



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:55 PM UTC

PDB ID : 5X1M / pdb_00005x1m
Title : Vanillate/3-O-methylgallate O-demethylase, LigM, protocatechuate-tetrahydrofolate complex form
Authors : Harada, A.; Senda, T.
Deposited on : 2017-01-26
Resolution : 1.90 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

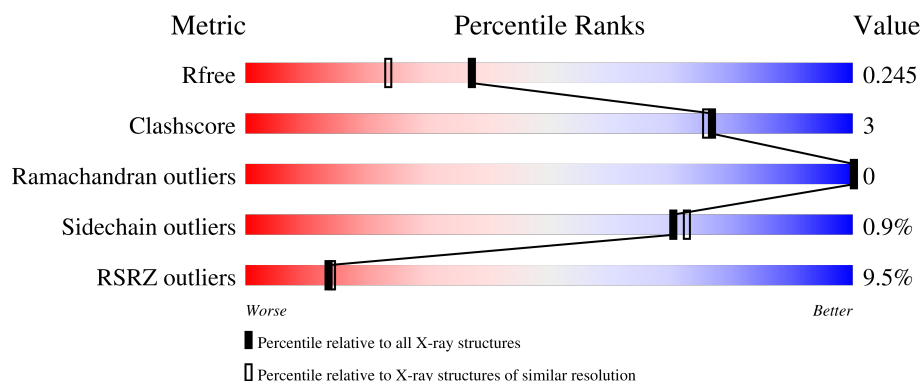
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	474	
1	B	474	
1	C	474	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11022 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.

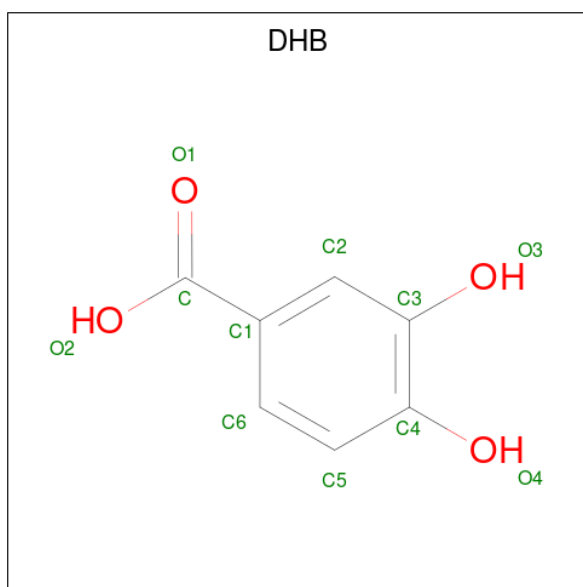
- Molecule 1 is a protein called Vanillate/3-O-methylgallate O-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	6	0
			3584	2302	608	661	13			
1	B	447	Total	C	N	O	S	0	2	0
			3491	2239	594	645	13			
1	C	455	Total	C	N	O	S	0	1	0
			3475	2234	587	640	14			

There are 9 discrepancies between the modelled and reference sequences:

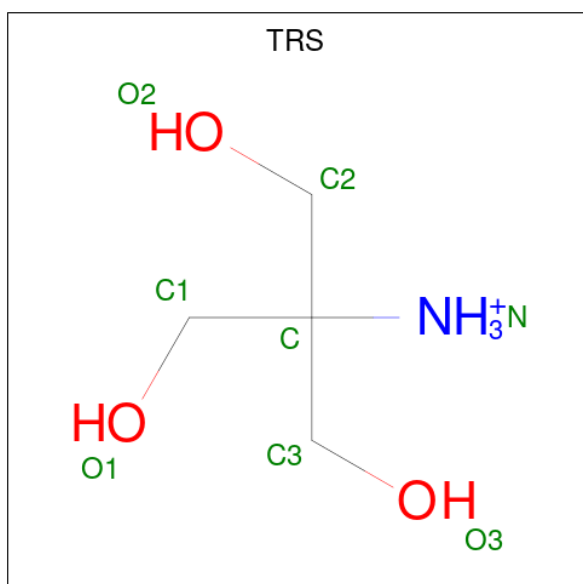
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G2IQS7
A	-1	SER	-	expression tag	UNP G2IQS7
A	0	SER	-	expression tag	UNP G2IQS7
B	-2	GLY	-	expression tag	UNP G2IQS7
B	-1	SER	-	expression tag	UNP G2IQS7
B	0	SER	-	expression tag	UNP G2IQS7
C	-2	GLY	-	expression tag	UNP G2IQS7
C	-1	SER	-	expression tag	UNP G2IQS7
C	0	SER	-	expression tag	UNP G2IQS7

- Molecule 2 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: C₇H₆O₄).



