Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:28 PM JST

PDB ID	:	6J1F
Title	:	Crystal structure of HypX from Aquifex aeolicus in complex with Tetrahydrofolic acid
Authors	:	Muraki, N.; Aono, S.
Deposited on	:	2018-12-28
Resolution	:	2.10 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:

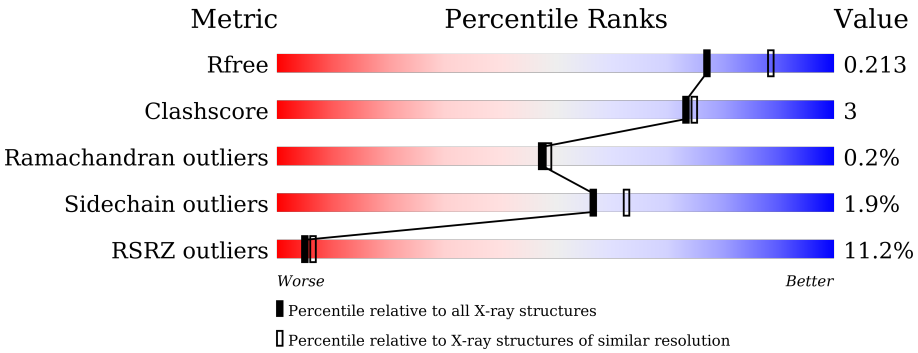
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	3% 88% 8% ·
2	B	576	18% 84% 12% · ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9405 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	564	4608	2958	791	841	18	0	1	0

There are 20 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

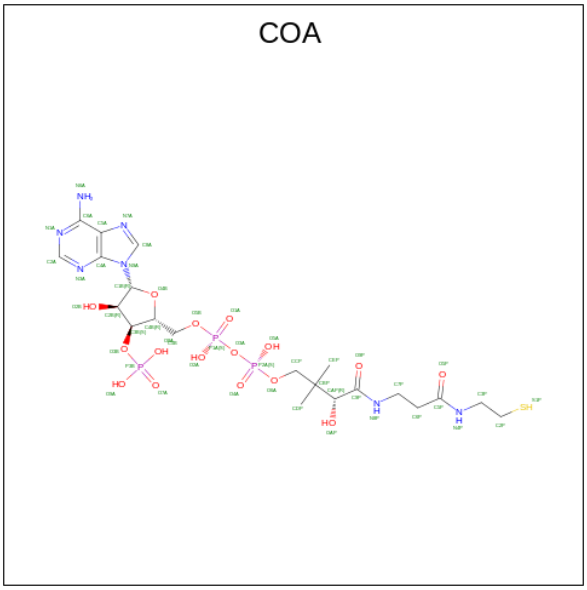
- Molecule 2 is a protein called Hydrogenase regulation HoxX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	557	4461	2863	761	820	17	0	12	0

There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

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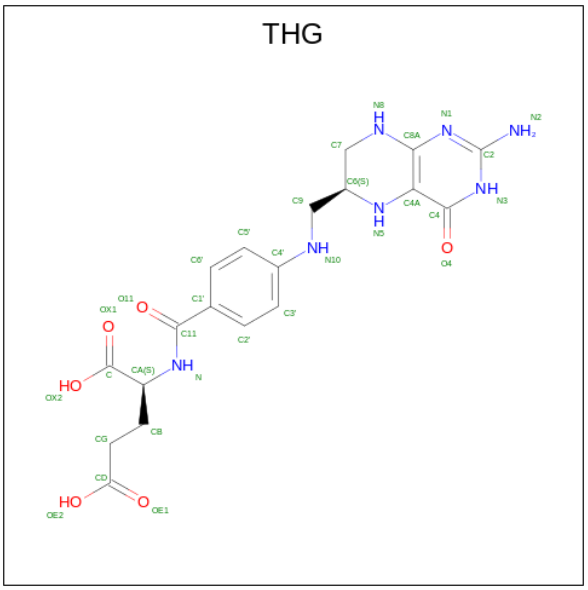
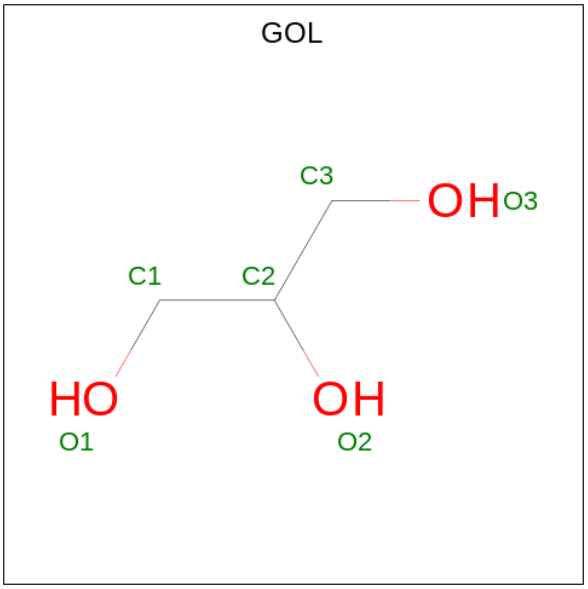
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

