



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:50 AM UTC

PDB ID : 9D3H / pdb_00009d3h
Title : Thermotoga maritima threonylcarbamoyl adenylate synthase (TsaC2) in complex with N-carboxy-L-threonine, magnesium and pyrophosphate.
Authors : Kutshuashvili, A.; Swairjo, M.A.
Deposited on : 2024-08-10
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

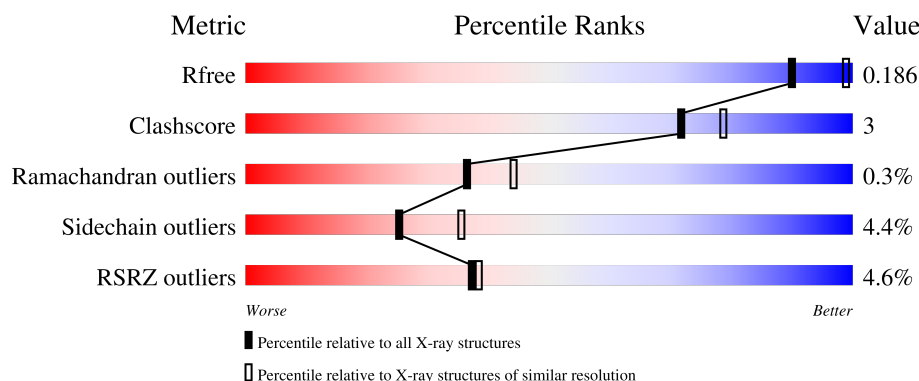
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	<div> <div>4%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	340	<div> <div>5%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5670 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.

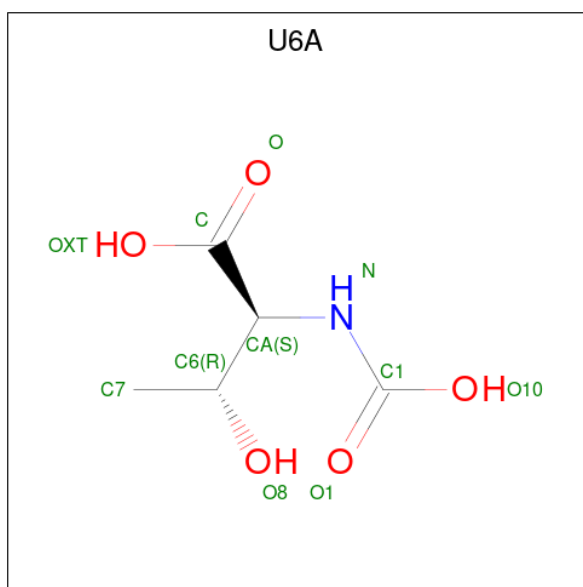
- Molecule 1 is a protein called Threonylcarbamoyl-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2688	1751	451	478	8			
1	B	336	Total	C	N	O	S	0	3	0
			2701	1755	457	481	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9WZV6
A	-3	SER	-	expression tag	UNP Q9WZV6
A	-2	HIS	-	expression tag	UNP Q9WZV6
A	-1	MET	-	expression tag	UNP Q9WZV6
A	0	ALA	-	expression tag	UNP Q9WZV6
A	1	SER	-	expression tag	UNP Q9WZV6
B	-4	GLY	-	expression tag	UNP Q9WZV6
B	-3	SER	-	expression tag	UNP Q9WZV6
B	-2	HIS	-	expression tag	UNP Q9WZV6
B	-1	MET	-	expression tag	UNP Q9WZV6
B	0	ALA	-	expression tag	UNP Q9WZV6
B	1	SER	-	expression tag	UNP Q9WZV6

- Molecule 2 is N-carboxy-L-threonine (CCD ID: U6A) (formula: $C_5H_9NO_5$) (labeled as "Ligand of Interest" by depositor).

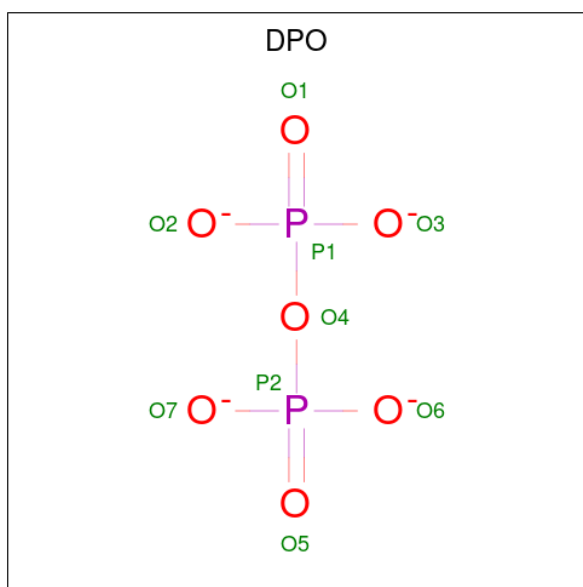


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	5	1	5		
2	B	1	Total	C	N	O	0	0
			11	5	1	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

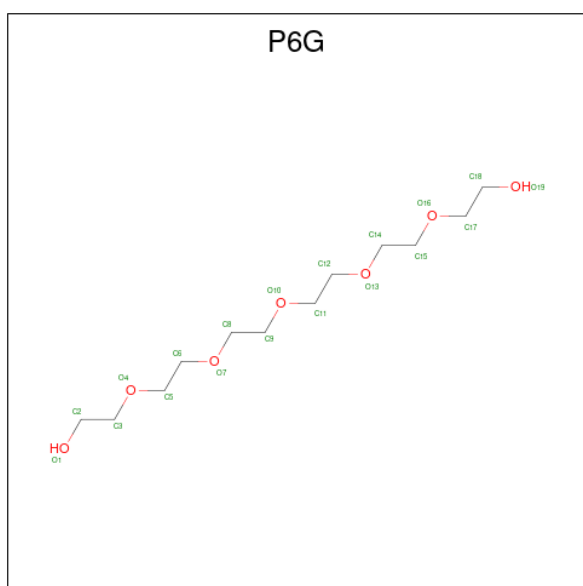
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



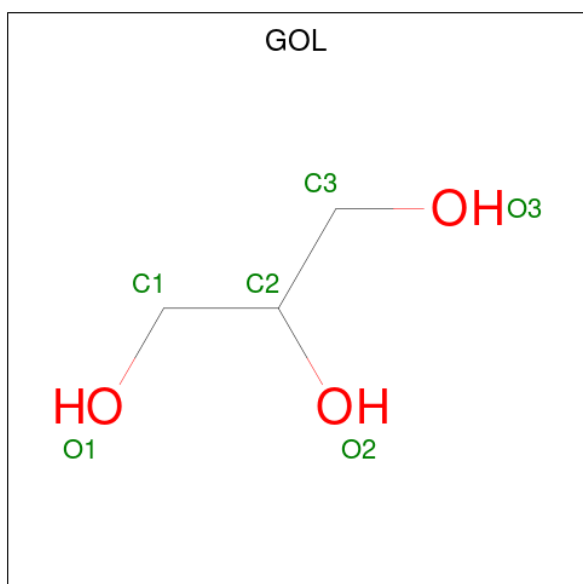
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			19	12 7		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



