Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 01:00 PM JST

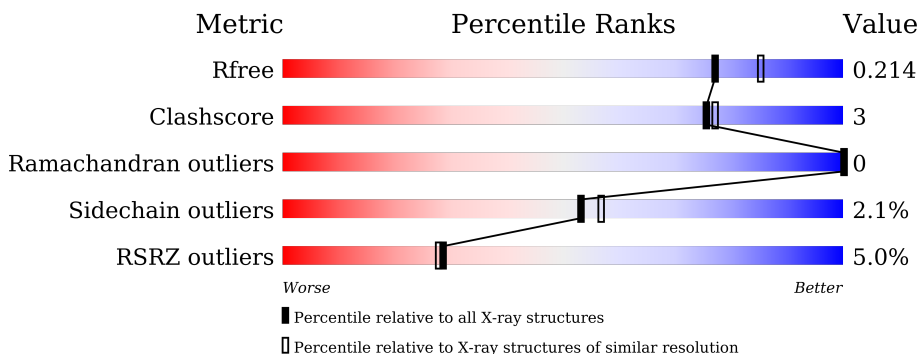|		
PDB ID	:	6J1J
Title	:	Crystal structure of HypX from Aquifex aeolicus, A392F-I419F variant in complex with Tetrahydrofolic acid
Authors	:	Muraki, N.; Aono, S.
Deposited on	:	2018-12-28
Resolution	:	2.00 Å(reported)

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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 2.00 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	Percentile Ranks	Value
Rfree		0.214
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		5.0%

Worse ——— Better

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	582	5% — 88% — 9% ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	A	601	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4778 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 Hydrogenase regulation HoxX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	4606	2963	791	834	18	0	6	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O67224
A	-18	GLY	-	expression tag	UNP O67224
A	-17	SER	-	expression tag	UNP O67224
A	-16	SER	-	expression tag	UNP O67224
A	-15	HIS	-	expression tag	UNP O67224
A	-14	HIS	-	expression tag	UNP O67224
A	-13	HIS	-	expression tag	UNP O67224
A	-12	HIS	-	expression tag	UNP O67224
A	-11	HIS	-	expression tag	UNP O67224
A	-10	HIS	-	expression tag	UNP O67224
A	-9	SER	-	expression tag	UNP O67224
A	-8	SER	-	expression tag	UNP O67224
A	-7	GLY	-	expression tag	UNP O67224
A	-6	LEU	-	expression tag	UNP O67224
A	-5	VAL	-	expression tag	UNP O67224
A	-4	PRO	-	expression tag	UNP O67224
A	-3	ARG	-	expression tag	UNP O67224
A	-2	GLY	-	expression tag	UNP O67224
A	-1	SER	-	expression tag	UNP O67224
A	0	HIS	-	expression tag	UNP O67224
A	392	PHE	ALA	engineered mutation	UNP O67224
A	419	PHE	ILE	engineered mutation	UNP O67224

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).

COA
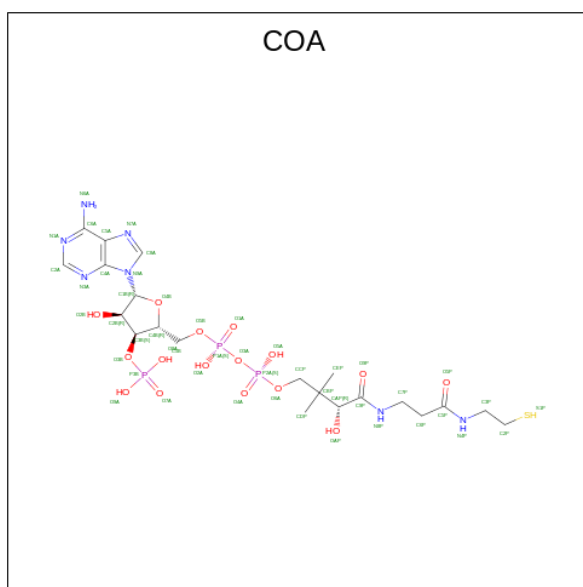
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0

- Molecule 3 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$) (labeled as "Ligand of Interest" by depositor).