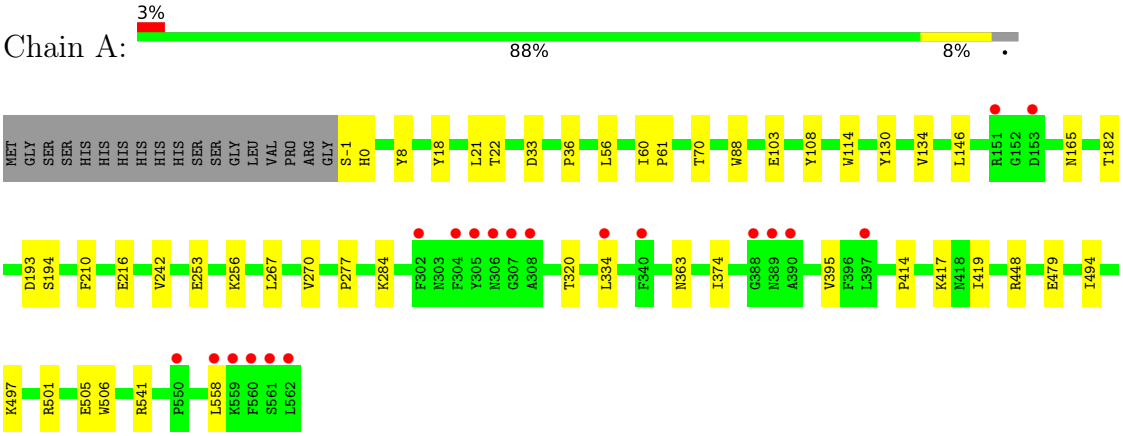
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	B	55	Total O 55 55	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

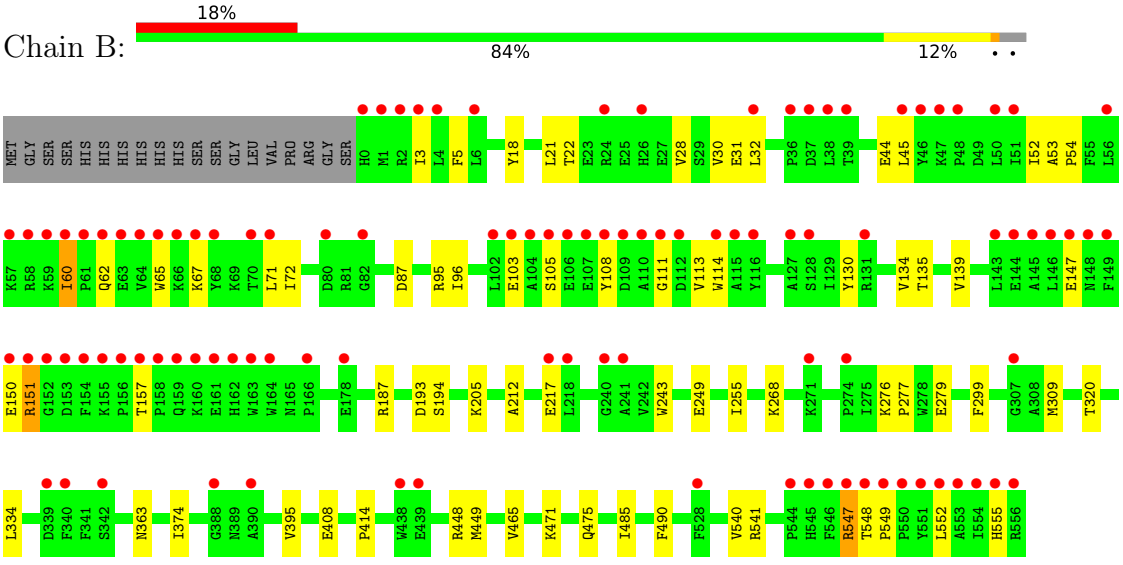
• Molecule 1: Hydrogenase regulation HoxX

Chain A:



• Molecule 2: Hydrogenase regulation HoxX

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	80.02Å 123.73Å 290.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 2.10 42.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.31-2.10) 99.9 (42.31-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.177 , 0.213 0.177 , 0.213	Depositor DCC
R_{free} test set	4205 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: THG, GOL, COA

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	0.46	0/4728	0.57	0/6387
2	B	9.13	2/4580 (0.0%)	0.78	4/6206 (0.1%)
All	All	6.41	2/9308 (0.0%)	0.68	4/12593 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	547[A]	ARG	CB-CG	436.44	13.30	1.52
2	B	547[B]	ARG	CB-CG	436.44	13.30	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	547[A]	ARG	CA-CB-CG	-30.95	45.31	113.40
2	B	547[B]	ARG	CA-CB-CG	-30.95	45.31	113.40
2	B	547[A]	ARG	CB-CG-CD	13.10	145.67	111.60
2	B	547[B]	ARG	CB-CG-CD	13.10	145.67	111.60

