Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 03:34 AM EDT

PDB ID	:	6SK4
Title	:	Methyltransferase MtgA from Desulfitobacterium hafniense in complex with methyl-tetrahydrofolate (P21)
Authors	:	Badmann, T.; Groll, M.
Deposited on	:	2019-08-14
Resolution	:	1.55 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:

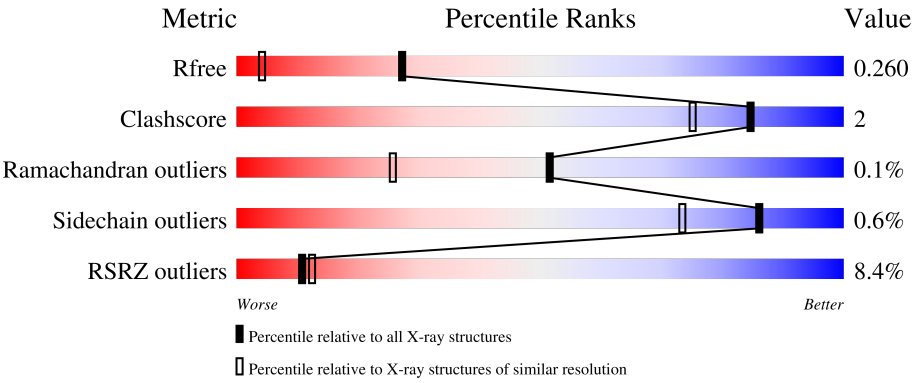
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	307	8% 92% 6% ·
1	B	307	10% 90% 6% ·
1	C	307	8% 93% · ·
1	D	307	7% 93% 6% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9768 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.

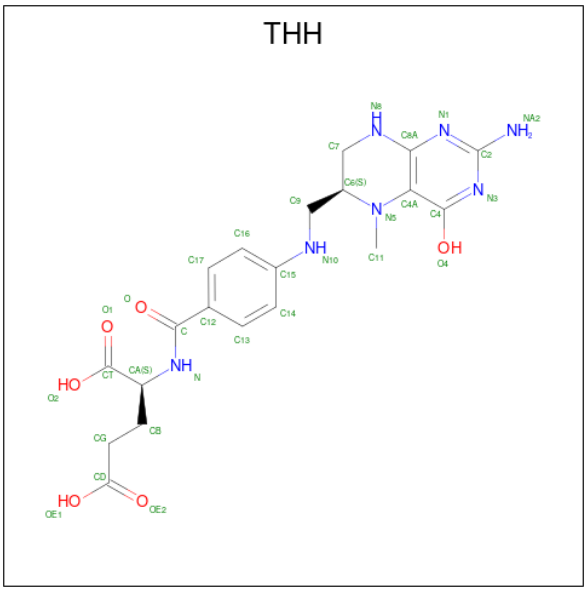
- Molecule 1 is a protein called Methylcorrinoid:tetrahydrofolate methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2307	1493	376	432	6			
1	B	296	Total	C	N	O	S	0	0	0
			2282	1475	371	430	6			
1	C	298	Total	C	N	O	S	0	0	0
			2296	1484	375	431	6			
1	D	304	Total	C	N	O	S	0	0	0
			2343	1511	383	443	6			

There are 8 discrepancies between the modelled and reference sequences:

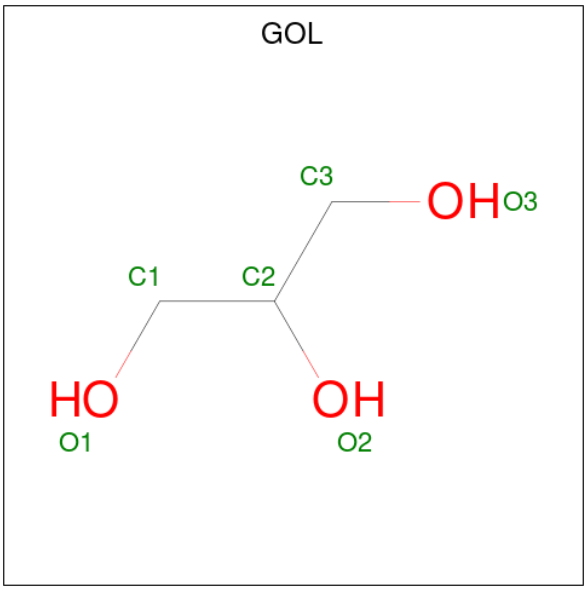
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q24SP6
A	1	SER	-	expression tag	UNP Q24SP6
B	0	GLY	-	expression tag	UNP Q24SP6
B	1	SER	-	expression tag	UNP Q24SP6
C	0	GLY	-	expression tag	UNP Q24SP6
C	1	SER	-	expression tag	UNP Q24SP6
D	0	GLY	-	expression tag	UNP Q24SP6
D	1	SER	-	expression tag	UNP Q24SP6

- Molecule 2 is N-[4-({[(6S)-2-AMINO-4-HYDROXY-5-METHYL-5,6,7,8-TETRAHYDROPTERIDIN-6-YL]METHYL}AMINO)BENZOYL]-L-GLUTAMIC ACID (three-letter code: THH) (formula: $C_{20}H_{25}N_7O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	20	7	6		
2	B	1	Total	C	N	O	0	0
			33	20	7	6		
2	C	1	Total	C	N	O	0	0
			33	20	7	6		
2	D	1	Total	C	N	O	0	0
			33	20	7	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