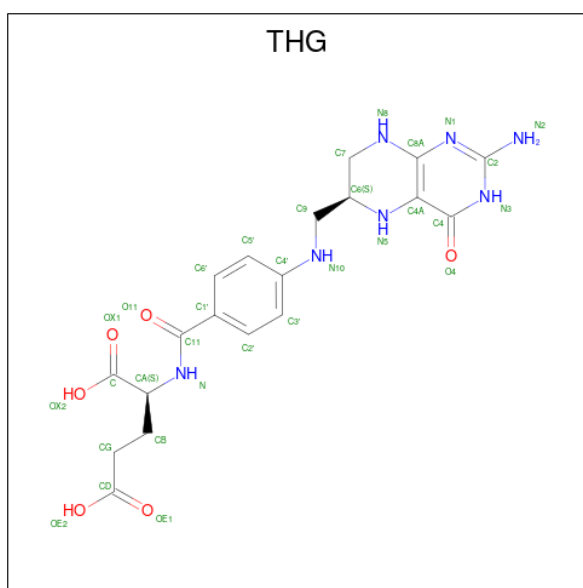
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	7	4		
2	A	1	Total	C	O	0	0
			11	7	4		
2	B	1	Total	C	O	0	0
			11	7	4		
2	C	1	Total	C	O	0	0
			11	7	4		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 4 is (6S)-5,6,7,8-TETRAHYDROFOLATE (CCD ID: THG) (formula: C₁₉H₂₃N₇O₆).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

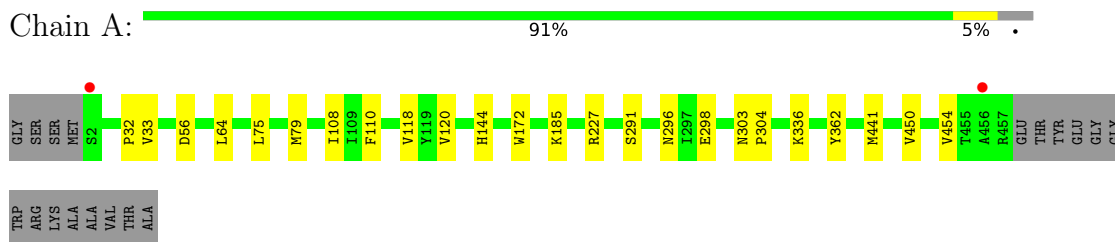
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	112	Total	O	0	0
			112	112		
6	C	43	Total	O	0	0
			43	43		

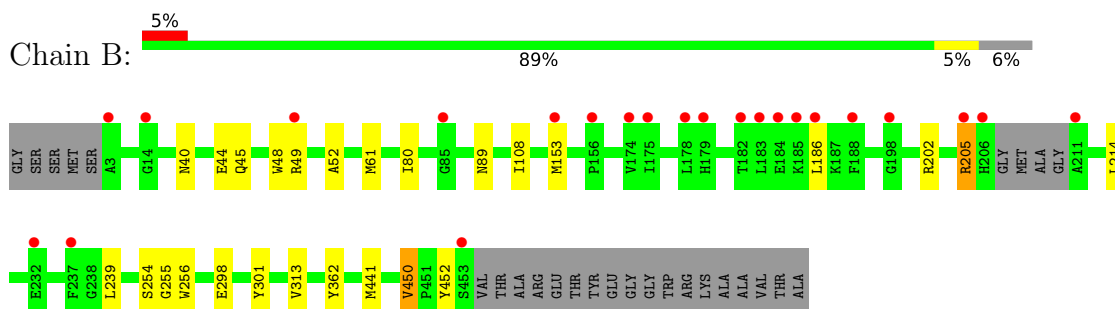
3 Residue-property plots

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.

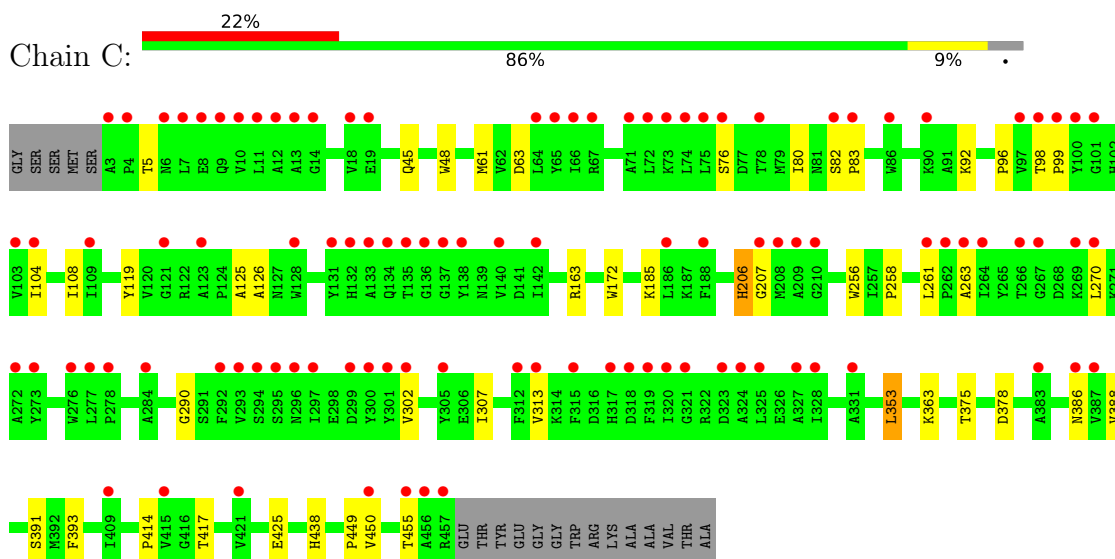
- Molecule 1: Vanillate/3-O-methylgallate O-demethylase



- Molecule 1: Vanillate/3-O-methylgallate O-demethylase



- Molecule 1: Vanillate/3-O-methylgallate O-demethylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.80Å 118.37Å 132.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 1.90 47.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.53-1.90) 87.7 (47.53-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.208 , 0.242 0.211 , 0.245	Depositor DCC
R_{free} test set	6311 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11022	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