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	4608	0	4530	22	0
2	B	4461	0	4288	37	0
3	A	48	0	32	0	0
3	B	48	0	32	1	0
4	A	32	0	21	0	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
6	A	141	0	0	0	0
6	B	55	0	0	0	0
All	All	9405	0	8919	60	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 (60) 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)
3:B:601:COA:O4B	3:B:601:COA:C1B	1.64	1.11
2:B:147:GLU:O	2:B:151:ARG:NH1	2.25	0.70
2:B:3:ILE:HD12	2:B:21:LEU:HD13	1.73	0.69
2:B:5:PHE:HB2	2:B:30:VAL:HG22	1.76	0.67
1:A:267:LEU:O	1:A:270:VAL:HG12	1.97	0.64
1:A:216:GLU:HG3	1:A:284:LYS:HB2	1.80	0.63
2:B:113:VAL:N	2:B:157:THR:O	2.32	0.59
2:B:32:LEU:HG	2:B:548[A]:THR:HG23	1.86	0.57
2:B:31:GLU:OE1	2:B:555[A]:HIS:NE2	2.29	0.55
1:A:36:PRO:HB3	1:A:61:PRO:HG3	1.89	0.54
2:B:193:ASP:OD1	2:B:194:SER:HA	2.08	0.54
2:B:60:ILE:HD13	2:B:65:TRP:HB3	1.91	0.52
1:A:417:LYS:HB2	1:A:448:ARG:HG3	1.91	0.52
1:A:334:LEU:HD11	1:A:374:ILE:HD11	1.92	0.52
2:B:71:LEU:HD21	2:B:114:TRP:CD2	2.46	0.51
1:A:210:PHE:CE2	1:A:256:LYS:HE2	2.46	0.50
2:B:395:VAL:HG11	2:B:414:PRO:HB3	1.93	0.50
1:A:193:ASP:OD1	1:A:194:SER:HA	2.11	0.49
2:B:299:PHE:CG	5:B:602:GOL:H12	2.48	0.49
2:B:334:LEU:HD11	2:B:374:ILE:HD11	1.95	0.49
2:B:95:ARG:O	2:B:96:ILE:HD13	2.13	0.49
2:B:205:LYS:NZ	2:B:249:GLU:OE1	2.30	0.48
2:B:255:ILE:HG21	2:B:540:VAL:HG12	1.95	0.48
2:B:103:GLU:O	2:B:111:GLY:HA3	2.13	0.47
1:A:277:PRO:HG2	1:A:320:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:LYS:O	2:B:475:GLN:HG3	2.13	0.47
1:A:253:GLU:O	1:A:541:ARG:NH1	2.47	0.47
1:A:21:LEU:HD22	1:A:146:LEU:HD11	1.96	0.45
2:B:212:ALA:HA	2:B:243:TRP:O	2.15	0.45
2:B:53:ALA:HB3	2:B:72:ILE:HA	1.98	0.45
2:B:62:GLN:HA	2:B:65:TRP:CD1	2.52	0.45
2:B:130:TYR:HA	2:B:134:VAL:HB	1.99	0.45
2:B:44:GLU:CD	2:B:67:LYS:HZ3	2.19	0.44
1:A:501:ARG:HD3	1:A:506:TRP:CZ2	2.53	0.44
2:B:52:ILE:HG22	2:B:54:PRO:HD3	1.99	0.43
2:B:485:ILE:HA	2:B:490:PHE:CG	2.53	0.43
1:A:8:TYR:HA	1:A:33:ASP:HB3	2.00	0.43
2:B:65:TRP:CH2	2:B:105:SER:HA	2.54	0.43
2:B:18:TYR:CE1	2:B:22:THR:HG21	2.54	0.43
2:B:277:PRO:HG2	2:B:320:THR:OG1	2.19	0.43
1:A:395:VAL:HG11	1:A:414:PRO:HB3	2.01	0.42
1:A:60:ILE:HD13	1:A:70:THR:HG21	2.01	0.42
1:A:130:TYR:HA	1:A:134:VAL:HB	2.01	0.42
2:B:135:THR:O	2:B:139:VAL:HG23	2.19	0.42
1:A:88:TRP:CD1	1:A:165:ASN:HB3	2.54	0.42
2:B:309:MET:HE3	2:B:309:MET:HB3	1.92	0.42
2:B:448:ARG:HD3	2:B:549[B]:PRO:HB3	2.01	0.42
1:A:494:ILE:HD13	1:A:494:ILE:HA	1.92	0.42
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.93	0.41
2:B:30:VAL:HB	2:B:552[A]:LEU:HD22	2.02	0.41
2:B:408:GLU:HG2	2:B:465:VAL:HG12	2.02	0.41
2:B:44:GLU:OE2	2:B:67:LYS:NZ	2.53	0.41
1:A:497:LYS:HG2	1:A:501:ARG:HG3	2.02	0.40
2:B:3:ILE:O	2:B:28:VAL:HA	2.22	0.40
2:B:62:GLN:HA	2:B:65:TRP:NE1	2.36	0.40
1:A:18:TYR:CZ	1:A:22:THR:HG21	2.56	0.40
1:A:103:GLU:HG3	1:A:114:TRP:NE1	2.37	0.40
1:A:182:THR:HG23	1:A:242:VAL:HG22	2.03	0.40
2:B:276:LYS:HB2	2:B:279:GLU:HG3	2.03	0.40
2:B:449:MET:SD	2:B:549[B]:PRO:HG3	2.61	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	563/582 (97%)	550 (98%)	13 (2%)	0	100	100
2	B	558/576 (97%)	534 (96%)	22 (4%)	2 (0%)	34	32
All	All	1121/1158 (97%)	1084 (97%)	35 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	45	LEU
2	B	268	LYS

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	486/511 (95%)	478 (98%)	8 (2%)	62	69
2	B	458/505 (91%)	447 (98%)	11 (2%)	49	53
All	All	944/1016 (93%)	925 (98%)	19 (2%)	57	60

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	0	HIS
1	A	108	TYR
1	A	363	ASN

