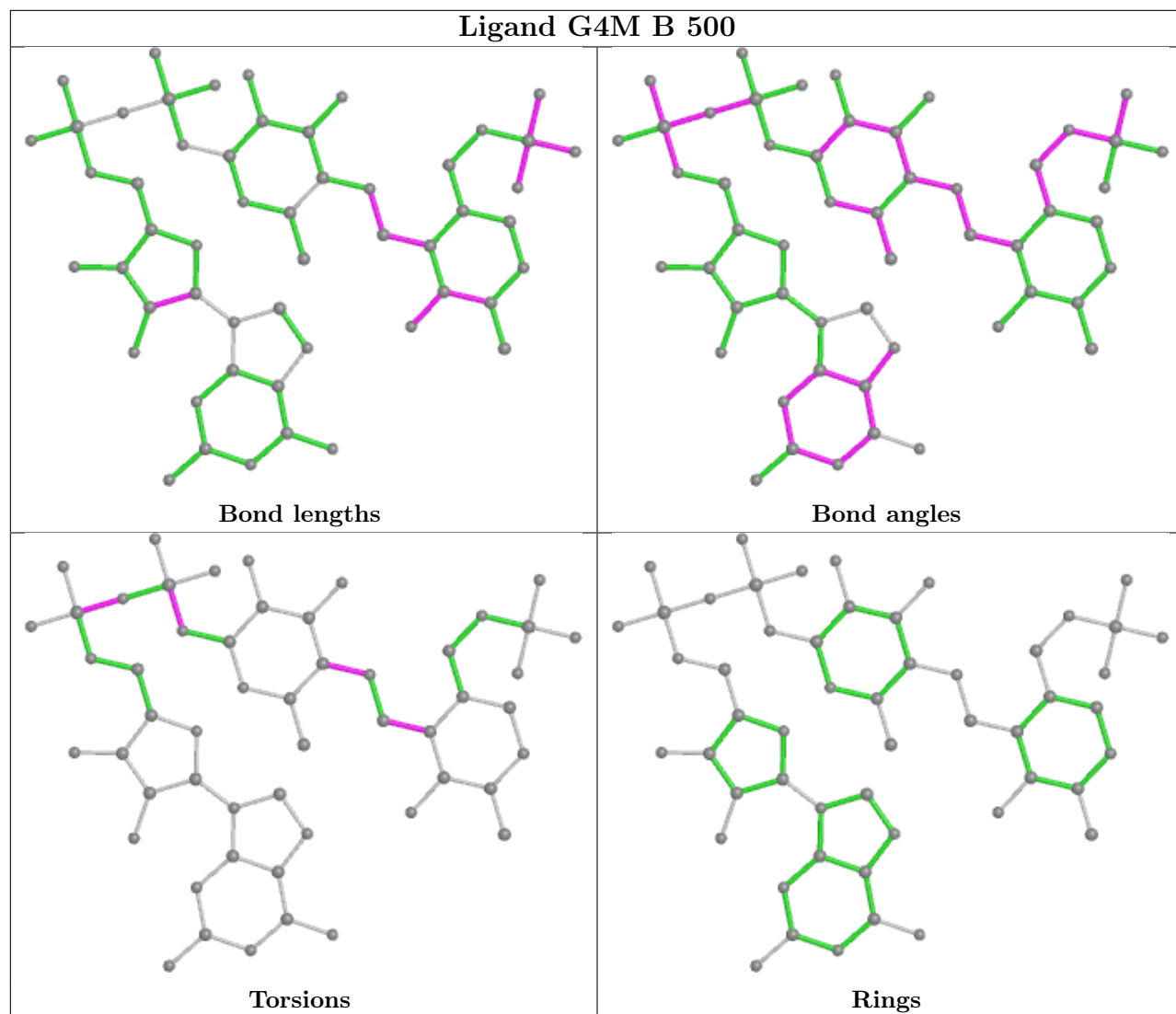
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	G4M	1	0
2	A	500	G4M	2	0
2	D	500	G4M	1	0

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.