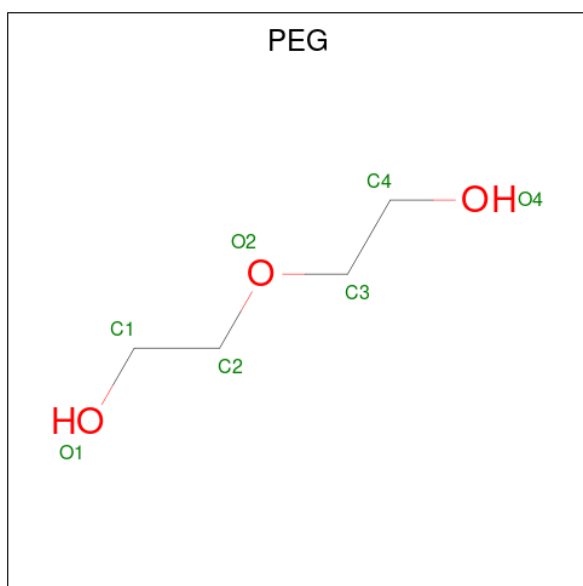
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

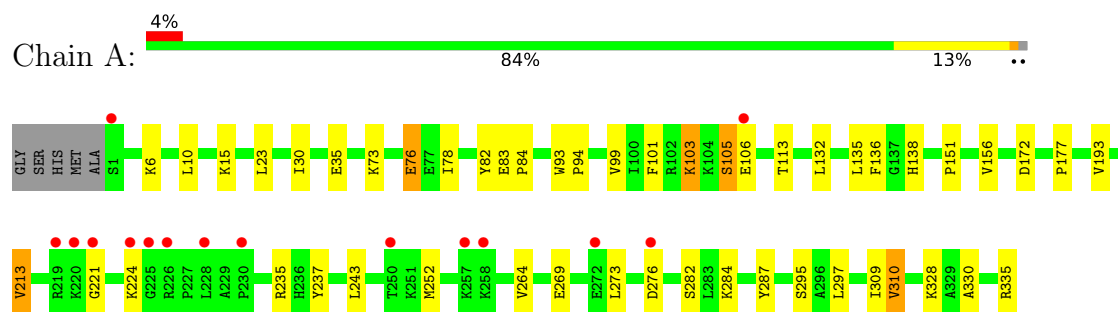
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	59	Total	O	0	0
			59	59		
9	B	92	Total	O	0	0
			92	92		

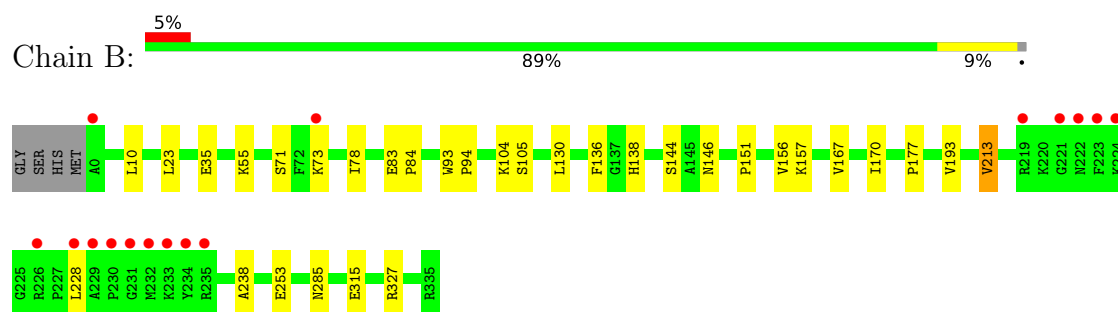
3 Residue-property plots [i](#)

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: Threonylcarbamoyl-AMP synthase



• Molecule 1: Threonylcarbamoyl-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.04Å 154.04Å 87.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.09 – 2.28 34.09 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.09-2.28) 99.0 (34.09-2.28)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.212 0.191 , 0.186	Depositor DCC
R_{free} test set	2771 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5670	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, U6A, GOL, ACT, P6G, DPO, PEG

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	1.05	0/2753	1.37	1/3728 (0.0%)
1	B	1.02	0/2763	1.31	2/3741 (0.1%)
All	All	1.03	0/5516	1.34	3/7469 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	CA-C-N	6.39	128.84	120.28
1	B	253	GLU	C-N-CA	6.39	128.84	120.28
1	A	287	TYR	CB-CA-C	5.32	119.62	110.79

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	2688	0	2808	26	0
1	B	2701	0	2815	14	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	19	0	26	0	0
6	A	8	0	6	0	0
6	B	12	0	9	0	0
7	B	42	0	56	1	0
8	B	7	0	10	0	0
9	A	59	0	0	0	0
9	B	92	0	0	0	0
All	All	5670	0	5730	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (37) 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:156:VAL:HG21	1:A:172:ASP:CB	2.31	0.60
1:A:252:MET:HE1	1:A:309:ILE:HG21	1.84	0.60
1:A:156:VAL:HG21	1:A:172:ASP:HB2	1.84	0.60
1:A:78:ILE:HA	1:A:105:SER:HB2	1.87	0.57
1:B:156:VAL:HG23	1:B:170:ILE:HG21	1.89	0.55
1:B:144:SER:OG	1:B:146:ASN:ND2	2.32	0.53
1:A:136:PHE:CE2	1:A:138:HIS:HB2	2.44	0.52
1:B:167:VAL:HA	7:B:407:GOL:C1	2.40	0.51
1:A:252:MET:HE3	1:A:252:MET:HA	1.93	0.51
1:A:93:TRP:HA	1:A:94:PRO:C	2.36	0.50
1:A:35:GLU:HA	1:A:177:PRO:HD2	1.93	0.49
1:A:252:MET:HE1	1:A:309:ILE:CG2	2.43	0.49
1:B:83:GLU:HB2	1:B:84:PRO:HD3	1.94	0.49
1:A:243:LEU:HD21	1:A:310:VAL:CG2	2.44	0.48
1:B:78:ILE:HA	1:B:105:SER:HB2	1.95	0.48
1:A:30:ILE:HD11	1:A:132:LEU:HD21	1.96	0.48
1:B:35:GLU:HA	1:B:177:PRO:HD2	1.96	0.47
1:A:193:VAL:HG13	1:A:213[A]:VAL:CG2	2.46	0.46
1:B:93:TRP:HA	1:B:94:PRO:C	2.41	0.46
1:A:235:ARG:NH2	1:A:330:ALA:O	2.50	0.45
1:A:284:LYS:O	1:A:284:LYS:HG3	2.18	0.44
1:A:10:LEU:CD2	1:B:10:LEU:HD23	2.47	0.44
1:A:135[B]:LEU:HD22	1:A:135[B]:LEU:HA	1.86	0.44
1:B:136:PHE:CE2	1:B:138:HIS:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD21	1:B:10:LEU:HD23	2.01	0.43
1:A:156:VAL:HG21	1:A:172:ASP:CG	2.43	0.43
1:A:264:VAL:HA	1:A:309:ILE:O	2.18	0.42
1:A:76:GLU:HA	1:A:82:TYR:OH	2.19	0.42
1:A:10:LEU:HD23	1:B:10:LEU:CD2	2.49	0.42
1:B:193:VAL:HG13	1:B:213:VAL:HG22	2.00	0.42
1:A:269:GLU:OE2	1:A:282:SER:OG	2.37	0.42
1:A:151:PRO:HA	1:A:237:TYR:HA	2.00	0.42
1:A:83:GLU:N	1:A:84:PRO:CD	2.83	0.41
1:A:99[A]:VAL:HG11	1:A:101:PHE:CZ	2.55	0.41
1:B:315:GLU:OE1	1:B:327:ARG:NH1	2.54	0.41
1:B:151:PRO:HD3	1:B:238:ALA:O	2.20	0.41
1:A:103:LYS:HE2	1:A:113:THR:HG21	2.04	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	336/340 (99%)	324 (96%)	10 (3%)	2 (1%)	21	25
1	B	337/340 (99%)	326 (97%)	11 (3%)	0	100	100
All	All	673/680 (99%)	650 (97%)	21 (3%)	2 (0%)	36	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLY
1	A	105	SER