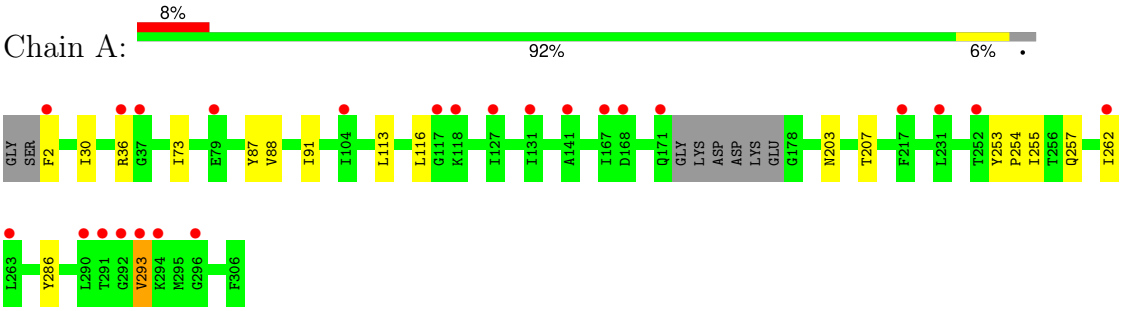
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	B	111	Total O 111 111	0	0
4	C	97	Total O 97 97	0	0
4	D	94	Total O 94 94	0	0

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.

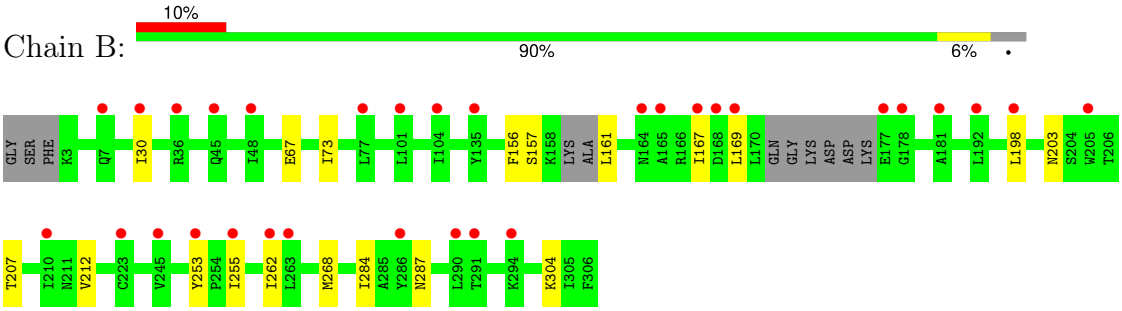
• Molecule 1: Methylcorrinoid:tetrahydrofolate methyltransferase

Chain A:



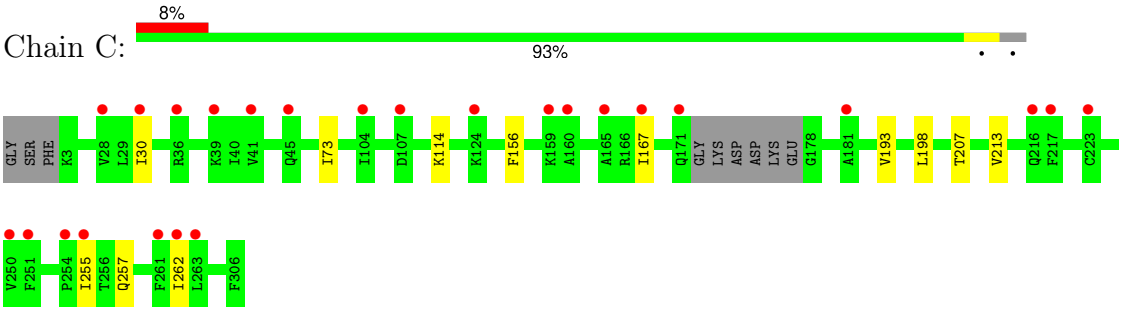
• Molecule 1: Methylcorrinoid:tetrahydrofolate methyltransferase

Chain B:



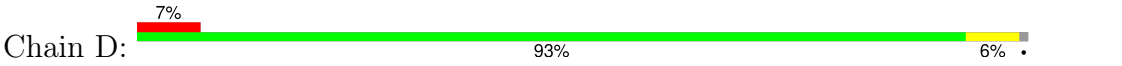
• Molecule 1: Methylcorrinoid:tetrahydrofolate methyltransferase

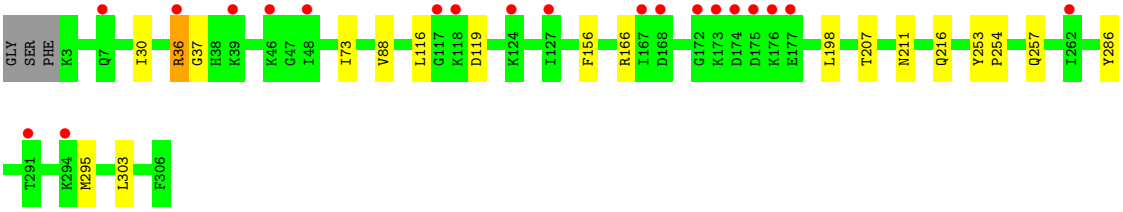
Chain C:



• Molecule 1: Methylcorrinoid:tetrahydrofolate methyltransferase

Chain D:




GLY
SER
PHE
K3
Q7
I30
R36
G37
H38
K39
K46
G47
I48
I73
V88
L116
G117
K118
D119
K124
I127
F156
R166
I167
D168
G172
K173
D174
D175
K176
E177
L198
T207
N211
Q216
Y253
P254
Q257
I262
Y286
T291
K294
M295
L303
F306