THG
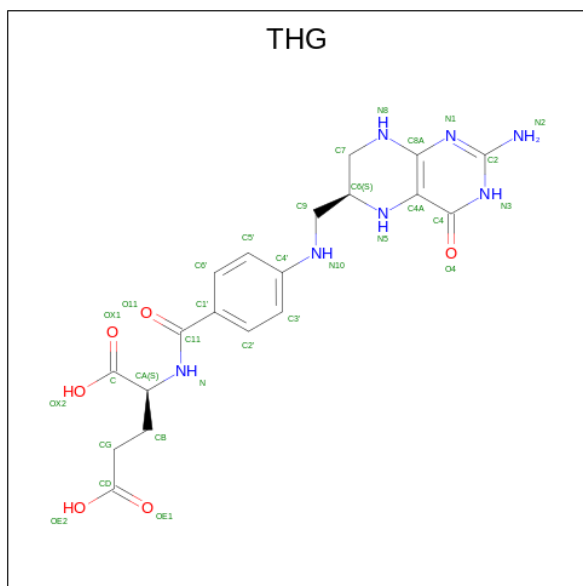
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	19	7	6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1　　C2

HO　　　　OH

O1　　　　O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total　C　O 6　　3　3			0	0
4	A	1	Total　C　O 6　　3　3			0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total　O 80　　80		0	0

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: Hydrogenase regulation HoxX
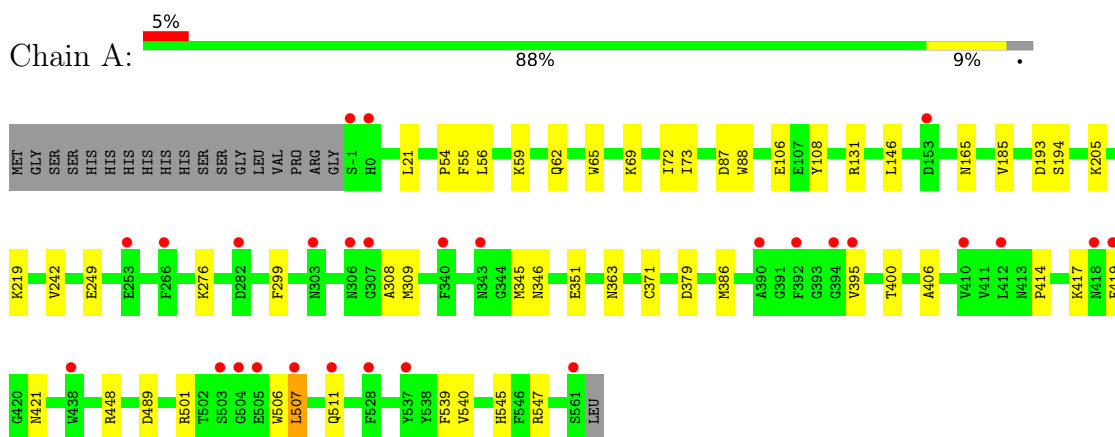
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	69.43Å 141.89Å 170.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 2.00 39.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.09-2.00) 99.9 (39.09-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.180 , 0.214 0.180 , 0.214	Depositor DCC
R_{free} test set	2000 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4778	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: COA, THG, GOL

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	0.38	0/4743	0.53	0/6414

There are no bond length outliers.

There are no bond angle outliers.