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	296/296 (100%)	279 (94%)	17 (6%)	18	25
1	B	296/296 (100%)	286 (97%)	10 (3%)	32	46
All	All	592/592 (100%)	565 (95%)	27 (5%)	25	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	15	LYS
1	A	23	LEU
1	A	73	LYS
1	A	76	GLU
1	A	103	LYS
1	A	106	GLU
1	A	213[A]	VAL
1	A	213[B]	VAL
1	A	224	LYS
1	A	273	LEU
1	A	276	ASP
1	A	295	SER
1	A	297	LEU
1	A	310	VAL
1	A	328	LYS
1	A	335	ARG
1	B	23	LEU
1	B	55	LYS
1	B	71	SER
1	B	73	LYS
1	B	104	LYS
1	B	130	LEU
1	B	157	LYS
1	B	213	VAL
1	B	228	LEU
1	B	285	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	292	ASN
1	B	146	ASN
1	B	236	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z > 2$
6	ACT	A	406	-	3,3,3	1.09	0	3,3,3	0.73	0
7	GOL	B	408	-	5,5,5	0.07	0	5,5,5	0.38	0
6	ACT	B	414	-	3,3,3	0.96	0	3,3,3	0.77	0
5	P6G	A	404	-	18,18,18	0.58	0	17,17,17	0.28	0
6	ACT	B	412	-	3,3,3	1.04	0	3,3,3	0.86	0
7	GOL	B	410	-	5,5,5	0.13	0	5,5,5	0.43	0
2	U6A	A	401	-	10,10,10	3.43	6 (60%)	12,13,13	1.65	3 (25%)
7	GOL	B	404	-	5,5,5	0.14	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	B	409	-	6,6,6	0.13	0	5,5,5	0.10	0
7	GOL	B	407	-	5,5,5	0.12	0	5,5,5	0.41	0
2	U6A	B	401	-	10,10,10	4.37	4 (40%)	12,13,13	1.55	2 (16%)
4	DPO	A	403	3	6,8,8	1.07	0	12,13,13	0.83	0
7	GOL	B	413	-	5,5,5	0.14	0	5,5,5	0.41	0
6	ACT	B	411	-	3,3,3	1.11	0	3,3,3	0.76	0
4	DPO	B	403	3	6,8,8	1.01	0	12,13,13	0.89	0
7	GOL	B	406	-	5,5,5	0.12	0	5,5,5	0.34	0
6	ACT	A	405	-	3,3,3	1.00	0	3,3,3	0.85	0
7	GOL	B	405	-	5,5,5	0.18	0	5,5,5	0.47	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
7	GOL	B	408	-	-	2/4/4/4	-
5	P6G	A	404	-	-	8/16/16/16	-
7	GOL	B	410	-	-	2/4/4/4	-
2	U6A	A	401	-	-	2/12/12/12	-
7	GOL	B	404	-	-	2/4/4/4	-
8	PEG	B	409	-	-	2/4/4/4	-
7	GOL	B	407	-	-	2/4/4/4	-
2	U6A	B	401	-	-	2/12/12/12	-
4	DPO	A	403	3	-	3/6/6/6	-
7	GOL	B	413	-	-	0/4/4/4	-
4	DPO	B	403	3	-	3/6/6/6	-
7	GOL	B	406	-	-	2/4/4/4	-
7	GOL	B	405	-	-	1/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	U6A	C1-N	10.46	1.53	1.35
2	A	401	U6A	C1-N	8.48	1.50	1.35
2	B	401	U6A	CA-C	7.61	1.64	1.52
2	A	401	U6A	CA-C	4.23	1.59	1.52
2	B	401	U6A	O1-C1	2.89	1.27	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	U6A	C6-CA	2.80	1.61	1.53
2	A	401	U6A	CA-N	2.43	1.50	1.45
2	B	401	U6A	CA-N	2.37	1.50	1.45
2	A	401	U6A	C7-C6	2.20	1.58	1.51
2	A	401	U6A	OXT-C	-2.01	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	U6A	O1-C1-N	-3.76	118.69	124.86
2	B	401	U6A	C-CA-N	3.68	118.26	110.17
2	A	401	U6A	C-CA-N	3.04	116.86	110.17
2	B	401	U6A	O1-C1-N	-2.25	121.16	124.86
2	A	401	U6A	C7-C6-CA	2.01	116.26	112.29

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	DPO	P2-O4-P1-O3
7	B	404	GOL	O1-C1-C2-C3
7	B	406	GOL	C1-C2-C3-O3
7	B	407	GOL	O1-C1-C2-C3
7	B	410	GOL	C1-C2-C3-O3
5	A	404	P6G	O13-C14-C15-O16
5	A	404	P6G	O4-C5-C6-O7
7	B	406	GOL	O2-C2-C3-O3
7	B	407	GOL	O1-C1-C2-O2
5	A	404	P6G	C2-C3-O4-C5
7	B	408	GOL	C1-C2-C3-O3
7	B	404	GOL	O1-C1-C2-O2
8	B	409	PEG	O1-C1-C2-O2
5	A	404	P6G	C11-C12-O13-C14
7	B	410	GOL	O2-C2-C3-O3
7	B	405	GOL	C1-C2-C3-O3
5	A	404	P6G	C8-C9-O10-C11
4	A	403	DPO	P2-O4-P1-O1
2	A	401	U6A	C7-C6-CA-N
2	B	401	U6A	C7-C6-CA-N
5	A	404	P6G	C18-C17-O16-C15
2	A	401	U6A	O8-C6-CA-N
5	A	404	P6G	O10-C11-C12-O13

Continued on next page...

Continued from previous page...