## 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	364/391 (93%)	-0.16	19 (5%)	27 24	15, 27, 72, 100	0
1	B	366/391 (93%)	-0.40	1 (0%)	94 93	15, 25, 55, 83	0
1	C	368/391 (94%)	-0.64	1 (0%)	94 93	14, 21, 45, 77	0
1	D	367/391 (93%)	-0.59	1 (0%)	94 93	13, 21, 44, 72	0
All	All	1465/1564 (93%)	-0.45	22 (1%)	73 73	13, 23, 58, 100	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	VAL	5.7
1	A	296	LEU	3.9
1	A	218	ASN	3.6
1	A	311	GLY	3.6
1	A	269	GLY	3.5
1	A	268	LEU	3.5
1	A	265	LEU	3.2
1	A	266	ALA	3.1
1	C	4	LEU	3.1
1	A	370	LEU	3.0
1	A	267	ARG	3.0
1	A	357	ALA	2.8
1	A	263	GLN	2.5
1	A	369	VAL	2.4
1	A	310	LEU	2.3
1	B	6	ARG	2.3
1	A	365	ALA	2.2
1	D	6	ARG	2.2
1	A	309	ALA	2.2
1	A	368	GLN	2.1
1	A	366	LEU	2.1
1	A	364	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

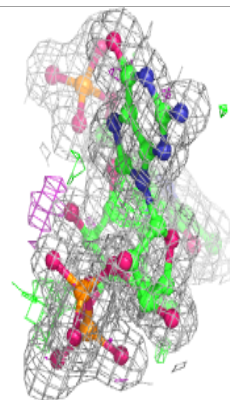
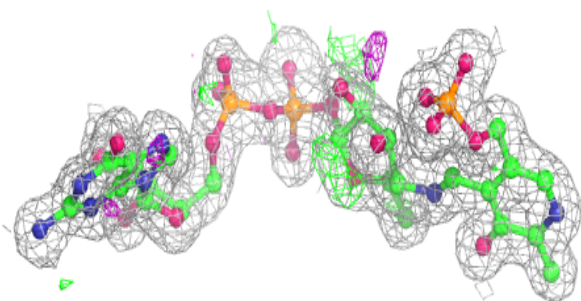
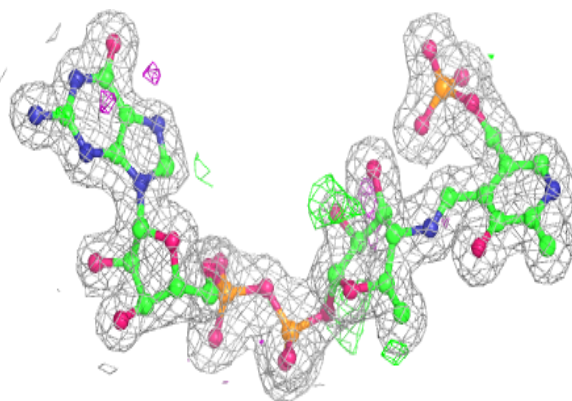
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	1261	4/4	0.71	0.16	71,97,100,100	0
3	EDO	B	1260	4/4	0.85	0.14	47,54,56,100	0
2	G4M	B	500	53/53	0.94	0.09	13,28,69,98	0
2	G4M	A	500	53/53	0.95	0.08	15,27,90,100	0
2	G4M	C	500	53/53	0.95	0.08	11,22,37,100	0
2	G4M	D	500	53/53	0.97	0.07	11,20,28,31	0

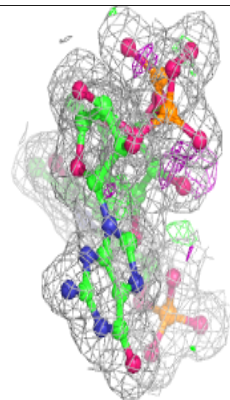
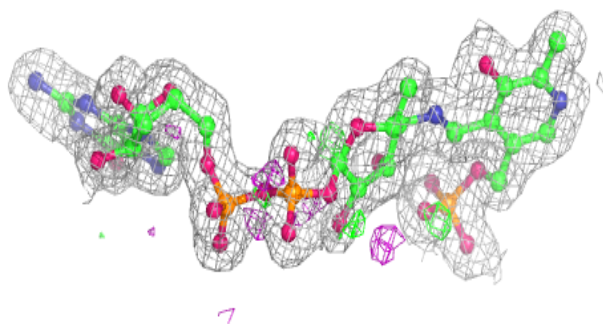
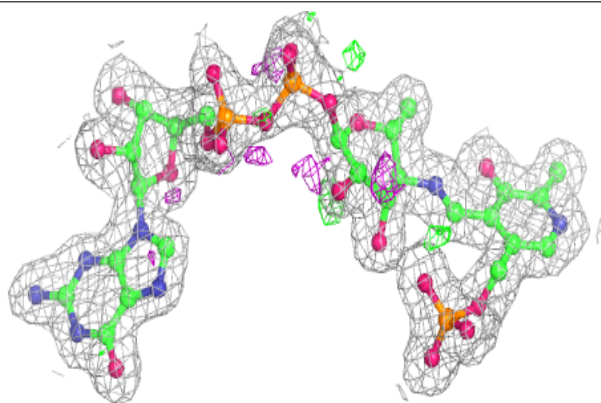
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around G4M B 500:**