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Mol	Chain	Res	Type
1	A	419	ILE
1	A	479	GLU
1	A	505	GLU
1	A	558	LEU
2	B	60	ILE
2	B	87	ASP
2	B	108	TYR
2	B	150	GLU
2	B	151	ARG
2	B	187	ARG
2	B	217	GLU
2	B	363	ASN
2	B	541	ARG
2	B	547[A]	ARG
2	B	547[B]	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	COA	A	601	-	41,50,50	3.99	13 (31%)	52,75,75	1.93	9 (17%)
3	COA	B	601	-	41,50,50	4.09	13 (31%)	52,75,75	1.86	8 (15%)
5	GOL	B	602	-	5,5,5	0.92	0	5,5,5	0.97	0
4	THG	A	602	-	32,34,34	4.04	19 (59%)	39,47,47	1.46	6 (15%)
5	GOL	A	603	-	5,5,5	1.03	0	5,5,5	1.03	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	COA	A	601	-	-	6/44/64/64	0/3/3/3
3	COA	B	601	-	-	7/44/64/64	0/3/3/3
5	GOL	B	602	-	-	1/4/4/4	-
4	THG	A	602	-	-	5/22/31/31	0/3/3/3
5	GOL	A	603	-	-	2/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	COA	O4B-C1B	16.74	1.64	1.41
3	A	601	COA	O4B-C1B	15.49	1.62	1.41
3	A	601	COA	C2B-C1B	-13.30	1.33	1.53
3	B	601	COA	C2B-C1B	-13.27	1.33	1.53
4	A	602	THG	C5'-C4'	8.98	1.54	1.39
4	A	602	THG	C2'-C3'	8.71	1.54	1.38
3	B	601	COA	C9P-N8P	8.58	1.52	1.33
3	A	601	COA	C9P-N8P	8.30	1.51	1.33
4	A	602	THG	C6'-C1'	7.94	1.52	1.39
4	A	602	THG	C2-N2	6.45	1.46	1.33
4	A	602	THG	O4-C4	6.25	1.40	1.24
3	A	601	COA	O4B-C4B	-5.84	1.32	1.45
4	A	602	THG	C4A-N5	5.73	1.49	1.38
4	A	602	THG	C11-N	5.59	1.46	1.34
3	B	601	COA	O4B-C4B	-5.57	1.32	1.45
3	B	601	COA	P3B-O3B	5.56	1.69	1.59
3	A	601	COA	P3B-O3B	5.43	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	THG	C2-N3	5.28	1.44	1.35
3	A	601	COA	C5P-N4P	4.13	1.42	1.33
3	A	601	COA	C2A-N3A	3.99	1.38	1.32
3	B	601	COA	C5P-N4P	3.95	1.42	1.33
4	A	602	THG	C4'-N10	3.92	1.50	1.38
3	B	601	COA	C2A-N3A	3.90	1.38	1.32
4	A	602	THG	C3'-C4'	-3.83	1.32	1.39
4	A	602	THG	C8A-N1	3.75	1.41	1.34
4	A	602	THG	C2-N1	3.70	1.42	1.35
4	A	602	THG	C2'-C1'	-3.65	1.33	1.39
4	A	602	THG	C4A-C4	3.64	1.46	1.41
4	A	602	THG	C4-N3	3.30	1.38	1.33
4	A	602	THG	C5'-C6'	-3.09	1.33	1.38
3	A	601	COA	C6A-N6A	2.65	1.43	1.34
3	A	601	COA	C7P-N8P	2.64	1.52	1.46
3	B	601	COA	O3B-C3B	-2.55	1.34	1.44
3	B	601	COA	C7P-N8P	2.49	1.51	1.46
3	B	601	COA	C5A-C4A	-2.46	1.34	1.40
3	B	601	COA	C6A-N6A	2.43	1.42	1.34
3	A	601	COA	C5A-C4A	-2.39	1.34	1.40
3	A	601	COA	C2A-N1A	2.38	1.38	1.33
3	A	601	COA	O3B-C3B	-2.36	1.35	1.44
3	B	601	COA	OAP-CAP	-2.33	1.38	1.42
4	A	602	THG	O11-C11	-2.24	1.18	1.23
4	A	602	THG	C9-N10	2.22	1.49	1.45
3	A	601	COA	C4A-N3A	2.20	1.38	1.35
3	B	601	COA	P1A-O5B	2.05	1.67	1.59
4	A	602	THG	CG-CD	2.05	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	COA	C7P-C6P-C5P	-7.32	100.17	112.36
3	B	601	COA	C7P-C6P-C5P	-6.21	102.02	112.36
3	B	601	COA	N3A-C2A-N1A	-6.10	119.14	128.68
3	A	601	COA	N3A-C2A-N1A	-5.86	119.52	128.68
3	B	601	COA	C5A-C6A-N6A	5.70	129.02	120.35
3	A	601	COA	C5A-C6A-N6A	5.24	128.32	120.35
4	A	602	THG	C8A-C4A-C4	5.00	119.01	114.57
3	B	601	COA	N6A-C6A-N1A	-3.69	110.92	118.57
4	A	602	THG	C4A-N5-C6	-3.48	112.32	121.48
3	A	601	COA	N6A-C6A-N1A	-3.35	111.61	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	COA	P2A-O3A-P1A	-3.24	121.72	132.83
3	A	601	COA	C1B-N9A-C4A	-3.12	121.16	126.64
3	B	601	COA	P2A-O3A-P1A	-2.48	124.33	132.83
3	A	601	COA	C6P-C5P-N4P	2.38	120.44	116.42
3	B	601	COA	C1B-N9A-C4A	-2.31	122.58	126.64
4	A	602	THG	C6-C7-N8	-2.30	106.35	110.68
3	A	601	COA	C3P-N4P-C5P	-2.21	118.73	122.84
4	A	602	THG	C2-N1-C8A	2.20	119.46	114.54
4	A	602	THG	CG-CB-CA	-2.18	109.07	113.16
3	B	601	COA	O6A-CCP-CBP	-2.10	107.17	110.55
4	A	602	THG	OX2-C-CA	2.04	120.17	113.40
3	B	601	COA	C3B-C2B-C1B	2.02	104.36	99.89
3	A	601	COA	O5P-C5P-C6P	-2.00	118.36	122.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