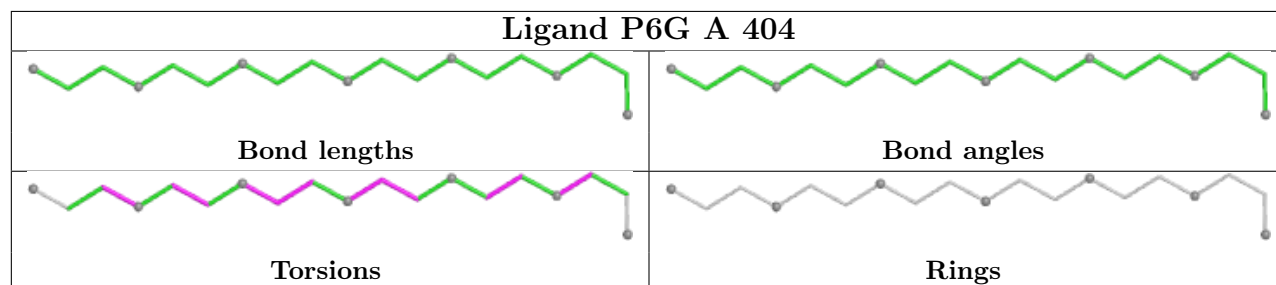
Mol	Chain	Res	Type	Atoms
7	B	408	GOL	O2-C2-C3-O3
8	B	409	PEG	C1-C2-O2-C3
4	A	403	DPO	P2-O4-P1-O2
4	A	403	DPO	P2-O4-P1-O3
4	B	403	DPO	P2-O4-P1-O2
2	B	401	U6A	O1-C1-N-CA
5	A	404	P6G	O7-C8-C9-O10
4	B	403	DPO	P2-O4-P1-O1

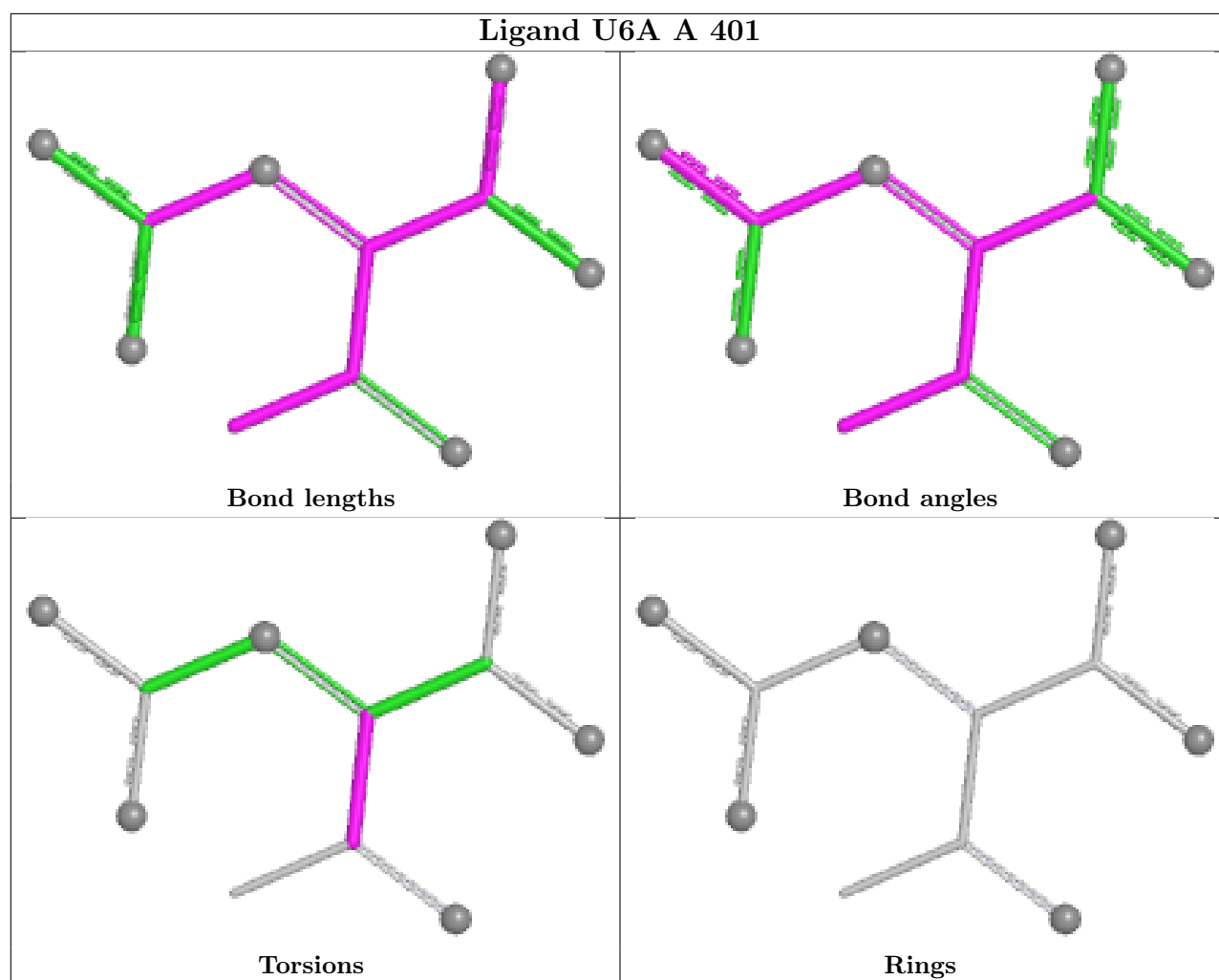
There are no ring outliers.