5.1 Standard geometry

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

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	0.34	0/3701	0.54	0/5047
1	B	0.28	0/3595	0.51	0/4904
1	C	0.22	0/3577	0.44	0/4889
All	All	0.29	0/10873	0.50	0/14840

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	3584	0	3469	14	0
1	B	3491	0	3338	19	0
1	C	3475	0	3271	28	0
2	A	22	0	10	1	0
2	B	11	0	5	2	0
2	C	11	0	5	2	0
3	A	16	0	24	2	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
4	B	32	0	21	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	32	0	21	3	0
5	B	4	0	6	0	0
6	A	173	0	0	0	0
6	B	112	0	0	1	0
6	C	43	0	0	1	0
All	All	11022	0	10194	61	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 (61) 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:C:61[A]:MET:HE2	2:C:502:DHB:H2	1.72	0.69
1:B:452:TYR:O	6:B:601:HOH:O	2.10	0.69
1:C:108:ILE:HD11	4:C:501:THG:HC5	1.76	0.68
1:B:61[B]:MET:HE3	4:B:501:THG:HC71	1.78	0.65
1:C:256:TRP:CH2	4:C:501:THG:HC6	2.33	0.64
1:C:256:TRP:CZ2	4:C:501:THG:HC6	2.34	0.63
1:A:75:LEU:HB3	1:A:79:MET:CE	2.30	0.61
1:B:256:TRP:CH2	4:B:501:THG:HC6	2.35	0.60
1:C:414:PRO:HD2	1:C:417:THR:HG21	1.85	0.58
1:A:291:SER:O	2:A:502:DHB:H5	2.03	0.58
1:B:61[B]:MET:HE2	2:B:502:DHB:H2	1.86	0.57
1:B:80:ILE:HD12	1:B:313:VAL:HG22	1.88	0.55
1:C:378:ASP:HB2	1:C:391:SER:HB3	1.89	0.54
1:A:56:ASP:OD2	1:A:227[A]:ARG:NH1	2.41	0.53
1:C:414:PRO:O	1:C:417:THR:HG23	2.09	0.52
1:A:108:ILE:HG12	3:A:504:TRS:H32	1.94	0.49
1:C:45:GLN:HG2	1:C:48:TRP:CH2	2.48	0.49
1:A:336:LYS:HE3	1:A:450:VAL:HG21	1.93	0.49
1:B:45:GLN:HG2	1:B:48:TRP:CH2	2.47	0.49
1:C:386:ASN:O	1:C:388:VAL:HG13	2.13	0.48
1:C:119:TYR:OH	1:C:125:ALA:HB3	2.14	0.48
1:C:449:PRO:HD3	1:C:455:THR:HG21	1.96	0.48
1:C:353:LEU:HD23	6:C:640:HOH:O	2.14	0.47
1:B:108:ILE:HD12	4:B:501:THG:C2	2.44	0.47
1:A:75:LEU:HB3	1:A:79:MET:HE3	1.96	0.47
1:C:63:ASP:OD2	1:C:163:ARG:NH1	2.47	0.47
1:C:261:LEU:HB2	1:C:375:THR:HG21	1.97	0.47
1:C:80:ILE:HD12	1:C:313:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HA	1:B:214:LEU:HD23	1.99	0.45
1:A:120:VAL:HG11	3:A:504:TRS:H22	1.98	0.45
1:B:61[B]:MET:CE	2:B:502:DHB:H2	2.47	0.45
1:C:99:PRO:HD2	1:C:270:LEU:HD21	1.98	0.44
1:C:76:SER:OG	1:C:83:PRO:HG3	2.18	0.44
1:C:363:LYS:HB2	1:C:438:HIS:CD2	2.53	0.44
1:C:96:PRO:HB2	1:C:104:ILE:HD12	2.00	0.44
1:C:98:THR:HG21	1:C:263:ALA:O	2.18	0.44
1:A:362:TYR:CD1	1:A:441:MET:HB2	2.53	0.43
1:C:172:TRP:CZ2	1:C:185:LYS:HG2	2.53	0.43
1:C:119:TYR:CE2	1:C:126:ALA:HB2	2.53	0.43
1:C:290:GLY:O	1:C:425:GLU:HG2	2.18	0.43
1:B:362:TYR:CD1	1:B:441:MET:HB2	2.54	0.43
1:B:186:LEU:O	1:B:205:ARG:NE	2.51	0.43
1:B:52:ALA:O	1:B:239:LEU:HA	2.18	0.43
1:A:110:PHE:HB2	1:A:118[B]:VAL:HG22	2.01	0.42
1:C:258:PRO:HD2	1:C:393:PHE:CD1	2.54	0.42
1:B:48:TRP:HD1	1:B:49:ARG:HG2	1.85	0.42
1:B:298:GLU:HG2	1:B:301:TYR:CE2	2.55	0.42
1:B:61[B]:MET:CE	4:B:501:THG:HC71	2.48	0.42
1:A:32:PRO:HB2	1:A:33:VAL:HG23	2.02	0.41
1:A:296:ASN:HB3	1:A:298:GLU:OE2	2.20	0.41
1:C:302:VAL:HG21	1:C:307:ILE:HG23	2.03	0.41
1:B:255:GLY:HA3	1:B:450:VAL:HG23	2.03	0.41
1:A:172:TRP:CZ2	1:A:185:LYS:HG2	2.55	0.41
1:C:82:SER:O	1:C:92:LYS:HE3	2.21	0.41
1:C:61[A]:MET:CE	2:C:502:DHB:H2	2.46	0.41
1:B:89:ASN:OD1	1:B:202:ARG:NH2	2.53	0.41
1:C:206:HIS:HB3	1:C:207:GLY:H	1.68	0.41
1:A:64[A]:LEU:HD12	1:A:144:HIS:HA	2.04	0.40
1:B:256:TRP:CZ2	4:B:501:THG:HC6	2.56	0.40
1:A:303:ASN:HB2	1:A:304:PRO:HD2	2.03	0.40
1:B:40:ASN:O	1:B:44:GLU:HG3	2.22	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	460/474 (97%)	452 (98%)	8 (2%)	0	100	100
1	B	445/474 (94%)	435 (98%)	10 (2%)	0	100	100
1	C	454/474 (96%)	440 (97%)	14 (3%)	0	100	100
All	All	1359/1422 (96%)	1327 (98%)	32 (2%)	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	367/382 (96%)	365 (100%)	2 (0%)	81	84
1	B	354/382 (93%)	350 (99%)	4 (1%)	65	67
1	C	339/382 (89%)	335 (99%)	4 (1%)	63	63
All	All	1060/1146 (92%)	1050 (99%)	10 (1%)	70	73