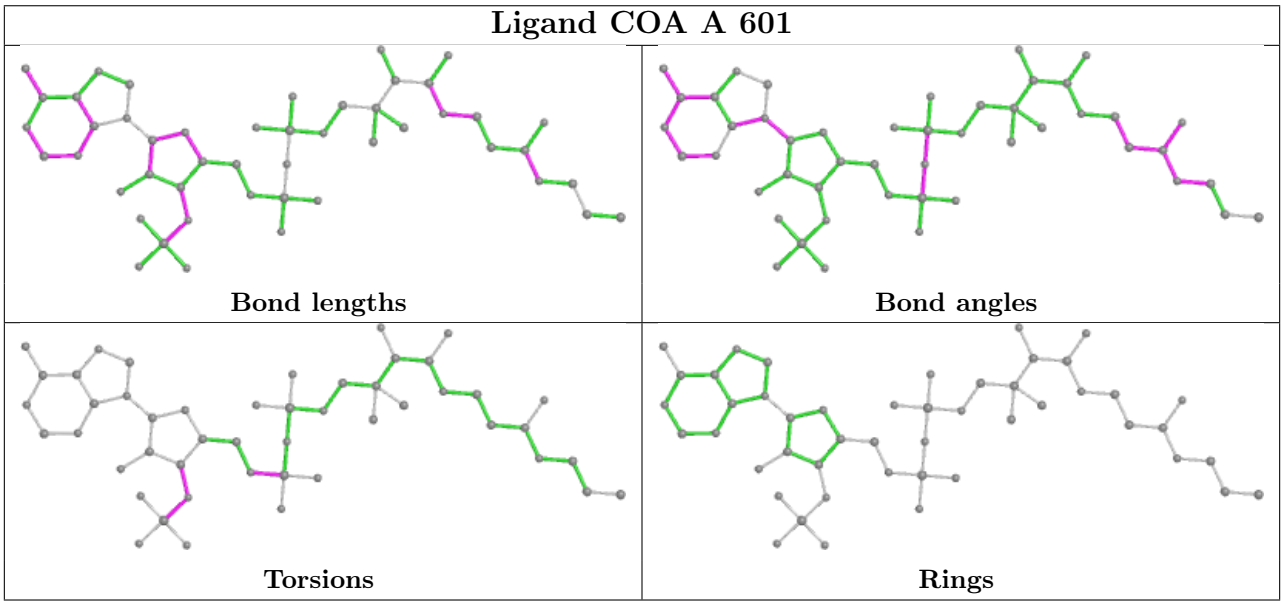
Mol	Chain	Res	Type	Atoms
3	A	601	COA	C5B-O5B-P1A-O2A
4	A	602	THG	C6-C9-N10-C4'
5	A	603	GOL	O1-C1-C2-C3
3	B	601	COA	C4B-C3B-O3B-P3B
3	A	601	COA	C4B-C3B-O3B-P3B
3	A	601	COA	C2B-C3B-O3B-P3B
3	B	601	COA	OAP-CAP-CBP-CEP
3	A	601	COA	C5B-O5B-P1A-O3A
3	B	601	COA	C5B-O5B-P1A-O3A
4	A	602	THG	C3'-C4'-N10-C9
3	A	601	COA	C5B-O5B-P1A-O1A
3	B	601	COA	C5B-O5B-P1A-O1A
4	A	602	THG	C5'-C4'-N10-C9
4	A	602	THG	OE1-CD-CG-CB
4	A	602	THG	OE2-CD-CG-CB
5	A	603	GOL	O1-C1-C2-O2
3	A	601	COA	C3B-O3B-P3B-O7A
3	B	601	COA	C3B-O3B-P3B-O7A
3	B	601	COA	C2B-C3B-O3B-P3B
3	B	601	COA	C3B-O3B-P3B-O8A
5	B	602	GOL	C1-C2-C3-O3

There are no ring outliers.