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.40Å 73.10Å 89.76Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 28.96 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-1.55) 97.3 (28.96-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.243 0.220 , 0.260	Depositor DCC
R_{free} test set	6984 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.920	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 43.1	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	0.96	EDS
Total number of atoms	9768	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0995e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: THH, 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	0.62	0/2357	0.71	0/3195
1	B	0.63	0/2330	0.70	0/3158
1	C	0.63	0/2345	0.70	0/3179
1	D	0.63	0/2393	0.72	0/3243
All	All	0.63	0/9425	0.71	0/12775

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	2307	0	2326	11	1
1	B	2282	0	2296	13	0
1	C	2296	0	2317	9	0
1	D	2343	0	2361	10	1
2	A	33	0	22	1	0
2	B	33	0	22	0	0
2	C	33	0	22	0	0
2	D	33	0	22	0	0
3	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	100	0	0	0	0
4	B	111	0	0	1	0
4	C	97	0	0	0	0
4	D	94	0	0	0	0
All	All	9768	0	9396	43	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 2.

All (43) 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:B:156:PHE:CZ	1:B:198:LEU:HD21	2.28	0.68
1:D:36:ARG:HD3	1:D:36:ARG:C	2.16	0.67
1:D:36:ARG:HD3	1:D:37:GLY:N	2.10	0.66
1:B:156:PHE:HZ	1:B:198:LEU:HD21	1.61	0.65
1:A:2:PHE:HE1	1:A:293:VAL:HB	1.67	0.60
1:A:36:ARG:HB3	3:A:902:GOL:H11	1.84	0.59
1:C:114:LYS:HA	1:C:114:LYS:HE3	1.87	0.57
1:A:207:THR:CG2	1:A:257:GLN:HB2	2.35	0.56
1:B:157:SER:HB2	1:B:169:LEU:HD11	1.87	0.56
1:A:2:PHE:CE1	1:A:293:VAL:HB	2.40	0.55
1:B:268:MET:HE3	4:B:1034:HOH:O	2.06	0.55
1:D:211:ASN:ND2	1:D:257:GLN:O	2.38	0.53
1:C:207:THR:HG21	1:C:257:GLN:HG3	1.92	0.51
1:C:167:ILE:HD12	1:C:213:VAL:CG2	2.40	0.51
1:B:167:ILE:HG13	1:B:212:VAL:HG11	1.92	0.51
1:B:161:LEU:HD22	1:B:198:LEU:HD11	1.93	0.51
1:B:203:ASN:O	1:B:207:THR:HG23	2.11	0.51
1:A:30:ILE:HA	1:A:73:ILE:O	2.11	0.51
1:D:88:VAL:HG11	1:D:116:LEU:HD13	1.95	0.49
1:A:36:ARG:O	2:A:901:THH:O1	2.31	0.49
1:D:36:ARG:C	1:D:36:ARG:CD	2.81	0.48
1:D:30:ILE:HA	1:D:73:ILE:O	2.12	0.48
1:D:295:MET:HE1	1:D:303:LEU:HD11	1.95	0.48
1:B:255:ILE:HD11	1:B:262:ILE:HG12	1.96	0.47
1:B:30:ILE:HA	1:B:73:ILE:O	2.14	0.47
1:A:88:VAL:HG11	1:A:116:LEU:HD13	1.97	0.47
1:C:255:ILE:HD11	1:C:262:ILE:HG12	1.97	0.47
1:C:207:THR:CG2	1:C:257:GLN:HG3	2.45	0.46
1:B:207:THR:HG21	1:B:253:TYR:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PHE:CZ	1:D:198:LEU:HD21	2.50	0.46
1:C:156:PHE:CZ	1:C:198:LEU:HD21	2.52	0.45
1:B:284:ILE:O	1:B:287:ASN:HB2	2.17	0.44
1:C:207:THR:CG2	1:C:257:GLN:HB2	2.48	0.44
1:A:87:TYR:O	1:A:91:ILE:HG12	2.19	0.43
1:D:207:THR:CG2	1:D:257:GLN:HB2	2.48	0.43
1:C:30:ILE:HA	1:C:73:ILE:O	2.17	0.43
1:A:253:TYR:HB3	1:A:254:PRO:HD3	2.01	0.42
1:D:253:TYR:HB3	1:D:254:PRO:HD3	2.01	0.42
1:A:255:ILE:HD11	1:A:262:ILE:HG12	2.01	0.42
1:B:67:GLU:O	1:B:304:LYS:HE3	2.20	0.42
1:B:207:THR:HG21	1:B:253:TYR:HD2	1.85	0.42
1:C:193:VAL:HG11	1:C:213:VAL:HG21	2.03	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.86	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:A:2:PHE:CZ	1:D:216:GLN:NE2[1_554]	2.19	0.01

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	295/307 (96%)	290 (98%)	5 (2%)	0	100	100
1	B	290/307 (94%)	289 (100%)	1 (0%)	0	100	100
1	C	294/307 (96%)	292 (99%)	2 (1%)	0	100	100
1	D	302/307 (98%)	296 (98%)	5 (2%)	1 (0%)	41	19
All	All	1181/1228 (96%)	1167 (99%)	13 (1%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	ASP

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	241/247 (98%)	238 (99%)	3 (1%)	71 49
1	B	239/247 (97%)	239 (100%)	0	100 100
1	C	240/247 (97%)	240 (100%)	0	100 100
1	D	245/247 (99%)	242 (99%)	3 (1%)	71 49
All	All	965/988 (98%)	959 (99%)	6 (1%)	86 73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	286	TYR
1	A	293	VAL
1	D	36	ARG
1	D	166	ARG
1	D	286	TYR