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

Mol	Chain	Res	Type
1	A	454[A]	VAL
1	A	454[B]	VAL
1	B	153	MET
1	B	205	ARG
1	B	254	SER

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Mol	Chain	Res	Type
1	B	450	VAL
1	C	5	THR
1	C	206	HIS
1	C	353	LEU
1	C	450	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	ASN
1	C	386	ASN
1	C	411	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](#)

11 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	$\# Z > 2$
4	THG	B	501	-	32,34,34	2.60	8 (25%)	39,47,47	3.33	19 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	THG	C	501	-	32,34,34	2.50	8 (25%)	39,47,47	1.58	7 (17%)
2	DHB	A	501	-	11,11,11	1.65	3 (27%)	15,15,15	1.16	1 (6%)
2	DHB	C	502	-	11,11,11	1.71	3 (27%)	15,15,15	1.02	1 (6%)
3	TRS	A	504	-	7,7,7	0.32	0	9,9,9	1.22	0
2	DHB	A	502	-	11,11,11	1.67	4 (36%)	15,15,15	1.00	0
3	TRS	B	503	-	7,7,7	0.20	0	9,9,9	0.72	0
5	EDO	B	504	-	3,3,3	0.36	0	2,2,2	0.93	0
3	TRS	C	503	-	7,7,7	0.33	0	9,9,9	0.55	0
3	TRS	A	503	-	7,7,7	0.33	0	9,9,9	0.69	0
2	DHB	B	502	-	11,11,11	1.80	3 (27%)	15,15,15	0.89	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
4	THG	B	501	-	-	12/22/31/31	0/3/3/3
4	THG	C	501	-	-	5/22/31/31	0/3/3/3
2	DHB	A	501	-	-	0/4/4/4	0/1/1/1
2	DHB	C	502	-	-	0/4/4/4	0/1/1/1
3	TRS	A	504	-	-	3/9/9/9	-
2	DHB	A	502	-	-	0/4/4/4	0/1/1/1
3	TRS	B	503	-	-	0/9/9/9	-
5	EDO	B	504	-	-	1/1/1/1	-
3	TRS	C	503	-	-	3/9/9/9	-
3	TRS	A	503	-	-	4/9/9/9	-
2	DHB	B	502	-	-	0/4/4/4	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	THG	C7-N8	-7.98	1.38	1.46
4	B	501	THG	C7-N8	-7.82	1.38	1.46
4	B	501	THG	C4A-N5	6.70	1.53	1.37
4	C	501	THG	C4A-N5	6.66	1.53	1.37
4	B	501	THG	C11-N	5.65	1.47	1.34
4	C	501	THG	C11-N	5.15	1.46	1.34
4	B	501	THG	C2-N2	4.54	1.44	1.34
4	C	501	THG	C2-N2	4.54	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	DHB	O4-C4	3.96	1.44	1.36
2	C	502	DHB	O4-C4	3.88	1.44	1.36
2	A	501	DHB	O4-C4	3.37	1.43	1.36
2	A	502	DHB	O4-C4	3.37	1.43	1.36
4	B	501	THG	C8A-N1	-2.94	1.31	1.36
4	B	501	THG	C4-N3	-2.67	1.33	1.38
4	B	501	THG	C4'-N10	2.56	1.45	1.38
2	A	501	DHB	O2-C	-2.44	1.23	1.30
4	C	501	THG	C8A-N1	-2.44	1.32	1.36
2	C	502	DHB	O2-C	-2.43	1.23	1.30
4	C	501	THG	C4-N3	-2.40	1.34	1.38
2	B	502	DHB	O2-C	-2.36	1.23	1.30
4	C	501	THG	O4-C4	-2.22	1.19	1.23
2	A	502	DHB	O2-C	-2.20	1.24	1.30
2	B	502	DHB	O1-C	2.20	1.29	1.22
4	B	501	THG	O4-C4	-2.19	1.19	1.23
4	C	501	THG	C4'-N10	2.17	1.44	1.38
2	A	501	DHB	O1-C	2.17	1.29	1.22
2	A	502	DHB	O1-C	2.13	1.29	1.22
2	A	502	DHB	O3-C3	2.07	1.40	1.36
2	C	502	DHB	O1-C	2.03	1.28	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	THG	C1'-C11-N	11.11	137.63	117.04
4	B	501	THG	CA-N-C11	10.43	146.58	121.56
4	B	501	THG	O11-C11-N	-5.94	111.17	122.47
4	B	501	THG	O11-C11-C1'	-4.91	111.17	120.90
4	B	501	THG	CG-CB-CA	-3.88	106.01	113.16
4	C	501	THG	C6-C7-N8	3.76	117.44	110.60
4	B	501	THG	CB-CA-N	3.62	118.07	110.91
4	B	501	THG	C2-N1-C8A	3.55	119.63	113.36
4	B	501	THG	C-CA-N	-3.55	102.34	110.57
4	C	501	THG	C2-N1-C8A	3.52	119.58	113.36
4	B	501	THG	C2-N3-C4	-3.13	119.44	125.11
4	C	501	THG	C2-N3-C4	-3.12	119.46	125.11
2	C	502	DHB	O2-C-C1	2.74	121.88	114.84
4	C	501	THG	O4-C4-C4A	-2.74	120.66	127.26
4	C	501	THG	C4A-C4-N3	2.53	119.07	112.13
4	B	501	THG	O4-C4-C4A	-2.50	121.22	127.26
4	B	501	THG	C4A-C4-N3	2.50	119.00	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	THG	OE2-CD-CG	2.46	121.78	114.00
4	B	501	THG	C6-C7-N8	2.45	115.05	110.60
4	B	501	THG	C6'-C1'-C11	-2.39	112.84	120.60
4	B	501	THG	C4-C4A-N5	2.36	122.71	116.27
2	A	501	DHB	C6-C5-C4	-2.36	118.14	120.50
4	C	501	THG	C4-C4A-N5	2.32	122.61	116.27
4	B	501	THG	C7-C6-C9	-2.28	108.28	112.96
4	B	501	THG	C2'-C1'-C11	2.24	127.86	120.60
4	B	501	THG	OE2-CD-OE1	-2.11	117.90	123.33
4	C	501	THG	N2-C2-N3	2.10	121.19	116.76
4	B	501	THG	OX2-C-OX1	-2.04	119.46	124.08