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	4606	0	4509	28	0
2	A	48	0	32	5	0
3	A	32	0	21	1	0
4	A	12	0	16	3	0
5	A	80	0	0	0	0
All	All	4778	0	4578	29	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 (29) 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)
2:A:601:COA:O4B	2:A:601:COA:C1B	1.66	1.23
1:A:56:LEU:H	2:A:601:COA:H22	1.56	0.69
1:A:345:MET:O	2:A:601:COA:N6A	2.31	0.61
1:A:185:VAL:HG11	1:A:242[A]:VAL:HG21	1.84	0.60
1:A:351:GLU:HG2	1:A:540:VAL:HG11	1.85	0.58
1:A:55:PHE:HE1	2:A:601:COA:H61	1.75	0.52
1:A:205:LYS:NZ	1:A:249:GLU:OE2	2.41	0.51
1:A:54:PRO:HA	1:A:73:ILE:HD13	1.93	0.51
1:A:545:HIS:HA	4:A:604:GOL:H31	1.93	0.49
1:A:276:LYS:HD3	1:A:276:LYS:HA	1.69	0.47
1:A:88:TRP:CD1	1:A:165:ASN:HB3	2.50	0.47
1:A:386:MET:HE2	1:A:406:ALA:HB2	1.97	0.46
1:A:308:ALA:HB1	1:A:346:ASN:HA	1.97	0.46
1:A:379:ASP:OD1	1:A:379:ASP:N	2.49	0.45
1:A:62:GLN:HG2	1:A:65:TRP:CZ2	2.52	0.44
1:A:309:MET:HE2	1:A:309:MET:HB3	1.59	0.44
1:A:59:LYS:HG3	1:A:108:TYR:CE1	2.53	0.43
1:A:395:VAL:HG11	1:A:414:PRO:HB3	2.00	0.43
1:A:299:PHE:CG	4:A:603:GOL:H12	2.53	0.43
1:A:507:LEU:O	1:A:511:GLN:HG2	2.20	0.42
1:A:62:GLN:NE2	1:A:106:GLU:OE2	2.53	0.42
1:A:419:PHE:HZ	1:A:539:PHE:CG	2.37	0.41
1:A:131:ARG:NH1	2:A:601:COA:O5B	2.52	0.41
1:A:545:HIS:ND1	4:A:604:GOL:H31	2.35	0.41
1:A:72:ILE:HD13	3:A:602:THG:C4A	2.51	0.41
1:A:371:CYS:HB3	1:A:400:THR:HG21	2.03	0.41
1:A:417:LYS:HB2	1:A:448:ARG:HG2	2.03	0.41
1:A:193:ASP:OD1	1:A:194:SER:HA	2.20	0.40
1:A:501:ARG:HD3	1:A:506:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/582 (97%)	548 (97%)	19 (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	483/512 (94%)	473 (98%)	10 (2%)	53	57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	69	LYS
1	A	87	ASP
1	A	146	LEU
1	A	219	LYS
1	A	363	ASN
1	A	421	ASN
1	A	489	ASP
1	A	507	LEU
1	A	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	#$|Z| > 2$
3	THG	A	602	-	32,34,34	4.03	19 (59%)	39,47,47	1.41	5 (12%)
4	GOL	A	603	-	5,5,5	1.04	0	5,5,5	1.02	0
2	COA	A	601	-	41,50,50	4.35	15 (36%)	52,75,75	1.63	7 (13%)
4	GOL	A	604	-	5,5,5	1.01	0	5,5,5	0.84	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
3	THG	A	602	-	-	6/22/31/31	0/3/3/3
4	GOL	A	603	-	-	2/4/4/4	-
2	COA	A	601	-	-	24/44/64/64	0/3/3/3
4	GOL	A	604	-	-	4/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	COA	O4B-C1B	18.08	1.66	1.41
2	A	601	COA	C2B-C1B	-13.57	1.33	1.53
2	A	601	COA	C9P-N8P	9.07	1.53	1.33
3	A	602	THG	C5'-C4'	8.88	1.54	1.39
3	A	602	THG	C2'-C3'	8.58	1.54	1.38
3	A	602	THG	C6'-C1'	8.10	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	THG	C2-N2	6.40	1.46	1.33
3	A	602	THG	C11-N	6.21	1.47	1.34
2	A	601	COA	P3B-O3B	6.16	1.70	1.59
3	A	602	THG	O4-C4	5.94	1.39	1.24
2	A	601	COA	O4B-C4B	-5.75	1.32	1.45
3	A	602	THG	C4A-N5	5.44	1.49	1.38
3	A	602	THG	C2-N3	5.33	1.44	1.35
2	A	601	COA	C5P-N4P	4.28	1.43	1.33
3	A	602	THG	C8A-N1	4.19	1.42	1.34
2	A	601	COA	C2A-N3A	3.99	1.38	1.32
3	A	602	THG	C4'-N10	3.78	1.49	1.38
3	A	602	THG	C3'-C4'	-3.76	1.32	1.39
3	A	602	THG	C2-N1	3.55	1.41	1.35
3	A	602	THG	C4A-C4	3.54	1.46	1.41
3	A	602	THG	C2'-C1'	-3.49	1.33	1.39
2	A	601	COA	C7P-N8P	3.45	1.54	1.46
3	A	602	THG	C4-N3	3.26	1.38	1.33
3	A	602	THG	C5'-C6'	-2.94	1.33	1.38
2	A	601	COA	C6A-N6A	2.50	1.43	1.34
2	A	601	COA	O3B-C3B	-2.45	1.35	1.44
2	A	601	COA	C5A-C4A	-2.36	1.34	1.40
2	A	601	COA	C6P-C5P	2.35	1.55	1.51
2	A	601	COA	P2A-O6A	2.32	1.68	1.59
3	A	602	THG	CG-CD	2.23	1.55	1.50
2	A	601	COA	OAP-CAP	-2.17	1.38	1.42
3	A	602	THG	O11-C11	-2.12	1.19	1.23
3	A	602	THG	C9-N10	2.11	1.49	1.45
2	A	601	COA	P1A-O5B	2.02	1.67	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	COA	C5A-C6A-N6A	5.63	128.90	120.35
2	A	601	COA	N3A-C2A-N1A	-4.63	121.44	128.68
3	A	602	THG	C8A-C4A-C4	4.38	118.46	114.57
2	A	601	COA	N6A-C6A-N1A	-3.89	110.50	118.57
2	A	601	COA	CAP-C9P-N8P	3.74	124.02	116.58
3	A	602	THG	C4A-N5-C6	-3.71	111.72	121.48
2	A	601	COA	O6A-CCP-CBP	2.88	115.17	110.55
2	A	601	COA	O9P-C9P-N8P	-2.68	117.24	122.99
2	A	601	COA	C6P-C5P-N4P	2.35	120.37	116.42
3	A	602	THG	C4-C4A-N5	2.25	121.01	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	THG	C2-N1-C8A	2.24	119.57	114.54
3	A	602	THG	OX2-C-CA	2.03	120.16	113.40