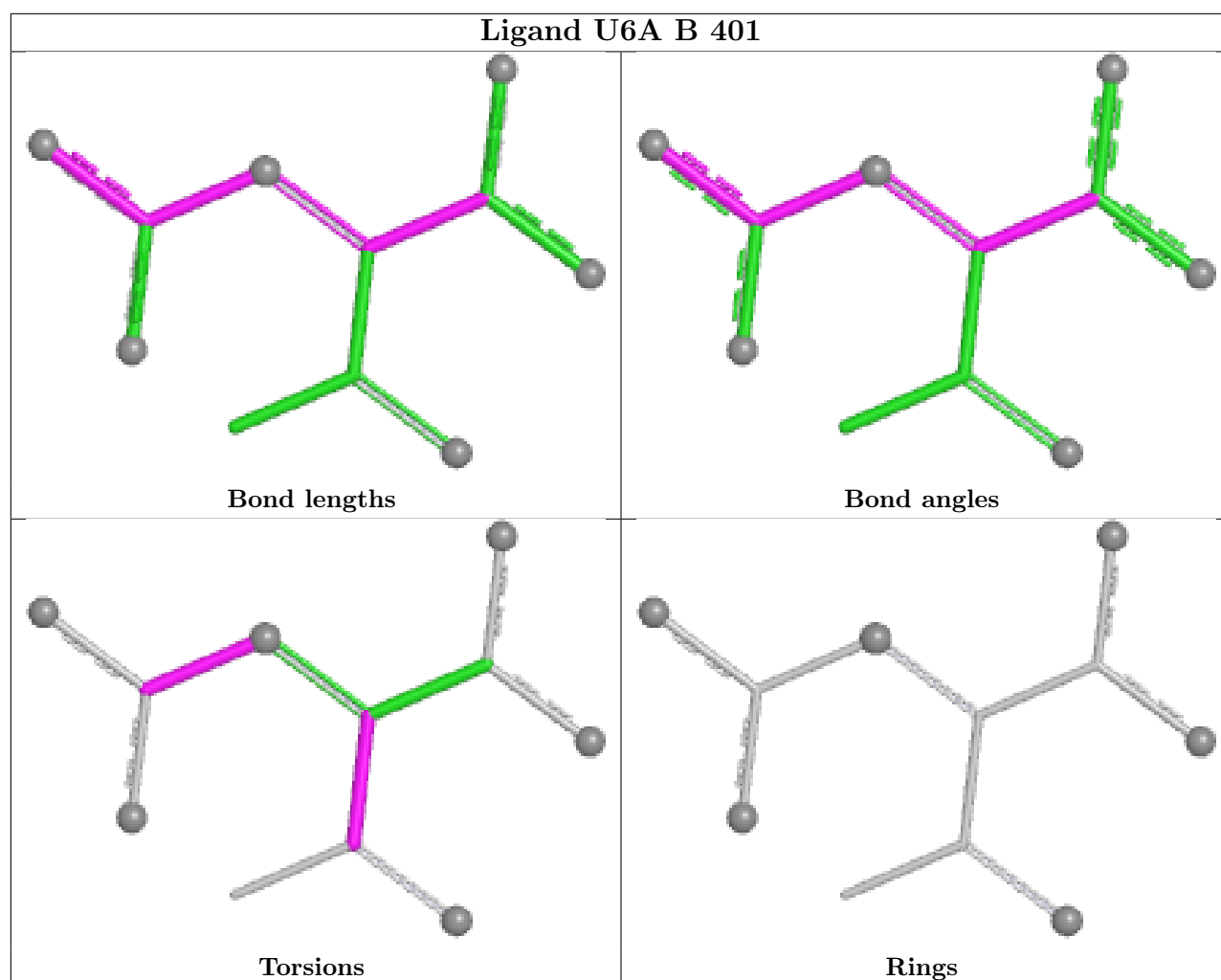
1 monomer is involved in 1 short contact:

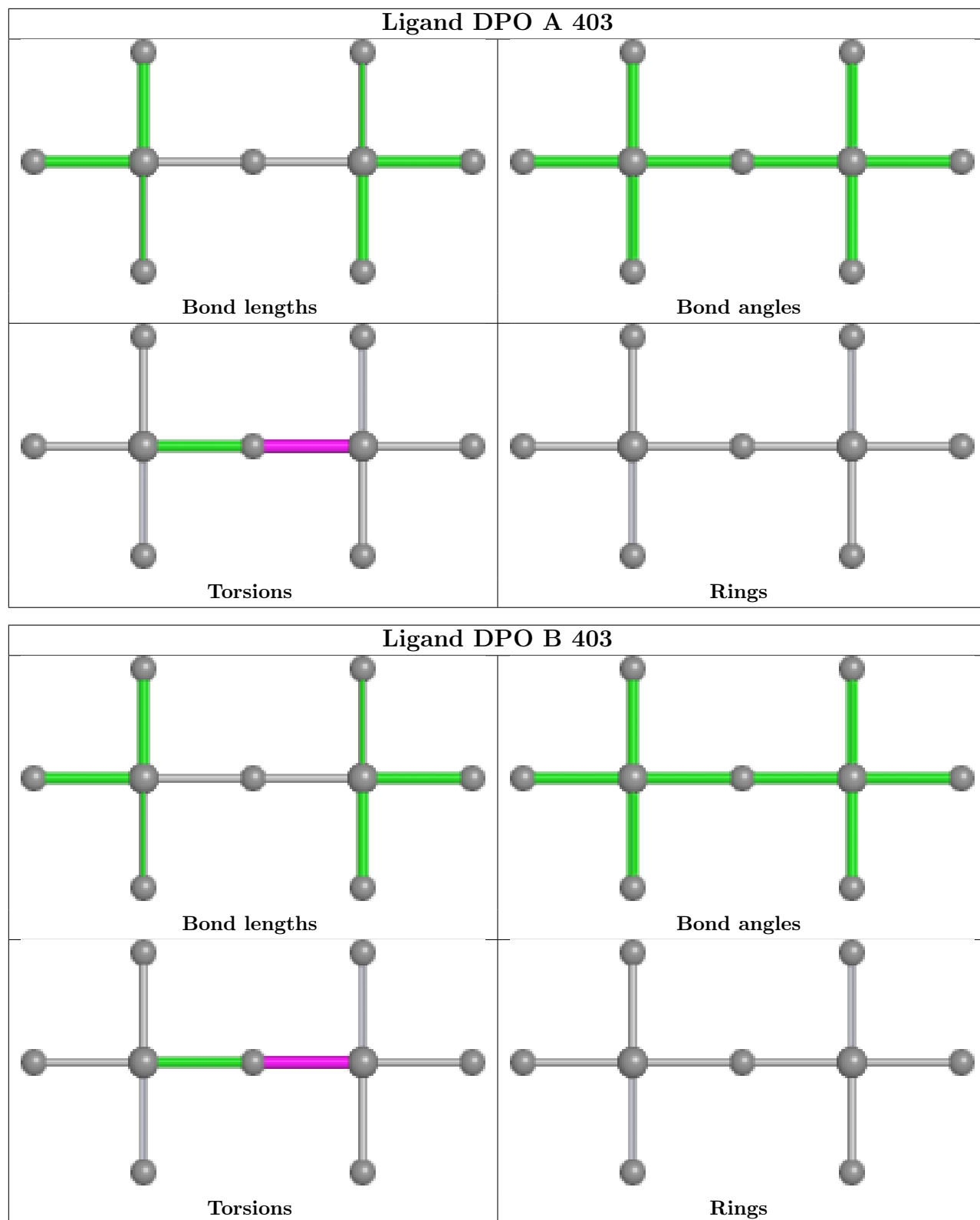
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	407	GOL	1	0