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	TRS	C2-C-C1-O1
3	A	503	TRS	C3-C-C1-O1
3	A	504	TRS	C1-C-C3-O3
3	A	504	TRS	C2-C-C3-O3
3	A	504	TRS	N-C-C3-O3
3	C	503	TRS	N-C-C3-O3
4	B	501	THG	C7-C6-C9-N10
4	B	501	THG	N5-C6-C9-N10
4	B	501	THG	C1'-C11-N-CA
4	B	501	THG	O11-C11-N-CA
4	B	501	THG	CB-CA-N-C11
4	C	501	THG	N-CA-CB-CG
4	C	501	THG	C-CA-CB-CG
3	C	503	TRS	C2-C-C3-O3
4	B	501	THG	OX2-C-CA-N
3	A	503	TRS	N-C-C1-O1
4	B	501	THG	CA-CB-CG-CD
4	B	501	THG	OX1-C-CA-N
4	B	501	THG	C5'-C4'-N10-C9
4	C	501	THG	OX2-C-CA-CB
4	C	501	THG	OX1-C-CA-CB
3	C	503	TRS	C1-C-C3-O3
4	B	501	THG	OE1-CD-CG-CB
4	B	501	THG	OE2-CD-CG-CB
4	B	501	THG	C3'-C4'-N10-C9
3	A	503	TRS	C3-C-C2-O2