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	COA	C5B-O5B-P1A-O1A
2	A	601	COA	C5B-O5B-P1A-O3A
2	A	601	COA	P2A-O3A-P1A-O5B
2	A	601	COA	CCP-O6A-P2A-O3A
2	A	601	COA	CCP-O6A-P2A-O4A
2	A	601	COA	CCP-O6A-P2A-O5A
2	A	601	COA	CAP-CBP-CCP-O6A
2	A	601	COA	OAP-CAP-CBP-CCP
2	A	601	COA	C9P-CAP-CBP-CCP
2	A	601	COA	OAP-CAP-CBP-CDP
2	A	601	COA	C9P-CAP-CBP-CDP
2	A	601	COA	OAP-CAP-CBP-CEP
2	A	601	COA	C9P-CAP-CBP-CEP
2	A	601	COA	O9P-C9P-CAP-CBP
2	A	601	COA	N8P-C9P-CAP-CBP
2	A	601	COA	C5P-C6P-C7P-N8P
4	A	603	GOL	C1-C2-C3-O3
4	A	603	GOL	O2-C2-C3-O3
3	A	602	THG	N-CA-CB-CG
2	A	601	COA	C3B-C4B-C5B-O5B
2	A	601	COA	O4B-C4B-C5B-O5B
3	A	602	THG	C-CA-CB-CG
2	A	601	COA	CDP-CBP-CCP-O6A
2	A	601	COA	CEP-CBP-CCP-O6A
4	A	604	GOL	O1-C1-C2-C3
4	A	604	GOL	C1-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
3	A	602	THG	CA-CB-CG-CD
4	A	604	GOL	O1-C1-C2-O2
2	A	601	COA	N8P-C9P-CAP-OAP
3	A	602	THG	C6-C9-N10-C4'
3	A	602	THG	OE1-CD-CG-CB
3	A	602	THG	OE2-CD-CG-CB
2	A	601	COA	P2A-O3A-P1A-O1A
2	A	601	COA	P1A-O3A-P2A-O5A