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/340 (98%)	0.13	15 (4%) 38 39	19, 51, 89, 111	3 (0%)
1	B	336/340 (98%)	-0.09	16 (4%) 35 36	21, 40, 65, 85	3 (0%)
All	All	671/680 (98%)	0.02	31 (4%) 37 38	19, 46, 79, 111	6 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	GLY	5.1
1	B	228	LEU	5.0
1	A	272	GLU	3.8
1	B	224	LYS	3.3
1	B	230	PRO	3.1
1	B	234	TYR	3.0
1	A	221	GLY	3.0
1	A	276	ASP	3.0
1	B	222	ASN	3.0
1	B	73	LYS	3.0
1	B	223	PHE	2.9
1	B	0	ALA	2.7
1	A	257	LYS	2.6
1	A	1	SER	2.5
1	A	228	LEU	2.5
1	B	231	GLY	2.5
1	B	219[A]	ARG	2.5
1	B	232	MET	2.3
1	B	229	ALA	2.2
1	B	233	LYS	2.2
1	A	226	ARG	2.2
1	A	250	THR	2.2
1	B	235	ARG	2.2
1	A	258	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	ARG	2.1
1	A	224	LYS	2.1
1	A	106	GLU	2.1
1	A	225	GLY	2.1
1	A	220	LYS	2.0
1	A	230	PRO	2.0
1	B	226	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	B	414	4/4	0.77	0.24	64,68,69,77	0
6	ACT	A	406	4/4	0.79	0.20	64,67,67,68	0
8	PEG	B	409	7/7	0.83	0.21	62,66,73,73	0
7	GOL	B	408	6/6	0.84	0.21	56,68,68,73	0
7	GOL	B	413	6/6	0.84	0.18	55,61,62,68	0
7	GOL	B	405	6/6	0.84	0.16	52,58,61,61	0
5	P6G	A	404	19/19	0.85	0.21	76,81,90,92	0
7	GOL	B	404	6/6	0.85	0.20	64,65,67,69	0
6	ACT	B	412	4/4	0.85	0.18	65,68,69,70	0
6	ACT	A	405	4/4	0.86	0.24	66,69,70,70	0
6	ACT	B	411	4/4	0.88	0.14	50,51,53,53	0
7	GOL	B	410	6/6	0.89	0.16	49,61,62,62	0
7	GOL	B	406	6/6	0.90	0.14	65,74,76,79	0
7	GOL	B	407	6/6	0.91	0.13	46,52,58,64	0
2	U6A	A	401	11/11	0.95	0.08	39,42,47,53	0
2	U6A	B	401	11/11	0.95	0.08	35,38,44,48	0

Continued on next page...

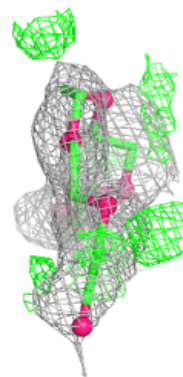
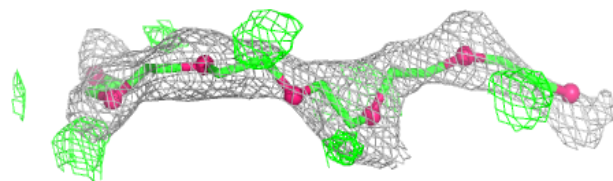
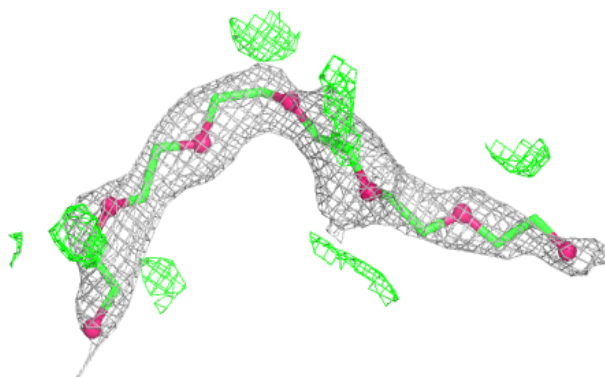
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	402	1/1	0.97	0.05	39,39,39,39	0
4	DPO	A	403	9/9	0.98	0.04	42,46,47,47	0
4	DPO	B	403	9/9	0.99	0.04	32,35,40,43	0
3	MG	A	402	1/1	1.00	0.02	41,41,41,41	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.

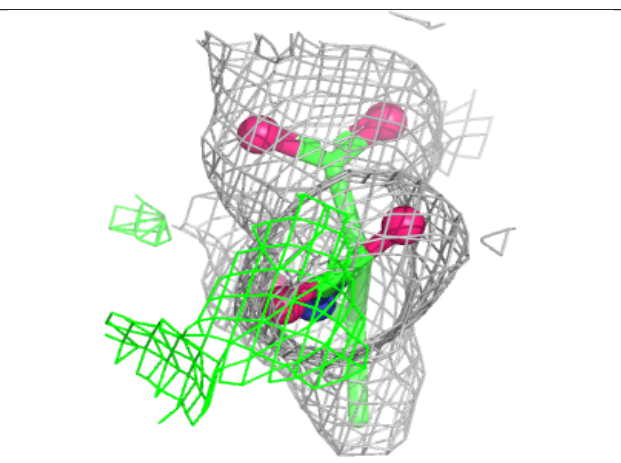
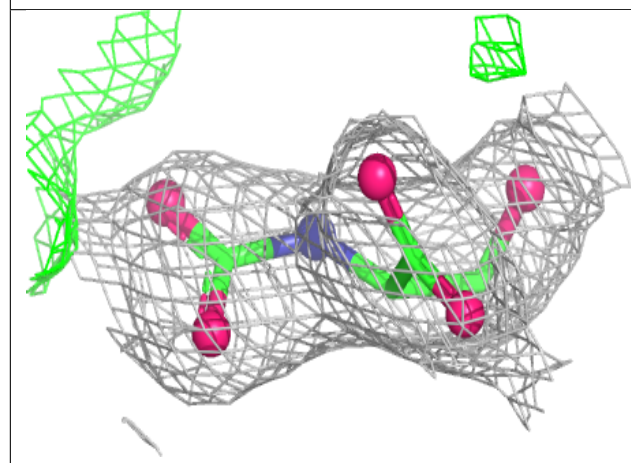
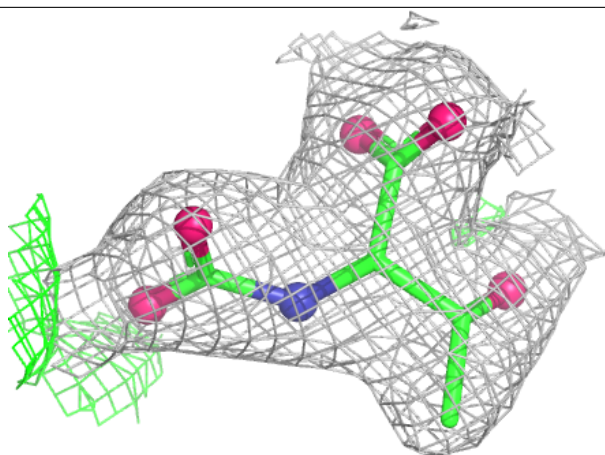
Electron density around P6G A 404:

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



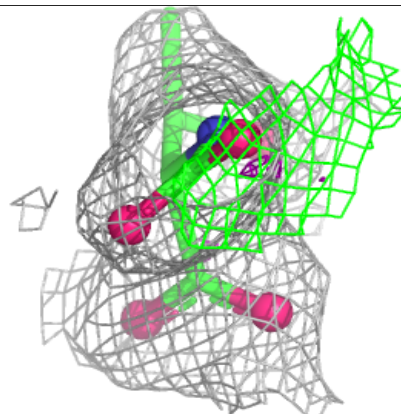
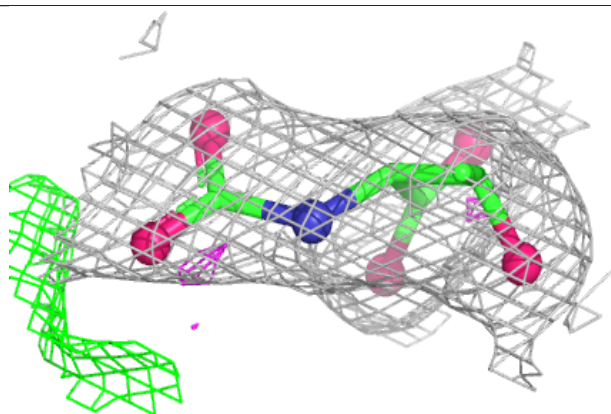
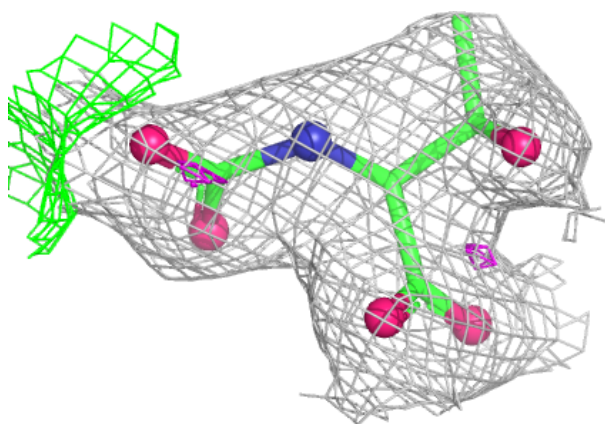
Electron density around U6A A 401:

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



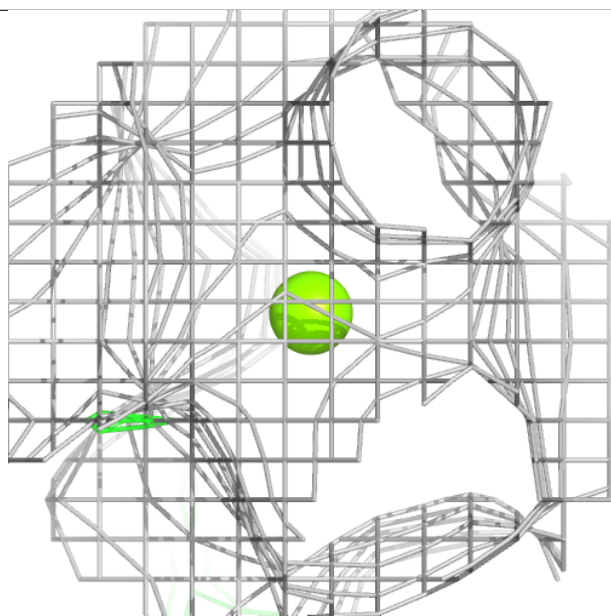
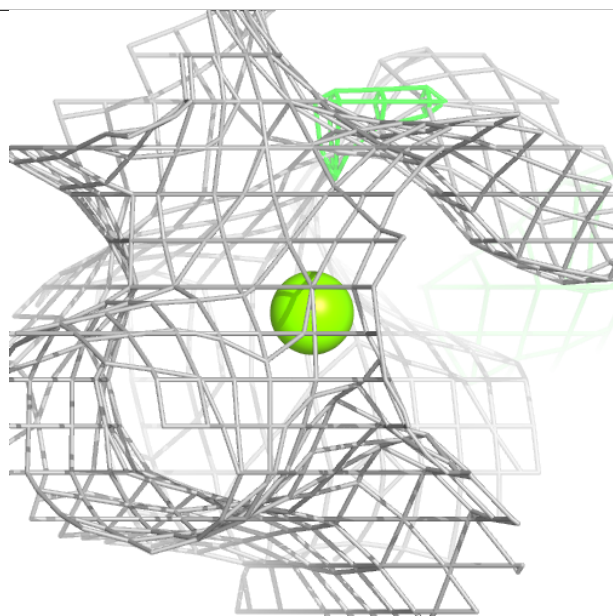
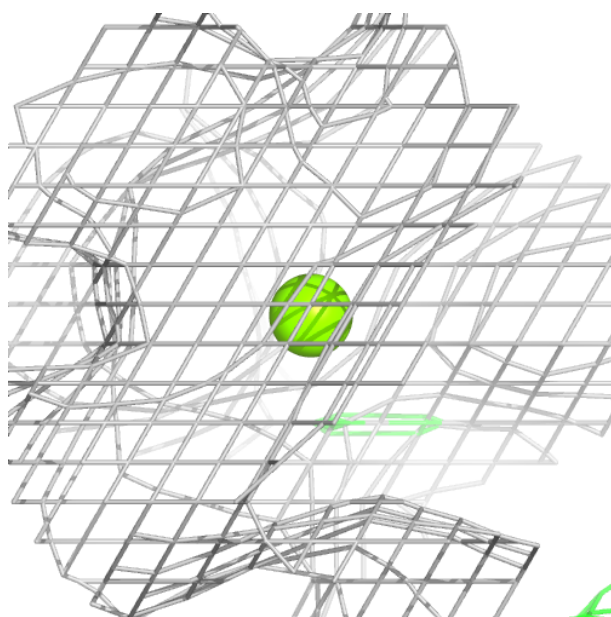
Electron density around U6A B 401:

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



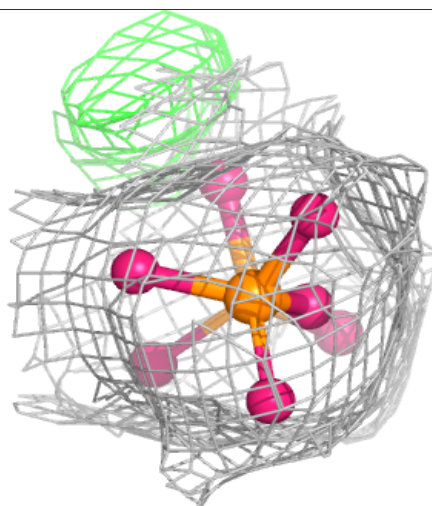
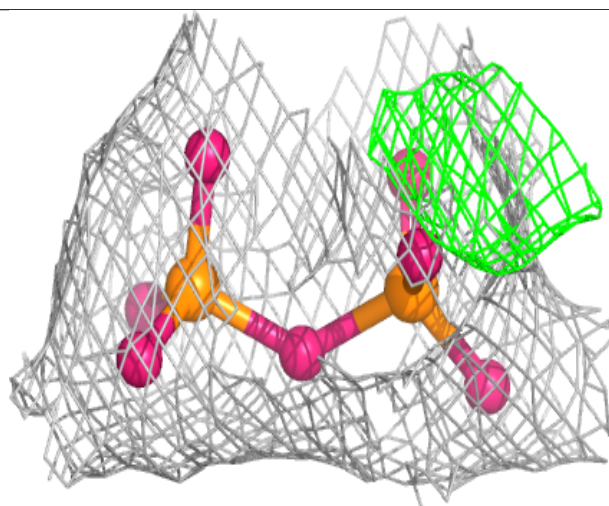
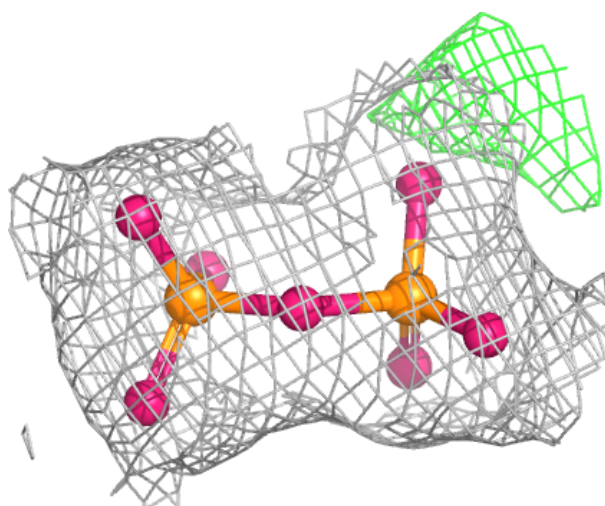
Electron density around MG B 402:

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



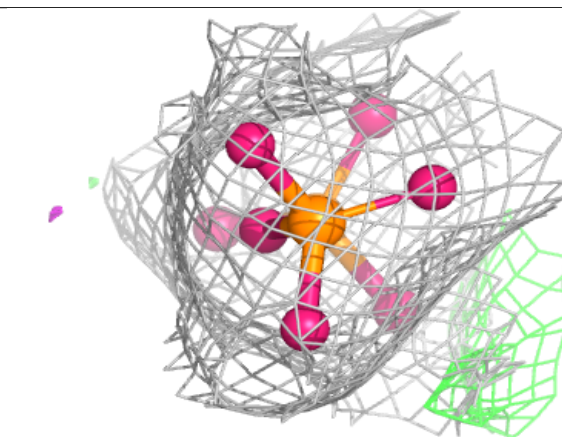
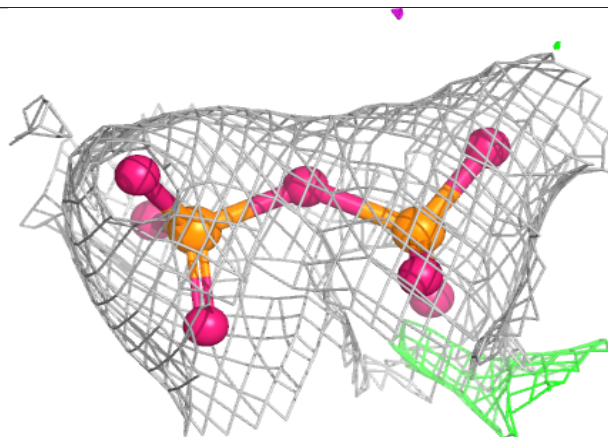
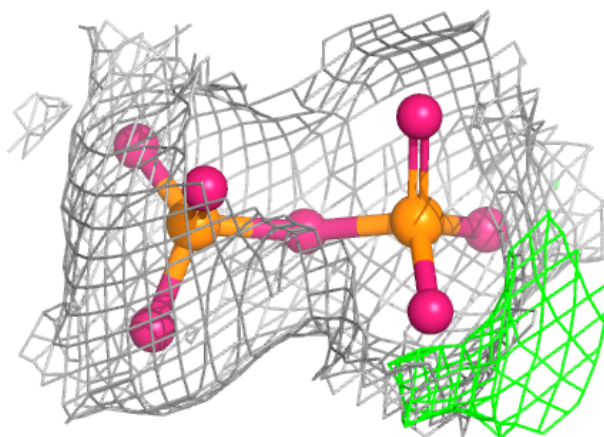
Electron density around DPO A 403:

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



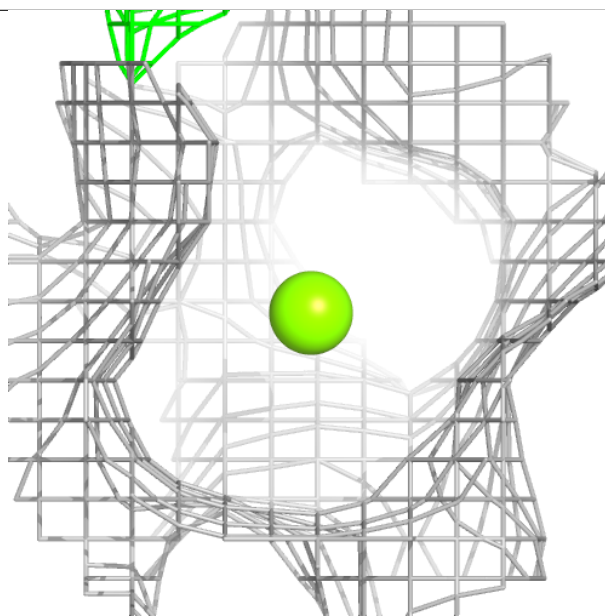
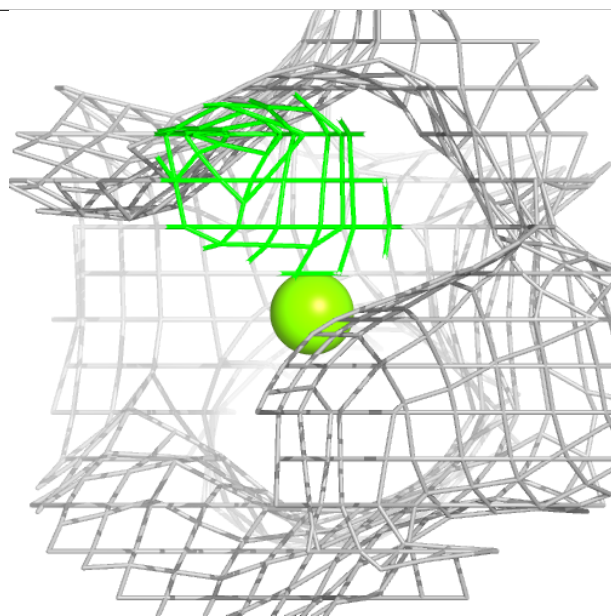
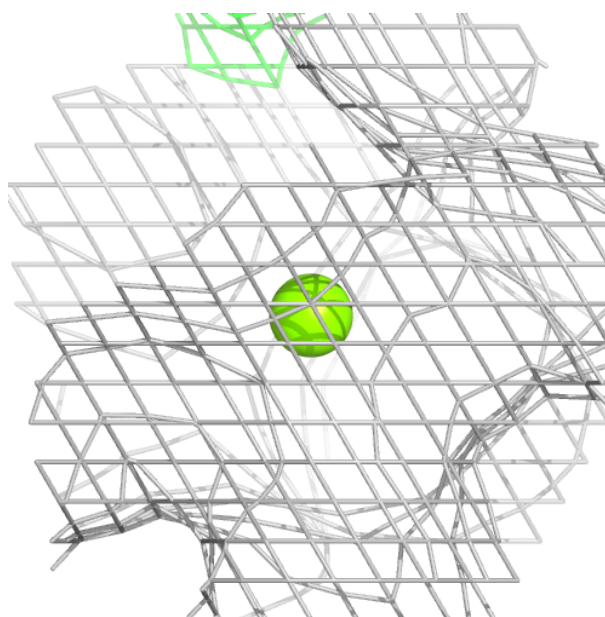
Electron density around DPO B 403:

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



Electron density around MG A 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.