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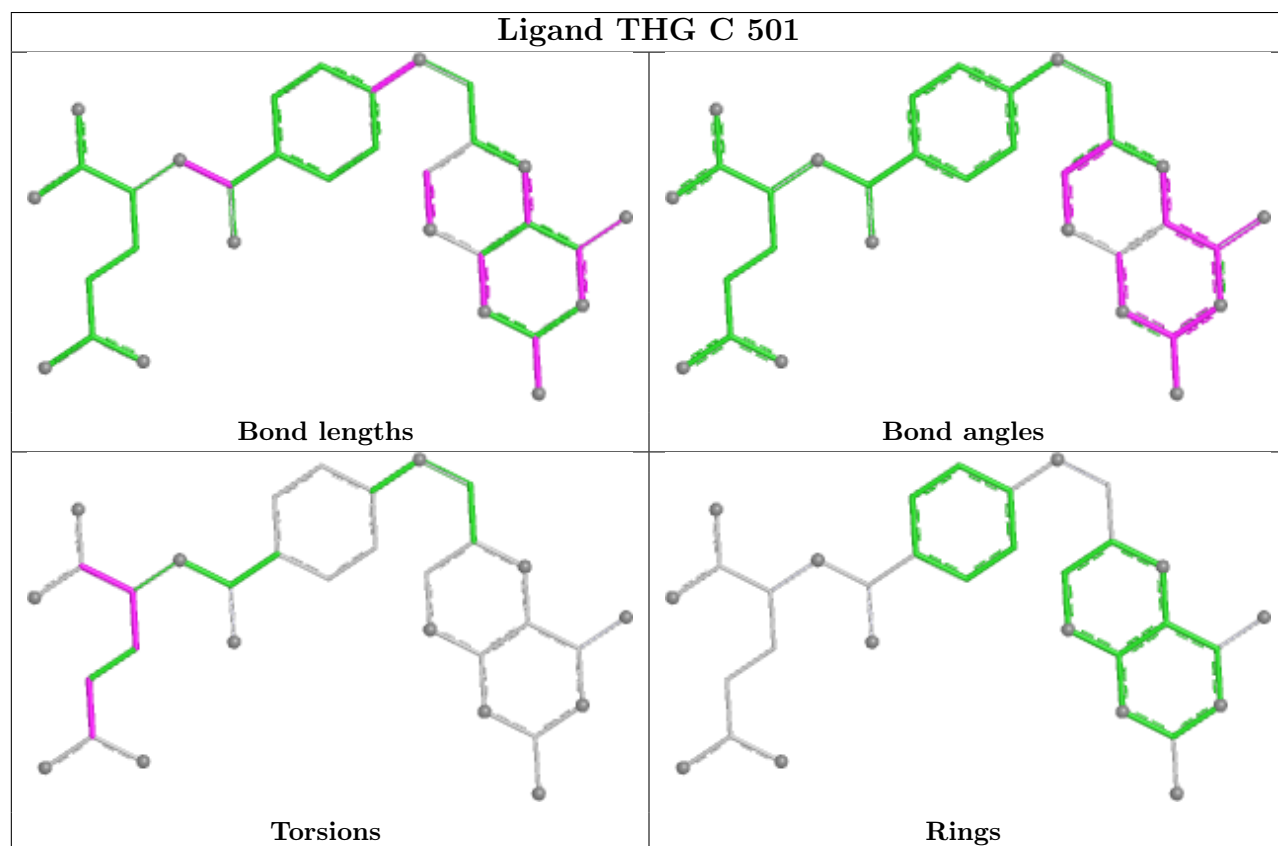
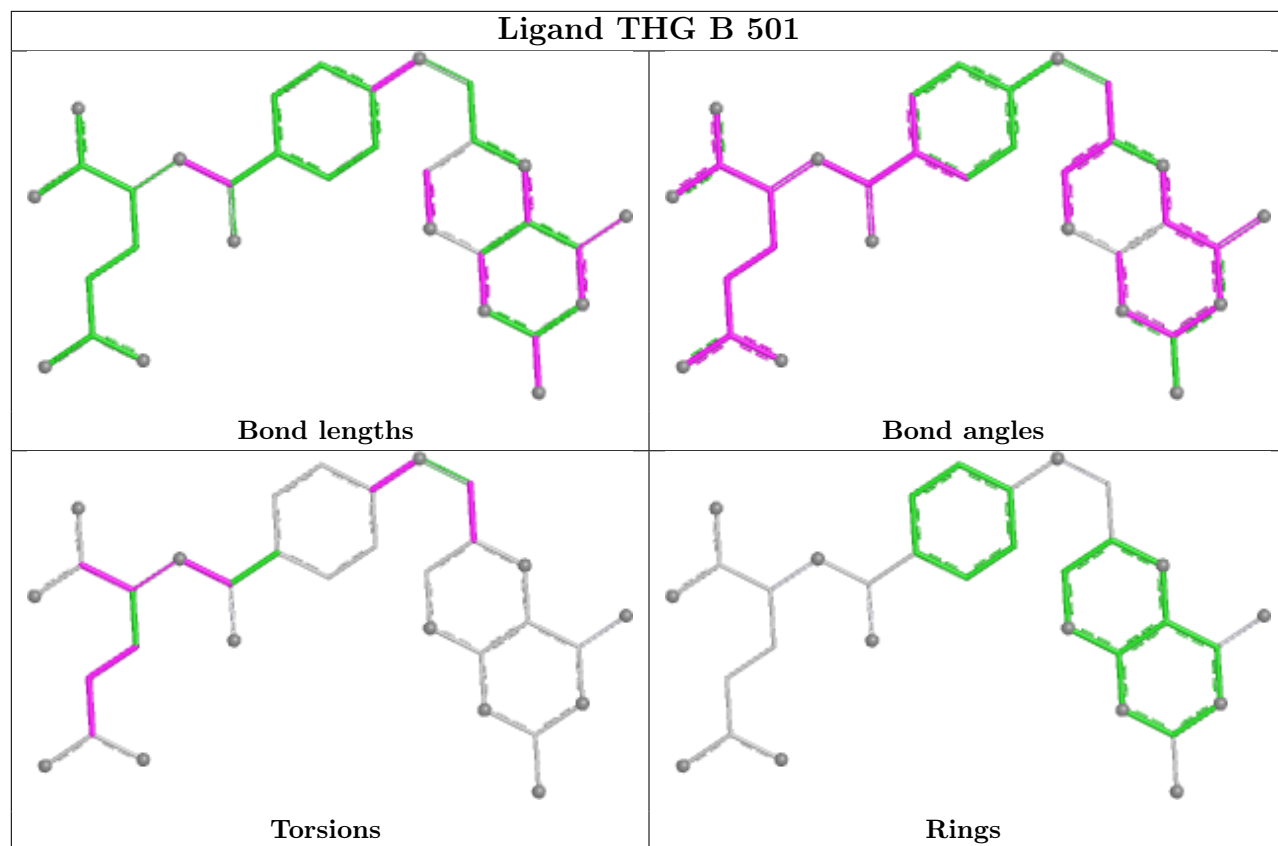
Mol	Chain	Res	Type	Atoms
4	C	501	THG	OE2-CD-CG-CB
5	B	504	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	THG	5	0
4	C	501	THG	3	0
2	C	502	DHB	2	0
3	A	504	TRS	2	0
2	A	502	DHB	1	0
2	B	502	DHB	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	456/474 (96%)	-0.01	2 (0%) 88 90	13, 26, 39, 60	6 (1%)
1	B	447/474 (94%)	0.41	23 (5%) 33 36	14, 32, 53, 64	2 (0%)
1	C	455/474 (95%)	1.31	104 (22%) 2 2	21, 47, 68, 73	1 (0%)
All	All	1358/1422 (95%)	0.57	129 (9%) 14 14	13, 33, 62, 73	9 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	4.9
1	C	325	LEU	4.9
1	C	133	ALA	4.2
1	C	137	GLY	4.2
1	B	3	ALA	4.1
1	C	327	ALA	4.1
1	C	328	ILE	4.0
1	C	312	PHE	3.9
1	B	206	HIS	3.8
1	C	210	GLY	3.7
1	C	263	ALA	3.7
1	C	302	VAL	3.6
1	C	138	TYR	3.5
1	C	323	ASP	3.5
1	C	315	PHE	3.5
1	C	318	ASP	3.3
1	C	295	SER	3.3
1	C	320	ILE	3.3
1	C	313	VAL	3.3
1	C	188	PHE	3.3
1	C	457	ARG	3.3
1	B	453	SER	3.3
1	C	134	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	456	ALA	3.2
1	C	266	THR	3.2
1	C	9	GLN	3.2
1	C	409	ILE	3.1
1	C	321	GLY	3.1
1	C	72	LEU	3.1
1	C	74	LEU	3.1
1	C	103	VAL	3.1
1	C	140	VAL	3.0
1	C	292	PHE	3.0
1	C	12	ALA	3.0
1	C	284	ALA	3.0
1	C	270	LEU	2.9
1	C	142	ILE	2.9
1	C	100	TYR	2.9
1	C	455	THR	2.9
1	C	277	LEU	2.9
1	C	97	VAL	2.8
1	C	75	LEU	2.8
1	A	2	SER	2.8
1	B	182	THR	2.8
1	B	183	LEU	2.8
1	C	109	ILE	2.8
1	C	208	MET	2.8
1	C	66	ILE	2.7
1	C	300	TYR	2.7
1	C	136	GLY	2.7
1	C	264	ILE	2.7
1	C	10	VAL	2.7
1	C	267	GLY	2.7
1	B	186	LEU	2.6
1	C	11	LEU	2.6
1	C	123	ALA	2.6
1	C	276	TRP	2.6
1	B	188	PHE	2.6
1	C	135	THR	2.6
1	C	14	GLY	2.6
1	C	71	ALA	2.6
1	C	383	ALA	2.6
1	C	4	PRO	2.5
1	C	65	TYR	2.5
1	C	186	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	386	ASN	2.5
1	C	297	ILE	2.5
1	C	128	TRP	2.5
1	C	331	ALA	2.5
1	C	73	LYS	2.5
1	C	415	VAL	2.4
1	C	299	ASP	2.4
1	C	98	THR	2.4
1	C	324	ALA	2.4
1	C	293	VAL	2.4
1	C	319	PHE	2.4
1	B	205	ARG	2.4
1	B	178	LEU	2.3
1	B	175	ILE	2.3
1	C	272	ALA	2.3
1	B	174	VAL	2.3
1	C	296	ASN	2.3
1	C	78	THR	2.3
1	B	232	GLU	2.3
1	C	83	PRO	2.2
1	C	131	TYR	2.2
1	C	269	LYS	2.2
1	B	198	GLY	2.2
1	C	3	ALA	2.2
1	C	13	ALA	2.2
1	C	273	TYR	2.2
1	C	294	SER	2.2
1	C	278	PRO	2.2
1	C	305	TYR	2.2
1	B	179	HIS	2.2
1	B	14	GLY	2.2
1	C	90	LYS	2.2
1	C	421	VAL	2.1
1	C	99	PRO	2.1
1	C	262	PRO	2.1
1	B	153	MET	2.1
1	A	456	ALA	2.1
1	C	18	VAL	2.1
1	B	185	LYS	2.1
1	C	7	LEU	2.1
1	C	261	LEU	2.1
1	B	211	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	104	ILE	2.1
1	C	301	TYR	2.1
1	C	76	SER	2.1
1	B	184	GLU	2.1
1	B	85	GLY	2.1
1	C	101	GLY	2.1
1	C	207	GLY	2.1
1	C	450	VAL	2.1
1	C	67	ARG	2.1
1	B	237	PHE	2.0
1	C	121	GLY	2.0
1	C	6	ASN	2.0
1	B	156	PRO	2.0
1	C	64	LEU	2.0
1	C	86	TRP	2.0
1	B	49	ARG	2.0
1	C	8	GLU	2.0
1	C	19	GLU	2.0
1	C	82	SER	2.0
1	C	132	HIS	2.0
1	C	317	HIS	2.0
1	C	387	VAL	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.