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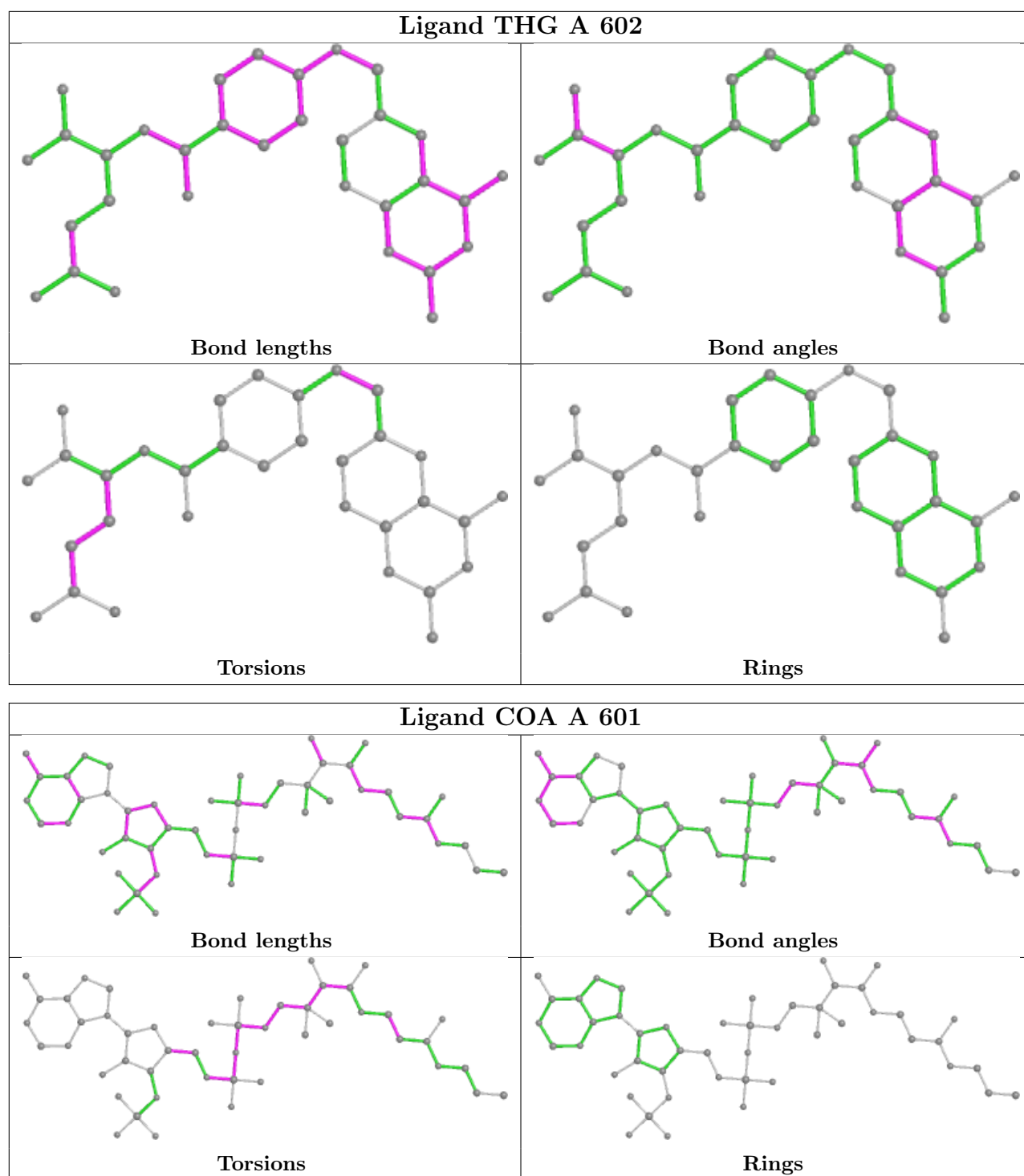| Mol	Chain	Res	Type	Atoms
2	A	601	COA	CBP-CCP-O6A-P2A

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	THG	1	0
4	A	603	GOL	1	0
2	A	601	COA	5	0
4	A	604	GOL	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand THG A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand COA A 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	563/582 (96%)	0.19	28 (4%)	28	28	33, 51, 82, 120	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	SER	5.8
1	A	561	SER	4.7
1	A	528	PHE	4.0
1	A	419	PHE	3.7
1	A	282	ASP	3.7
1	A	438	TRP	3.5
1	A	307	GLY	2.9
1	A	507	LEU	2.7
1	A	392	PHE	2.6
1	A	412[A]	LEU	2.6
1	A	503	SER	2.4
1	A	418	ASN	2.4
1	A	395	VAL	2.4
1	A	410	VAL	2.3
1	A	537	TYR	2.3
1	A	303[A]	ASN	2.3
1	A	343	ASN	2.2
1	A	505	GLU	2.2
1	A	511	GLN	2.2
1	A	306	ASN	2.2
1	A	266	PHE	2.2
1	A	253	GLU	2.2
1	A	0	HIS	2.2
1	A	390	ALA	2.2
1	A	153	ASP	2.1
1	A	340	PHE	2.1
1	A	504	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