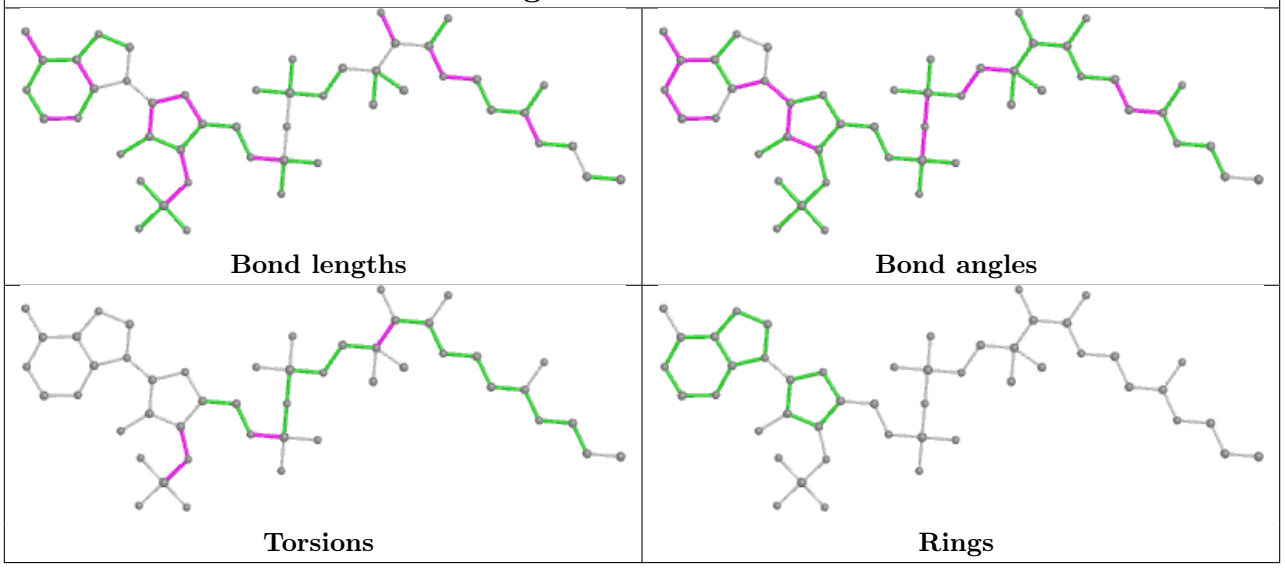
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	COA	1	0
5	B	602	GOL	1	0

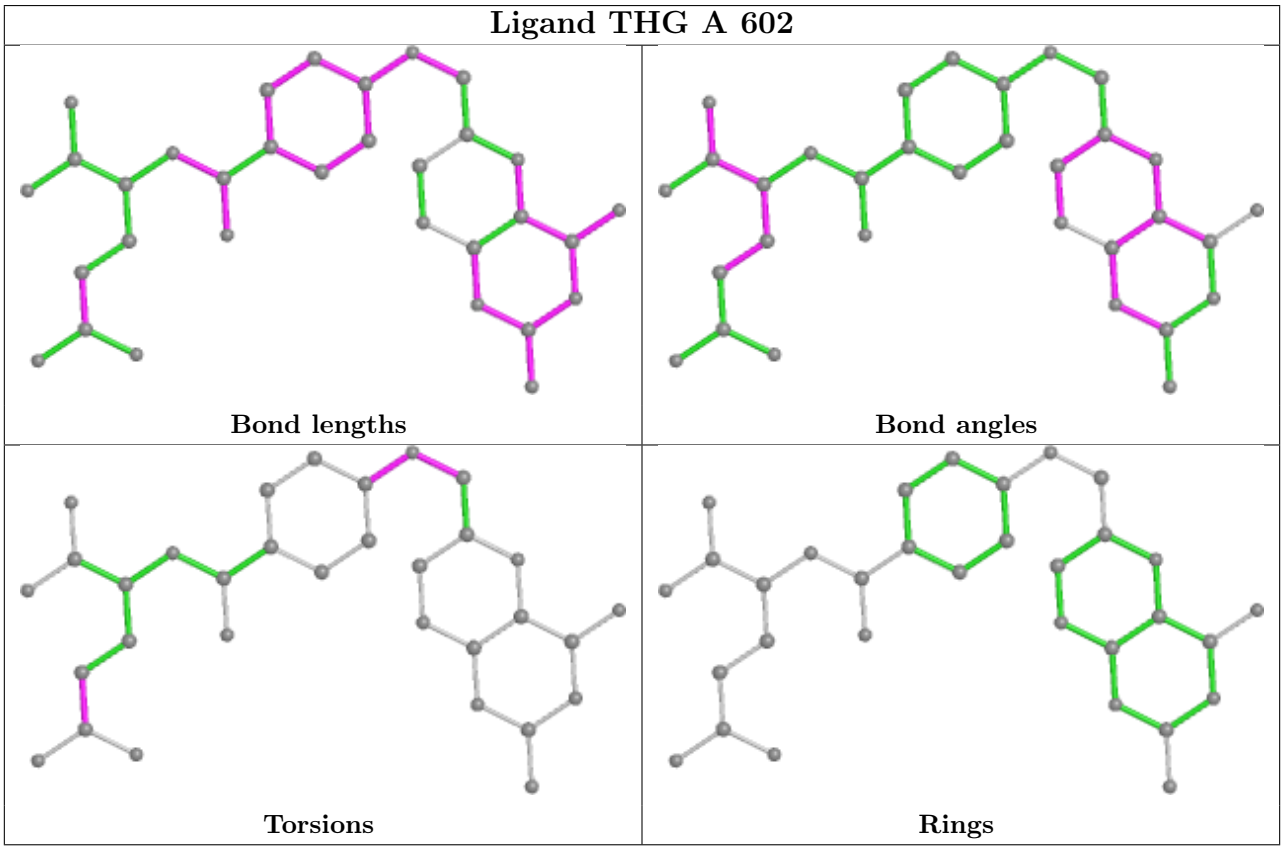
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 COA B 601