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	$\#\|Z\| > 2$
2	THH	D	901	-	33,35,35	1.30	5 (15%)	35,49,49	1.34	6 (17%)
3	GOL	A	902	-	5,5,5	0.08	0	5,5,5	0.22	0
2	THH	B	901	-	33,35,35	1.38	5 (15%)	35,49,49	1.33	6 (17%)
2	THH	A	901	-	33,35,35	1.40	5 (15%)	35,49,49	1.47	5 (14%)
2	THH	C	901	-	33,35,35	1.39	5 (15%)	35,49,49	1.25	5 (14%)

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	THH	D	901	-	-	0/22/35/35	0/3/3/3
3	GOL	A	902	-	-	2/4/4/4	-
2	THH	B	901	-	-	0/22/35/35	0/3/3/3
2	THH	A	901	-	-	0/22/35/35	0/3/3/3
2	THH	C	901	-	-	0/22/35/35	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	THH	C12-C	-4.31	1.40	1.50
2	B	901	THH	C12-C	-3.74	1.42	1.50
2	C	901	THH	C12-C	-3.69	1.42	1.50
2	D	901	THH	C12-C	-3.66	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	THH	C2-N3	3.15	1.40	1.35
2	B	901	THH	C2-N3	2.98	1.40	1.35
2	A	901	THH	C2-N3	2.77	1.40	1.35
2	A	901	THH	C6-N5	2.62	1.51	1.47
2	B	901	THH	C7-N8	2.53	1.49	1.44
2	B	901	THH	C9-N10	2.51	1.49	1.45
2	D	901	THH	C7-N8	2.24	1.48	1.44
2	D	901	THH	C6-N5	2.21	1.50	1.47
2	C	901	THH	C9-N10	2.20	1.49	1.45
2	D	901	THH	C9-N10	2.15	1.49	1.45
2	A	901	THH	C7-N8	2.15	1.48	1.44
2	A	901	THH	C9-N10	2.14	1.49	1.45
2	B	901	THH	C6-N5	2.14	1.50	1.47
2	D	901	THH	C2-N3	2.11	1.39	1.35
2	C	901	THH	C7-N8	2.11	1.48	1.44
2	C	901	THH	C7-C6	-2.10	1.49	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	THH	CB-CG-CD	-4.39	100.79	112.49
2	B	901	THH	N3-C2-N1	-3.54	120.06	125.48
2	D	901	THH	N3-C2-N1	-3.08	120.75	125.48
2	C	901	THH	N3-C2-N1	-3.05	120.80	125.48
2	C	901	THH	C11-N5-C6	-2.96	109.66	117.96
2	B	901	THH	C11-N5-C6	-2.93	109.73	117.96
2	D	901	THH	CG-CB-CA	-2.70	108.19	113.16
2	A	901	THH	N3-C2-N1	-2.60	121.50	125.48
2	C	901	THH	CG-CB-CA	-2.58	108.41	113.16
2	C	901	THH	C2-N1-C8A	2.45	120.41	114.59
2	D	901	THH	C11-N5-C6	-2.44	111.11	117.96
2	D	901	THH	C2-N3-C4	2.43	121.55	116.31
2	B	901	THH	C2-N1-C8A	2.41	120.31	114.59
2	D	901	THH	NA2-C2-N1	2.40	120.82	117.22
2	A	901	THH	NA2-C2-N3	2.38	120.80	117.22
2	B	901	THH	C2-N3-C4	2.37	121.42	116.31
2	B	901	THH	CG-CB-CA	-2.33	108.86	113.16
2	A	901	THH	C2-N3-C4	2.25	121.16	116.31
2	D	901	THH	C2-N1-C8A	2.21	119.84	114.59
2	B	901	THH	NA2-C2-N3	2.20	120.53	117.22
2	A	901	THH	C11-N5-C6	-2.13	111.98	117.96
2	C	901	THH	NA2-C2-N3	2.12	120.40	117.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

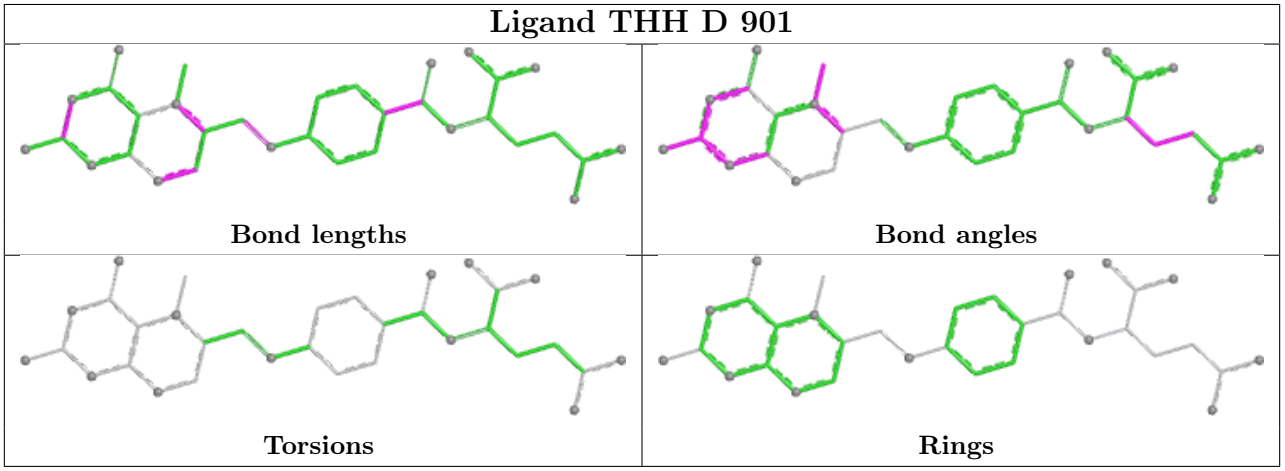
Mol	Chain	Res	Type	Atoms
3	A	902	GOL	O1-C1-C2-C3
3	A	902	GOL	O1-C1-C2-O2

