



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:14 PM BST

PDB ID : 4DM6  
Title : Crystal structure of RARb LBD homodimer in complex with TTNPB  
Authors : Osz, J.; Brelivet, Y.; Peluso-Iltis, C.; Cura, V.; Eiler, S.; Ruff, M.; Bourguet, W.; Rochel, N.; Moras, D.  
Deposited on : 2012-02-07  
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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

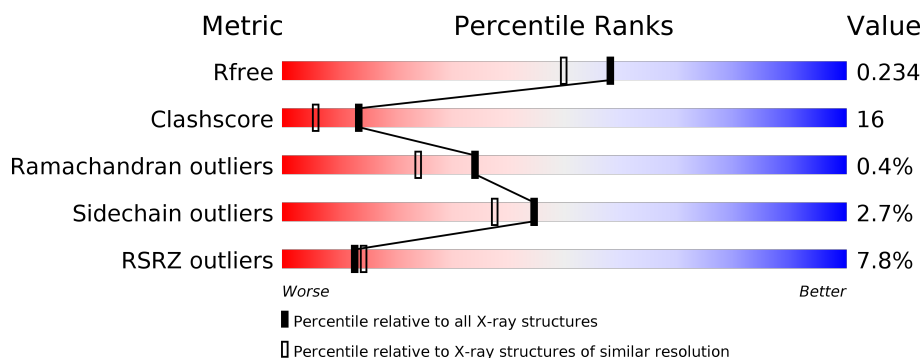
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	267	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>27%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	267	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>10%</div> </div> </div>
2	E	25	<div> <div>16%</div> <div> <div></div> <div>32%</div> <div>8%</div> <div>•</div> <div>56%</div> </div> </div>
2	F	25	<div> <div>4%</div> <div> <div></div> <div>32%</div> <div>12%</div> <div>•</div> <div>52%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4203 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 Retinoic acid receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	5	0	0
			1894	1205	318	356	15			
1	B	239	Total	C	N	O	S	2	0	0
			1890	1204	317	354	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	MET	-	INITIATING METHIONINE	UNP P10826
A	158	GLY	-	EXPRESSION TAG	UNP P10826
A	159	SER	-	EXPRESSION TAG	UNP P10826
A	160	SER	-	EXPRESSION TAG	UNP P10826
A	161	HIS	-	EXPRESSION TAG	UNP P10826
A	162	HIS	-	EXPRESSION TAG	UNP P10826
A	163	HIS	-	EXPRESSION TAG	UNP P10826
A	164	HIS	-	EXPRESSION TAG	UNP P10826
A	165	HIS	-	EXPRESSION TAG	UNP P10826
A	166	HIS	-	EXPRESSION TAG	UNP P10826
A	167	SER	-	EXPRESSION TAG	UNP P10826
A	168	SER	-	EXPRESSION TAG	UNP P10826
A	169	GLY	-	EXPRESSION TAG	UNP P10826
A	170	LEU	-	EXPRESSION TAG	UNP P10826
A	171	VAL	-	EXPRESSION TAG	UNP P10826
A	172	PRO	-	EXPRESSION TAG	UNP P10826
A	173	ARG	-	EXPRESSION TAG	UNP P10826
A	174	GLY	-	EXPRESSION TAG	UNP P10826
A	175	SER	-	EXPRESSION TAG	UNP P10826
A	176	HIS	-	EXPRESSION TAG	UNP P10826
A	177	MET	-	EXPRESSION TAG	UNP P10826
B	1157	MET	-	INITIATING METHIONINE	UNP P10826
B	1158	GLY	-	EXPRESSION TAG	UNP P10826
B	1159	SER	-	EXPRESSION TAG	UNP P10826
B	1160	SER	-	EXPRESSION TAG	UNP P10826

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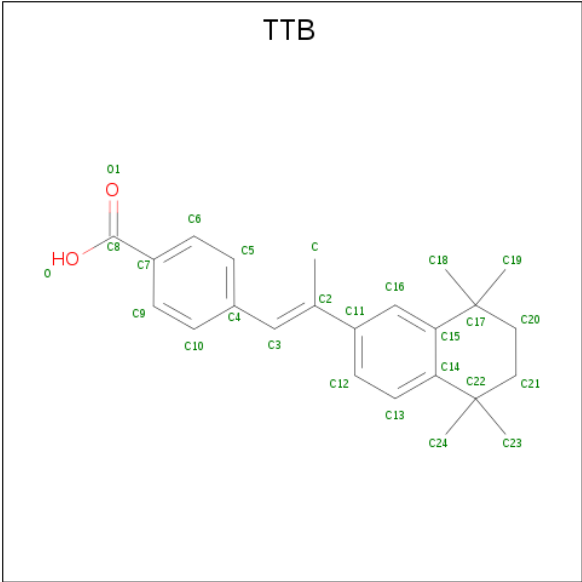
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1161	HIS	-	EXPRESSION TAG	UNP P10826
B	1162	HIS	-	EXPRESSION TAG	UNP P10826
B	1163	HIS	-	EXPRESSION TAG	UNP P10826
B	1164	HIS	-	EXPRESSION TAG	UNP P10826
B	1165	HIS	-	EXPRESSION TAG	UNP P10826
B	1166	HIS	-	EXPRESSION TAG	UNP P10826
B	1167	SER	-	EXPRESSION TAG	UNP P10826
B	1168	SER	-	EXPRESSION TAG	UNP P10826
B	1169	GLY	-	EXPRESSION TAG	UNP P10826
B	1170	LEU	-	EXPRESSION TAG	UNP P10826
B	1171	VAL	-	EXPRESSION TAG	UNP P10826
B	1172	PRO	-	EXPRESSION TAG	UNP P10826
B	1173	ARG	-	EXPRESSION TAG	UNP P10826
B	1174	GLY	-	EXPRESSION TAG	UNP P10826
B	1175	SER	-	EXPRESSION TAG	UNP P10826
B	1176	HIS	-	EXPRESSION TAG	UNP P10826
B	1177	MET	-	EXPRESSION TAG	UNP P10826