Ligand THG A 602



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^{th} 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	564/582 (96%)	0.08	20 (3%) 44 50	33, 47, 75, 112	0
2	B	557/576 (96%)	0.95	105 (18%) 1 1	37, 65, 131, 170	10 (1%)
All	All	1121/1158 (96%)	0.51	125 (11%) 5 6	33, 53, 119, 170	10 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	547[A]	ARG	10.5
2	B	149	PHE	9.0
2	B	146	LEU	8.9
2	B	51	ILE	8.5
2	B	154	PHE	8.0
2	B	108	TYR	7.7
2	B	46	TYR	7.5
2	B	528	PHE	7.3
2	B	152	GLY	7.3
2	B	550[A]	PRO	7.3
2	B	50	LEU	7.1
2	B	552[A]	LEU	6.9
2	B	115	ALA	6.9
2	B	48	PRO	6.8
2	B	551[A]	TYR	6.7
2	B	65	TRP	6.6
2	B	6	LEU	6.5
2	B	70	THR	6.5
2	B	71	LEU	6.3
2	B	546[B]	PHE	6.3
2	B	549[A]	PRO	6.1
2	B	104	ALA	6.1
2	B	162	HIS	5.9
2	B	61	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	151	ARG	5.8
2	B	554[A]	ILE	5.7
2	B	107	GLU	5.7
2	B	553[A]	ALA	5.6
2	B	110	ALA	5.5
2	B	156	PRO	5.4
2	B	548[A]	THR	5.3
1	A	558	LEU	5.2
2	B	114	TRP	5.1
2	B	58	ARG	4.9
2	B	68	TYR	4.9
2	B	153	ASP	4.8
2	B	116	TYR	4.6
2	B	163	TRP	4.6
2	B	3	ILE	4.5
2	B	102	LEU	4.4
2	B	63	GLU	4.4
2	B	4	LEU	4.4
1	A	562	LEU	4.3
2	B	105	SER	4.3
2	B	64	VAL	4.3
2	B	159	GLN	4.2
2	B	544	PRO	4.2
2	B	2	ARG	4.2
2	B	555[A]	HIS	4.1
2	B	106	GLU	4.0
2	B	112	ASP	4.0
2	B	56	LEU	3.9
2	B	62	GLN	3.8
2	B	60	ILE	3.8
2	B	66	LYS	3.7
2	B	545[B]	HIS	3.7
1	A	153	ASP	3.6
2	B	164	TRP	3.6
1	A	561	SER	3.6
1	A	560	PHE	3.5
2	B	59	LYS	3.5
2	B	109	ASP	3.5
2	B	150	GLU	3.4
2	B	45	LEU	3.4
2	B	158	PRO	3.4
2	B	38	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	37	ASP	3.3
2	B	32	LEU	3.3
2	B	556[A]	ARG	3.3
2	B	241	ALA	3.3
2	B	147	GLU	3.2
2	B	157	THR	3.2
2	B	82	GLY	3.2
2	B	131	ARG	3.2
2	B	26	HIS	3.1
2	B	148	ASN	3.1
2	B	111	GLY	3.0
2	B	340	PHE	3.0
1	A	151	ARG	3.0
2	B	145	ALA	2.9
1	A	305	TYR	2.9
2	B	438	TRP	2.8
2	B	178	GLU	2.8
2	B	80	ASP	2.7
2	B	439	GLU	2.7
2	B	36	PRO	2.7
1	A	304	PHE	2.7
1	A	559	LYS	2.6
2	B	103	GLU	2.6
2	B	271	LYS	2.6
1	A	388	GLY	2.6
2	B	67	LYS	2.5
2	B	161	GLU	2.5
1	A	308	ALA	2.5
1	A	390	ALA	2.5
2	B	57	LYS	2.5
1	A	302	PHE	2.5
2	B	160	LYS	2.4
2	B	342	SER	2.4
2	B	166	PRO	2.4
2	B	1	MET	2.3
2	B	127	ALA	2.3
1	A	550	PRO	2.3
2	B	24	ARG	2.3
1	A	340	PHE	2.2
1	A	306	ASN	2.2
1	A	389	ASN	2.2
1	A	307	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	0	HIS	2.2
1	A	397	LEU	2.2
2	B	47	LYS	2.2
2	B	128	SER	2.2
2	B	274	PRO	2.2
2	B	240	GLY	2.1
2	B	307	GLY	2.1
2	B	143	LEU	2.1
2	B	339	ASP	2.1
2	B	388	GLY	2.1
2	B	155	LYS	2.1
2	B	39	THR	2.1
2	B	144	GLU	2.0
1	A	334	LEU	2.0
2	B	390	ALA	2.0
2	B	217	GLU	2.0
2	B	218	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