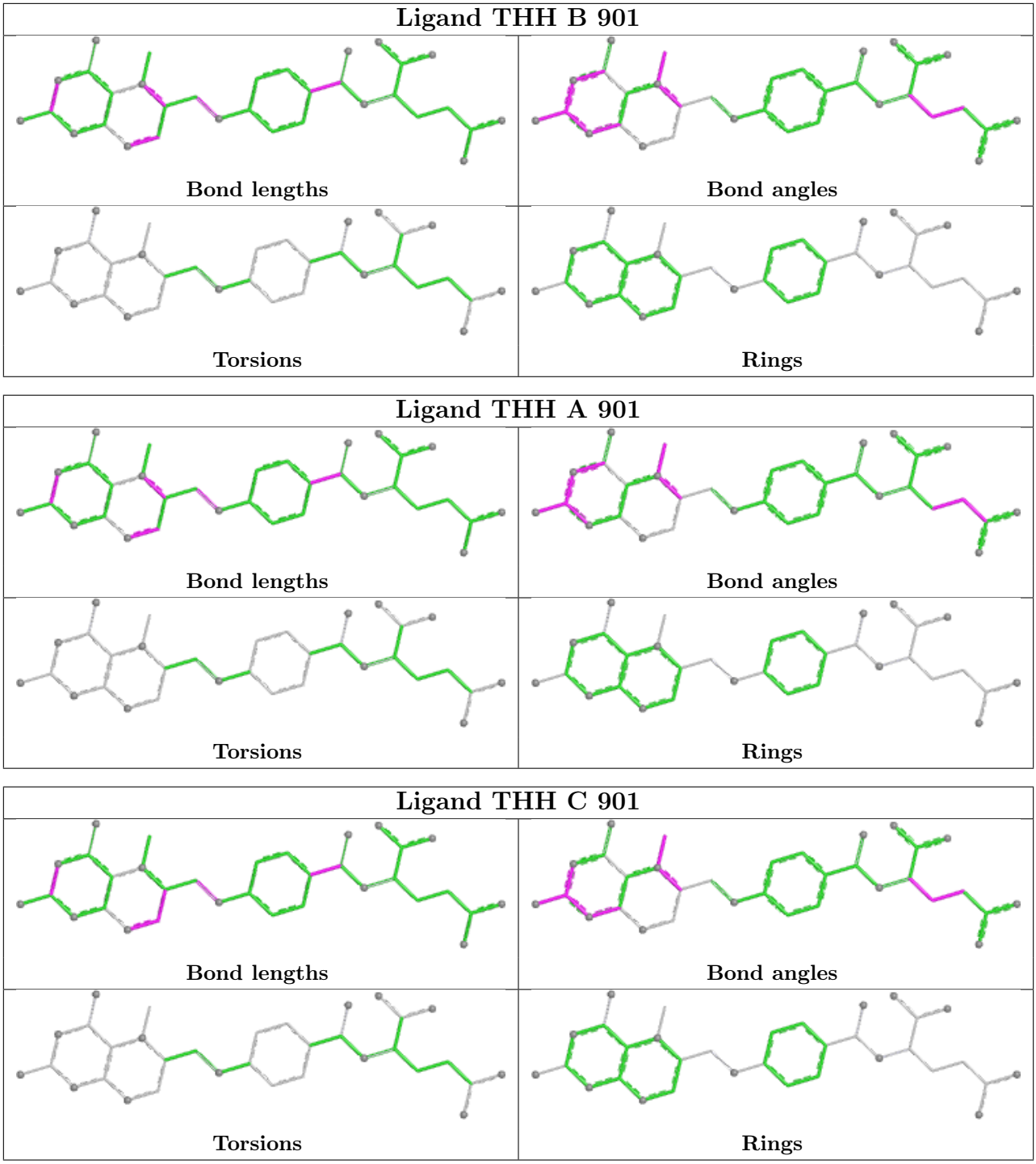
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GOL	1	0
2	A	901	THH	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.