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	5	0	0
			91	59	20	12			
2	F	12	Total	C	N	O	6	0	0
			98	62	21	15			

- Molecule 3 is 4-[(1E)-2-(5,5,8,8-TETRAMETHYL-5,6,7,8-TETRAHYDRONAPHTHALEN-2-YL)PROP-1-ENYL]BENZOIC ACID (three-letter code: TTB) (formula: C<sub>24</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	24	2		
3	B	1	Total	C	O	0	0
			26	24	2		

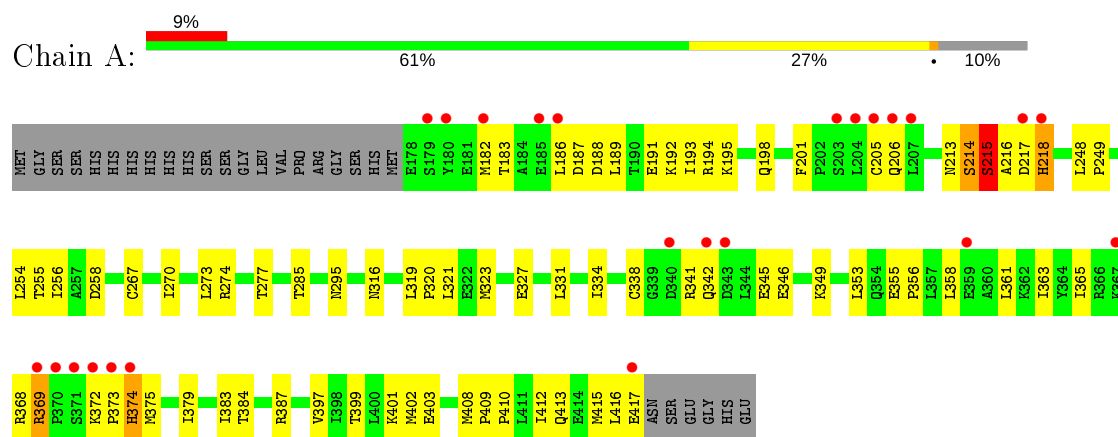
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	103	Total	O	0	0
			103	103		
4	F	2	Total	O	0	0
			2	2		

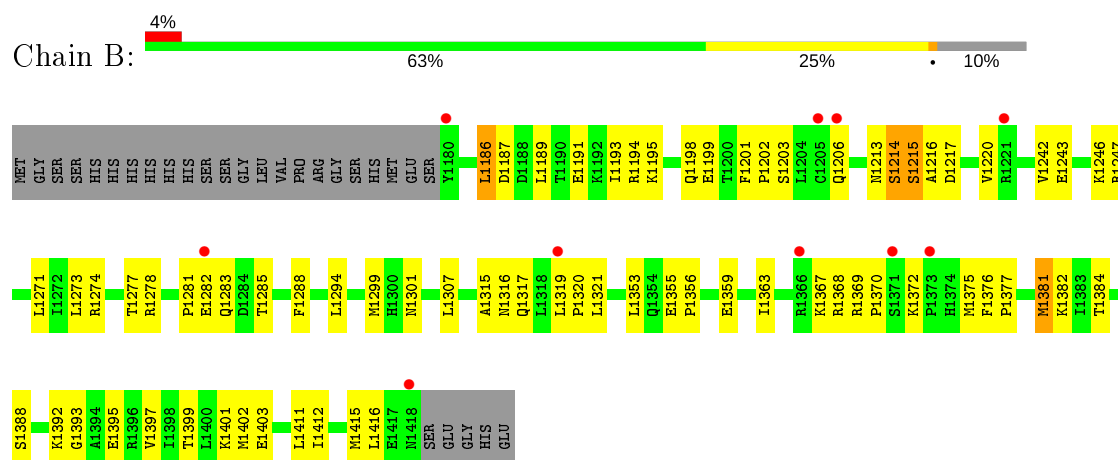
### 3 Residue-property plots [i](#)

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.