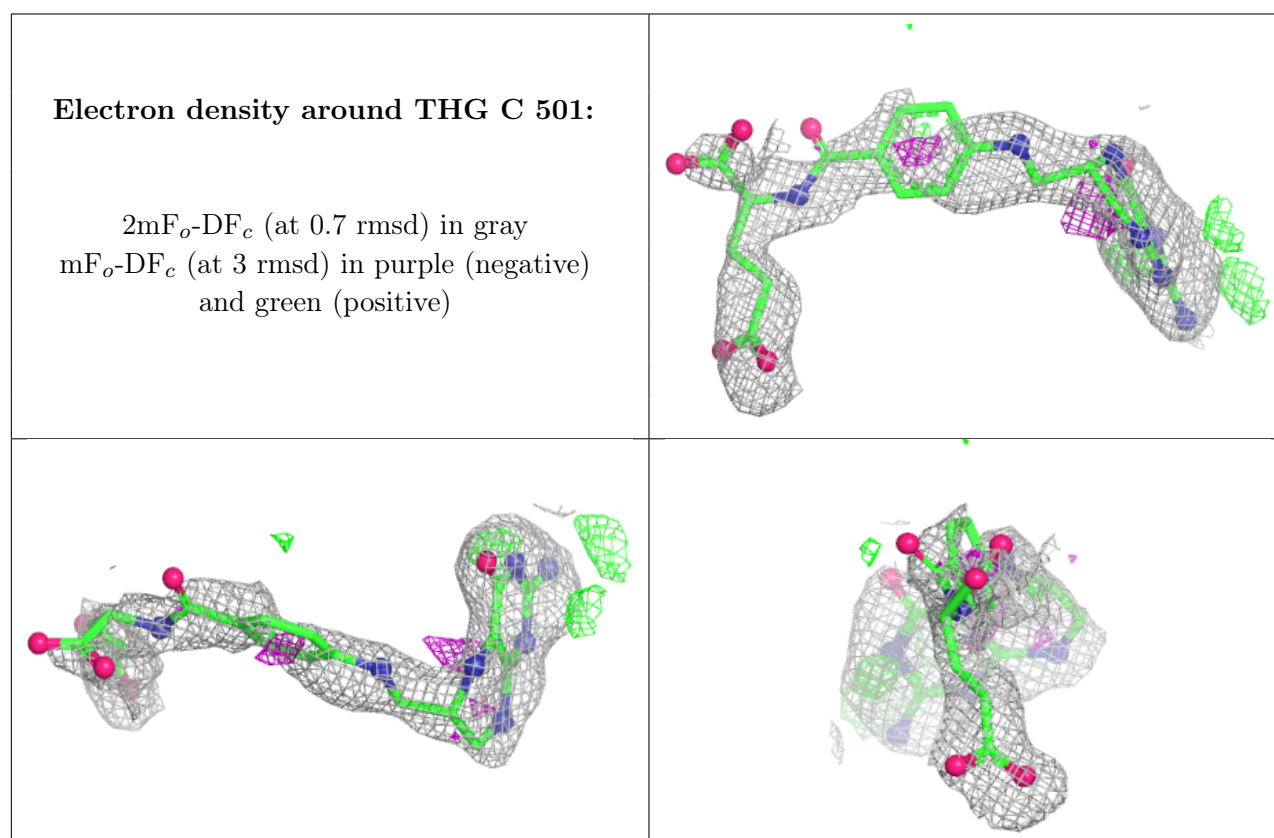
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	THG	C	501	32/32	0.69	0.18	52,62,82,84	0