5.7 Other polymers

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, 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	299/307 (97%)	0.77	24 (8%) 12 14	15, 21, 34, 59	0
1	B	296/307 (96%)	0.75	31 (10%) 6 6	15, 22, 35, 47	0
1	C	298/307 (97%)	0.70	25 (8%) 11 12	15, 22, 33, 48	0
1	D	304/307 (99%)	0.66	20 (6%) 18 21	14, 22, 35, 50	0
All	All	1197/1228 (97%)	0.72	100 (8%) 11 12	14, 22, 34, 59	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	10.8
1	A	293	VAL	9.6
1	D	167	ILE	8.1
1	A	167	ILE	6.0
1	A	294	LYS	5.9
1	A	2	PHE	5.6
1	A	291	THR	5.4
1	B	290	LEU	4.6
1	B	167	ILE	4.4
1	A	36	ARG	4.3
1	D	173	LYS	4.2
1	C	171	GLN	4.1
1	A	104	ILE	3.9
1	B	198	LEU	3.8
1	B	104	ILE	3.7
1	B	165	ALA	3.6
1	C	160	ALA	3.6
1	C	255	ILE	3.6
1	A	37	GLY	3.5
1	B	36	ARG	3.5
1	C	159	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	118	LYS	3.4
1	B	164	ASN	3.3
1	B	48	ILE	3.3
1	D	117	GLY	3.3
1	A	262	ILE	3.3
1	A	171	GLN	3.2
1	D	36	ARG	3.2
1	C	45	GLN	3.1
1	C	36	ARG	3.1
1	D	168	ASP	3.1
1	C	263	LEU	3.1
1	C	261	PHE	3.1
1	D	174	ASP	3.0
1	A	292	GLY	3.0
1	A	117	GLY	3.0
1	B	30	ILE	3.0
1	B	45	GLN	2.9
1	B	168	ASP	2.9
1	C	250	VAL	2.9
1	D	176	LYS	2.9
1	B	205	TRP	2.9
1	C	41	VAL	2.9
1	D	127	ILE	2.8
1	D	175	ASP	2.8
1	B	262	ILE	2.8
1	C	167	ILE	2.8
1	C	30	ILE	2.7
1	B	192	LEU	2.7
1	C	251	PHE	2.7
1	B	263	LEU	2.7
1	B	169	LEU	2.7
1	C	104	ILE	2.6
1	D	39	LYS	2.6
1	C	165	ALA	2.6
1	A	217	PHE	2.6
1	D	294	LYS	2.6
1	B	210	ILE	2.6
1	A	79	GLU	2.5
1	B	291	THR	2.5
1	C	217	PHE	2.5
1	C	28	VAL	2.5
1	A	168	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	178	GLY	2.5
1	C	223	CYS	2.5
1	A	296	GLY	2.5
1	A	141	ALA	2.4
1	A	263	LEU	2.4
1	D	172	GLY	2.4
1	B	7	GLN	2.3
1	A	127	ILE	2.3
1	C	262	ILE	2.3
1	C	181	ALA	2.3
1	B	177	GLU	2.3
1	A	118	LYS	2.3
1	C	124	LYS	2.3
1	C	216	GLN	2.2
1	D	124	LYS	2.2
1	C	107	ASP	2.2
1	B	135	TYR	2.2
1	B	223	CYS	2.2
1	A	131	ILE	2.2
1	B	294	LYS	2.2
1	C	39	LYS	2.1
1	D	46	LYS	2.1
1	D	291	THR	2.1
1	C	254	PRO	2.1
1	B	255	ILE	2.1
1	D	48	ILE	2.1
1	A	231	LEU	2.1
1	B	101	LEU	2.1
1	A	252	THR	2.1
1	D	177	GLU	2.1
1	B	245	VAL	2.1
1	B	77	LEU	2.1
1	B	181	ALA	2.1
1	D	7	GLN	2.0
1	B	253	TYR	2.0
1	B	286	TYR	2.0
1	D	262	ILE	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)

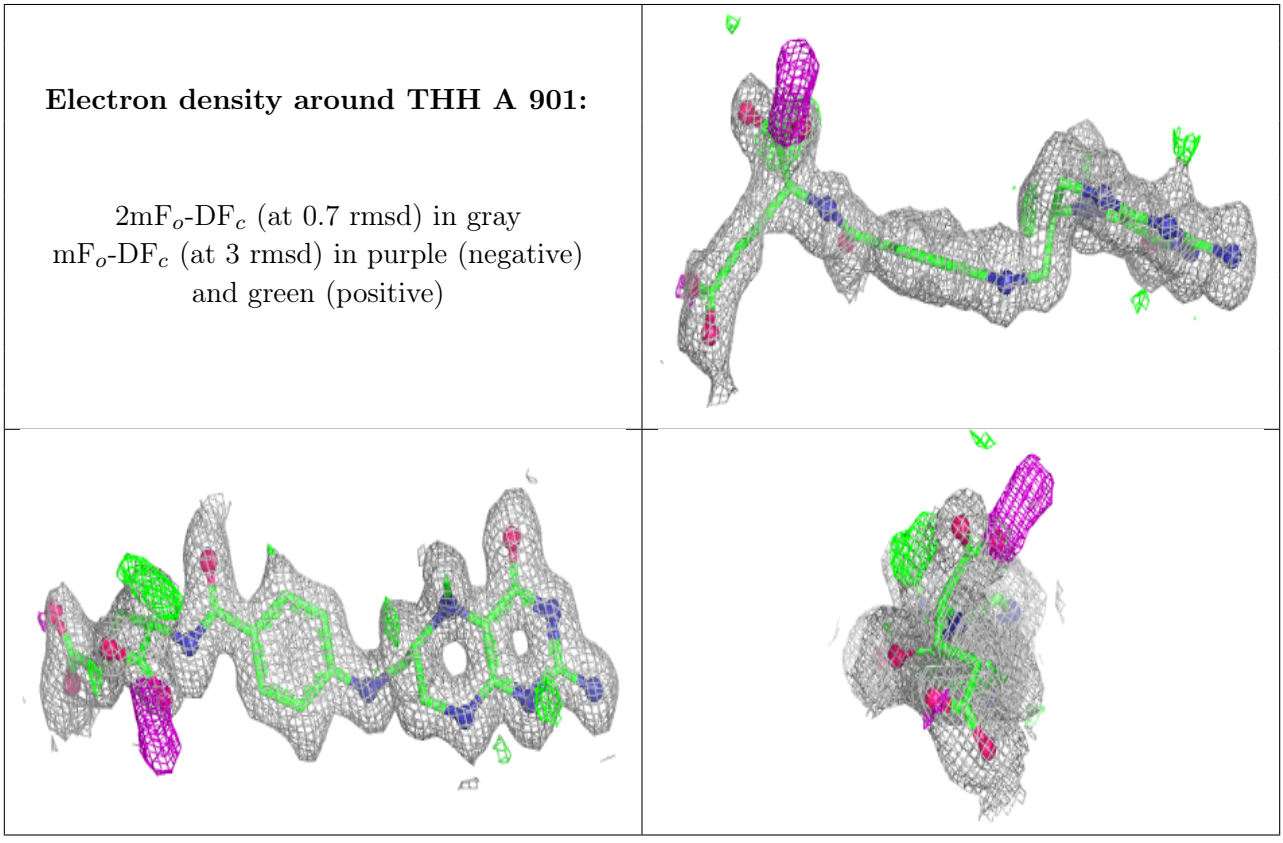
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	THH	A	901	33/33	0.83	0.14	14,18,31,35	0
2	THH	C	901	33/33	0.83	0.13	17,19,32,35	0
2	THH	D	901	33/33	0.84	0.14	16,18,29,34	0
2	THH	B	901	33/33	0.86	0.13	17,20,34,36	0
3	GOL	A	902	6/6	0.87	0.22	32,34,36,42	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.