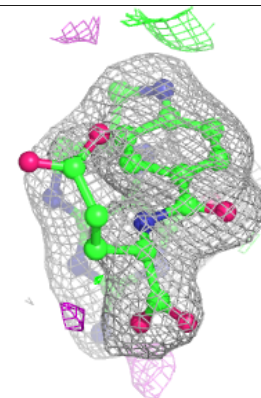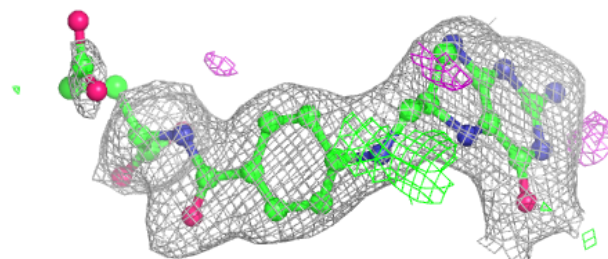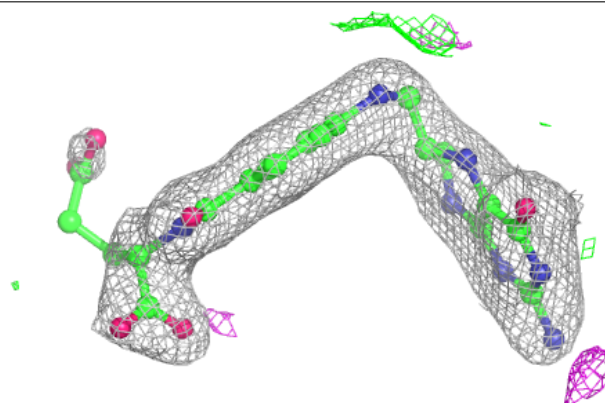| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	A	601	48/48	0.65	0.41	47,85,105,114	48
4	GOL	A	604	6/6	0.65	0.23	87,93,100,102	0
4	GOL	A	603	6/6	0.85	0.18	52,66,74,80	0
3	THG	A	602	32/32	0.94	0.14	47,55,106,108	0

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 COA A 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
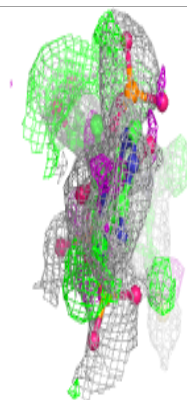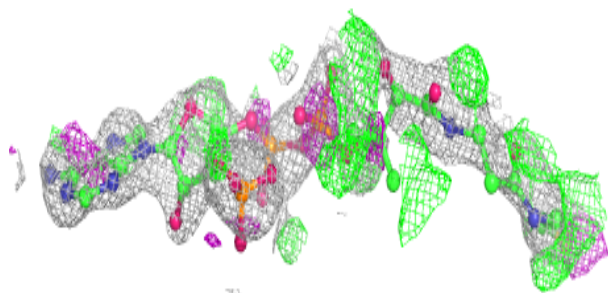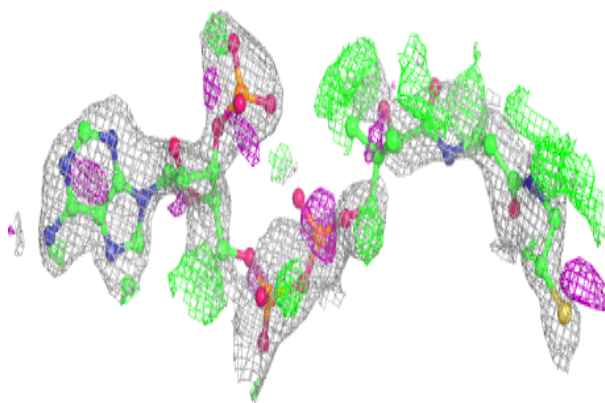
Electron density around THG A 602:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.