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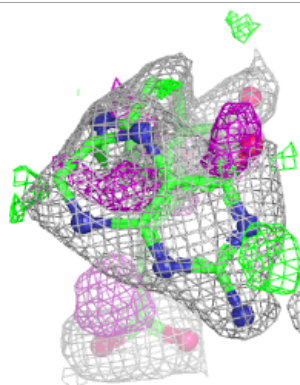
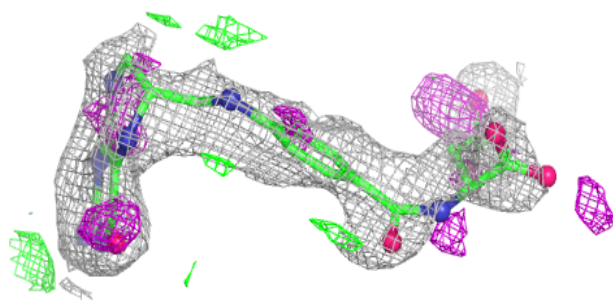
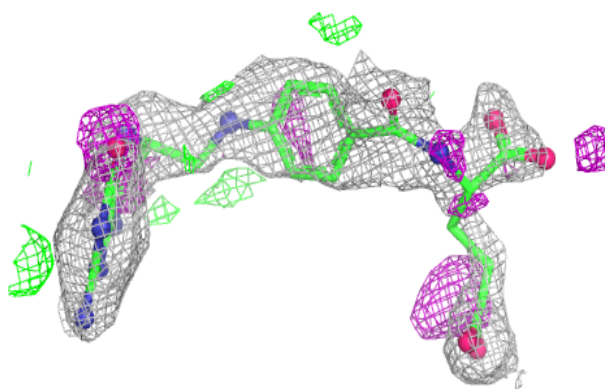
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DHB	A	502	11/11	0.71	0.17	42,51,62,66	0
4	THG	B	501	32/32	0.78	0.15	37,46,63,67	0
5	EDO	B	504	4/4	0.80	0.17	38,42,43,44	0
3	TRS	A	503	8/8	0.82	0.13	23,30,36,39	0
3	TRS	C	503	8/8	0.83	0.13	41,47,49,50	0
3	TRS	A	504	8/8	0.84	0.13	27,36,40,42	0
3	TRS	B	503	8/8	0.91	0.10	34,37,41,44	0
2	DHB	C	502	11/11	0.93	0.09	36,40,43,44	0
2	DHB	B	502	11/11	0.94	0.07	26,29,32,33	0
2	DHB	A	501	11/11	0.96	0.05	16,19,23,24	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 B 501:

$2mF_o-DF_c$ (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.