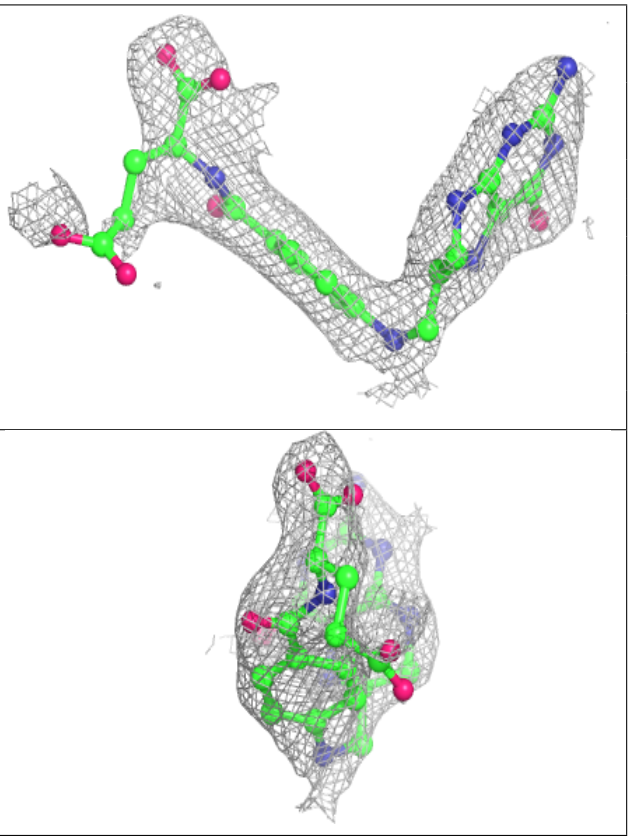
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

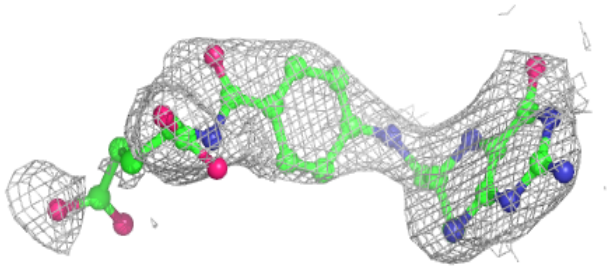
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	THG	A	602	32/32	0.87	0.21	69,87,123,125	0
5	GOL	A	603	6/6	0.90	0.15	53,60,66,71	0
5	GOL	B	602	6/6	0.92	0.17	61,66,75,85	0
3	COA	B	601	48/48	0.96	0.18	39,52,62,76	0
3	COA	A	601	48/48	0.96	0.17	32,40,45,48	0

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 THG A 602:

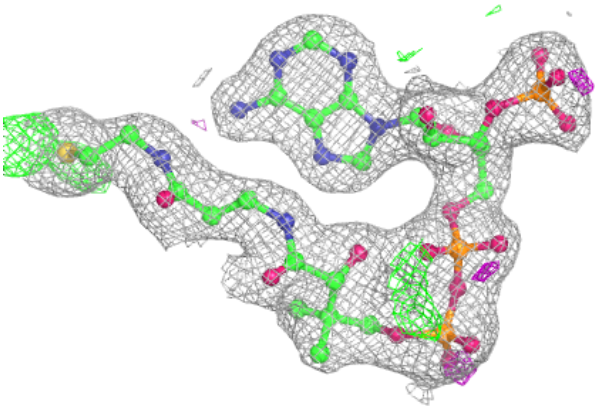
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

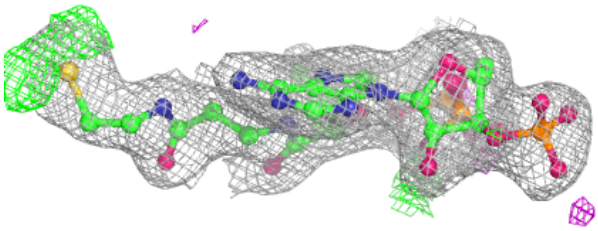


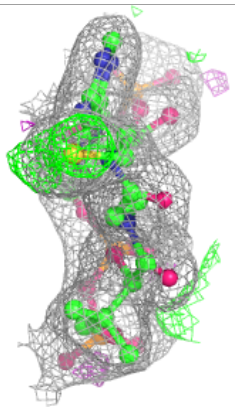


Electron density around COA B 601:

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

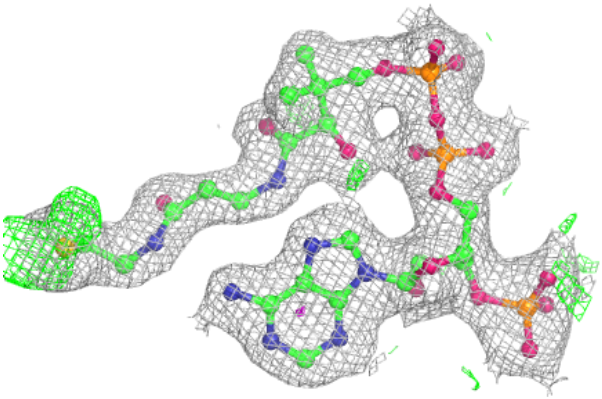


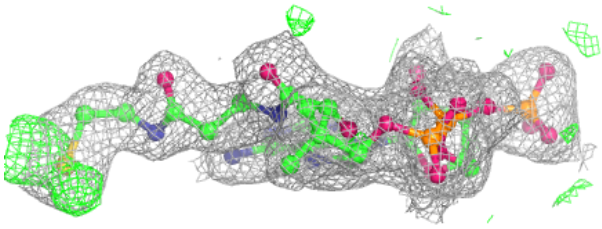


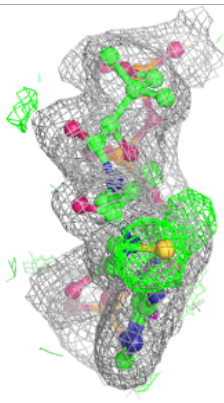


Electron density around COA A 601:

$2mF_o$-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.