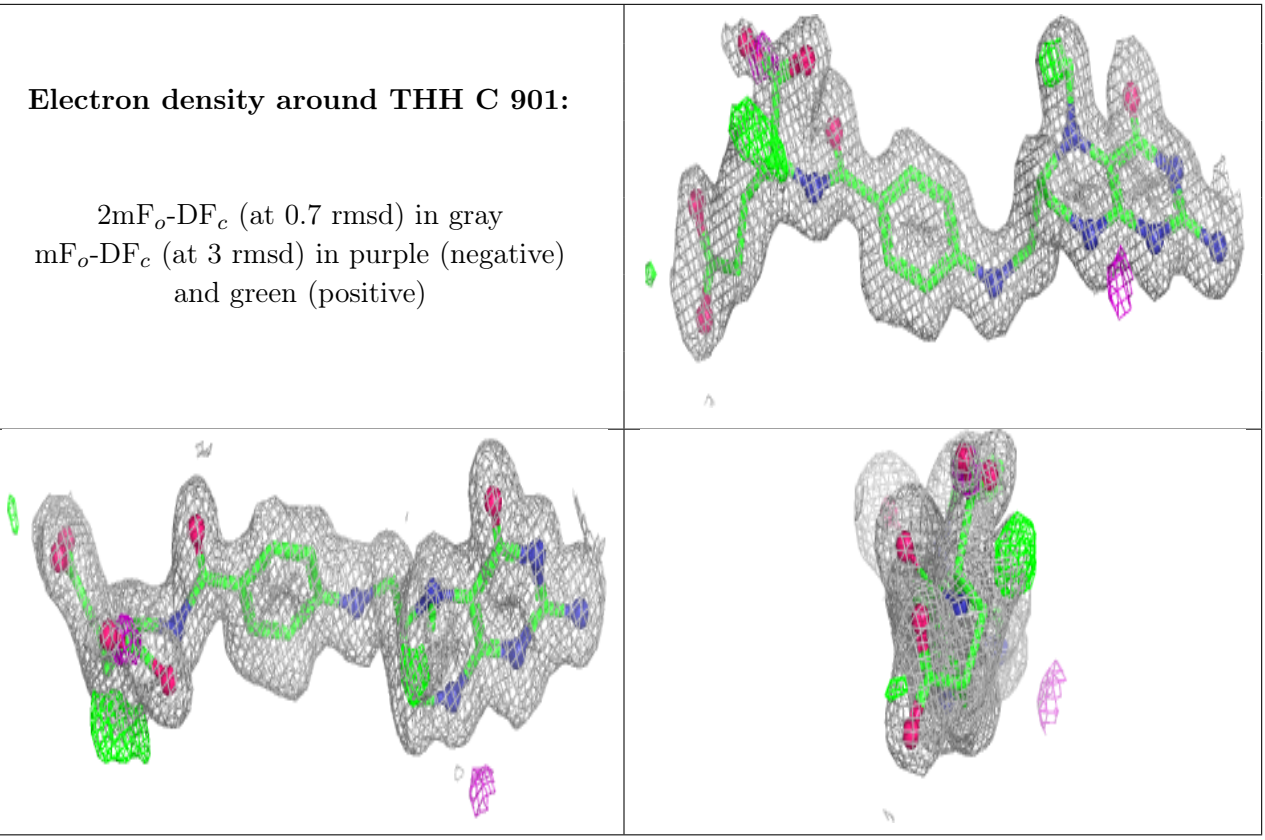
Electron density around THH A 901:

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



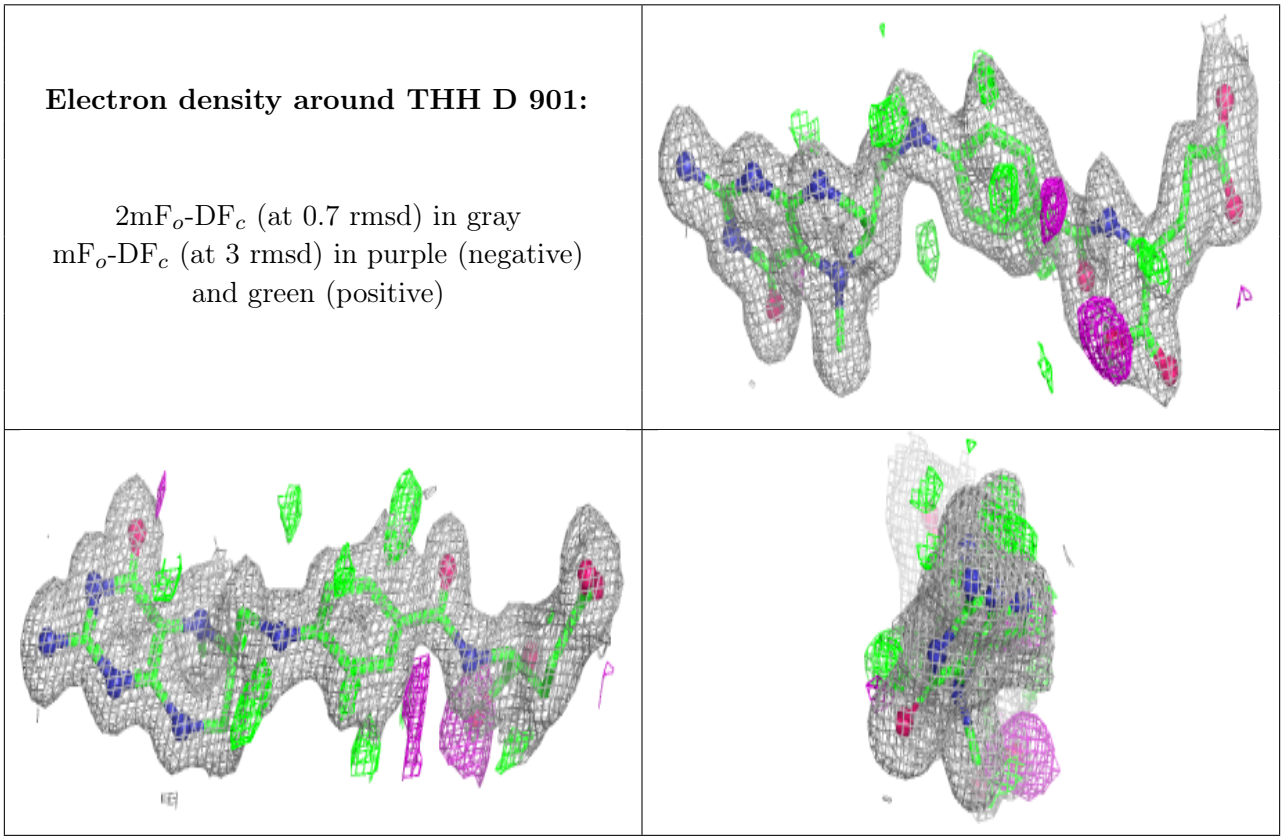
Electron density around THH C 901:

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



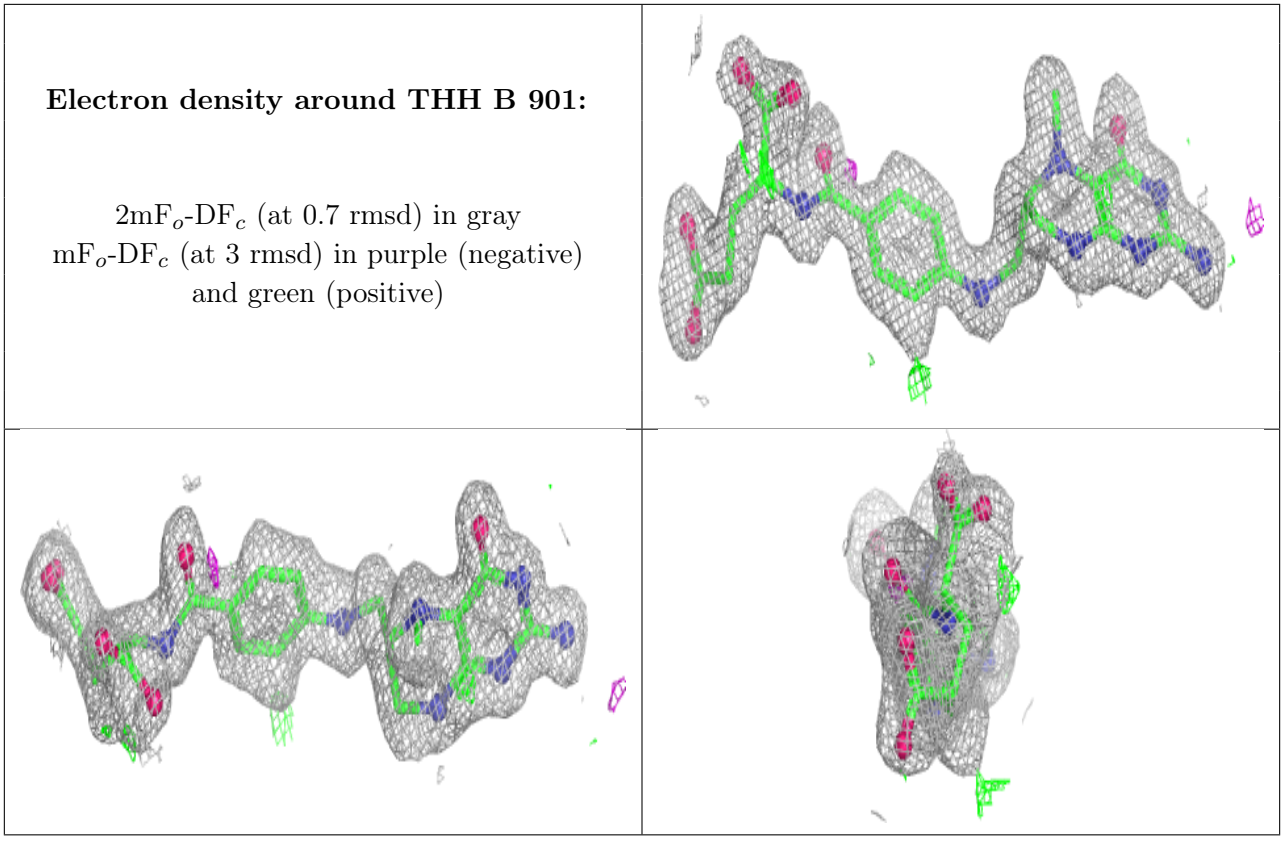
Electron density around THH D 901:

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



Electron density around THH B 901:

$2mF_o$-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.