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

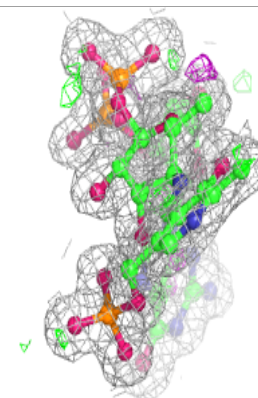
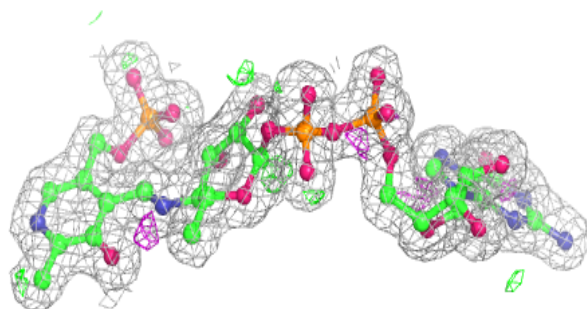
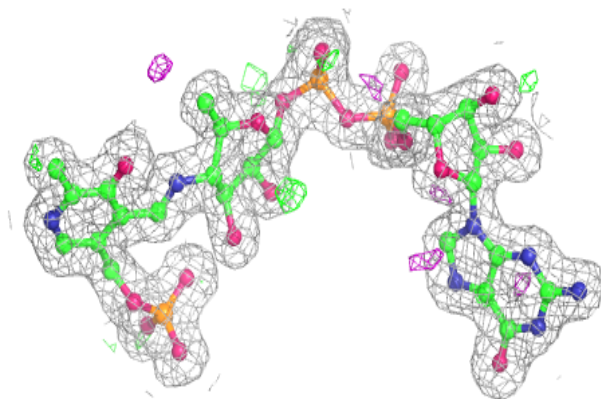
**Electron density around G4M A 500:**

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

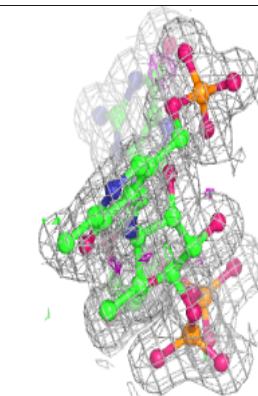
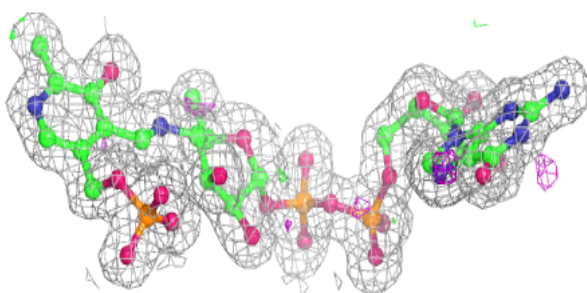
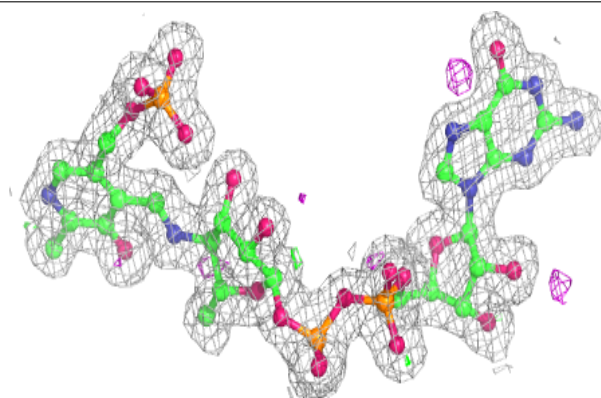


**Electron density around G4M C 500:**

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

**Electron density around G4M D 500:**

$2mF_o-DF_c$  (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.