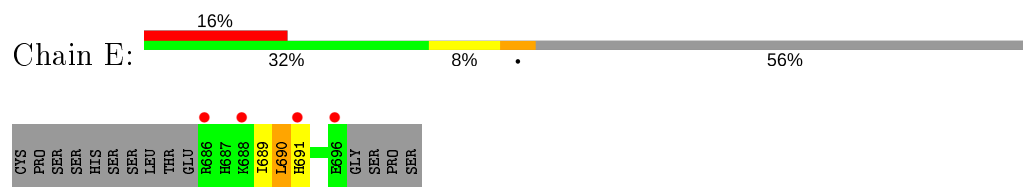
#### • Molecule 1: Retinoic acid receptor beta



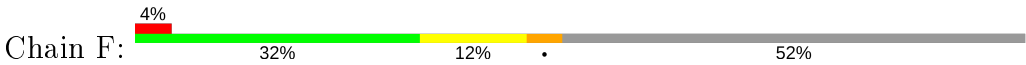
#### • Molecule 1: Retinoic acid receptor beta



#### • Molecule 2: Nuclear receptor coactivator 1



#### • Molecule 2: Nuclear receptor coactivator 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.09 Å 84.06 Å 102.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 99.8 (19.18-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.58 (at 1.90 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.239 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	2003 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TTB

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	0.55	6/1924 (0.3%)	0.56	1/2598 (0.0%)
1	B	0.66	7/1921 (0.4%)	0.57	1/2595 (0.0%)
2	E	1.52	3/92 (3.3%)	0.79	0/122
2	F	2.59	9/99 (9.1%)	1.01	0/130
All	All	0.75	25/4036 (0.6%)	0.59	2/5445 (0.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	796	GLU	CB-CG	-11.19	1.30	1.52
1	B	1215	SER	C-O	-10.25	1.03	1.23
2	F	794	LEU	C-O	-9.58	1.05	1.23
1	B	1214	SER	C-O	-9.17	1.05	1.23
1	B	1216	ALA	C-O	-8.37	1.07	1.23
1	B	1215	SER	CB-OG	-8.16	1.31	1.42
2	F	795	GLN	C-O	-7.81	1.08	1.23
1	A	216	ALA	CA-CB	-7.63	1.36	1.52
2	F	796	GLU	C-O	-7.53	1.09	1.23
1	A	214	SER	CB-OG	-6.96	1.33	1.42
1	A	214	SER	C-O	-6.87	1.10	1.23
2	E	690	LEU	C-O	-6.74	1.10	1.23
2	E	691	HIS	C-O	-6.28	1.11	1.23
1	A	213	ASN	CB-CG	-6.21	1.36	1.51
2	F	795	GLN	CD-OE1	-6.20	1.10	1.24
2	F	797	GLY	CA-C	-6.17	1.42	1.51
1	A	215	SER	CB-OG	-5.98	1.34	1.42
2	F	795	GLN	CD-NE2	-5.93	1.18	1.32
2	E	690	LEU	CG-CD1	-5.41	1.31	1.51
1	B	1213	ASN	C-O	-5.38	1.13	1.23
2	F	796	GLU	CD-OE2	-5.34	1.19	1.25
1	A	213	ASN	C-O	-5.18	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1217	ASP	C-O	-5.16	1.13	1.23
2	F	796	GLU	CD-OE1	-5.13	1.20	1.25
1	B	1213	ASN	CB-CG	-5.04	1.39	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1215	SER	N-CA-C	6.77	129.29	111.00
1	A	373	PRO	N-CA-CB	5.52	109.93	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1894	0	1955	68	0
1	B	1890	0	1956	67	0
2	E	91	0	95	2	0
2	F	98	0	101	0	0
3	A	26	0	27	1	0
3	B	26	0	27	3	0
4	A	73	0	0	1	0
4	B	103	0	0	2	0
4	F	2	0	0	1	0
All	All	4203	0	4161	130	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 16.

All (130) 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:1382:LYS:HE2	1:B:1382:LYS:HA	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HG23	1:A:258:ASP:H	1.32	0.94
1:B:1186:LEU:HD23	1:B:1363:ILE:HD12	1.49	0.94
1:B:1294:LEU:HD12	1:B:1299:MET:HE3	1.54	0.87
1:B:1412:ILE:O	1:B:1416:LEU:HD23	1.73	0.87
1:B:1294:LEU:HD12	1:B:1299:MET:CE	2.04	0.86
1:A:369:ARG:HB3	1:A:372:LYS:HG2	1.58	0.85
1:A:372:LYS:HB2	1:A:375:MET:HG2	1.58	0.84
1:B:1376:PHE:HB3	1:B:1377:PRO:HD3	1.64	0.78
1:B:1299:MET:HA	1:B:1299:MET:HE2	1.72	0.70
1:A:191:GLU:HG3	1:A:195:LYS:HE3	1.73	0.70
1:A:374:HIS:HA	1:B:1359:GLU:OE1	1.91	0.70
1:A:319:LEU:HB2	1:A:320:PRO:HD3	1.76	0.68
1:B:1368:ARG:HH12	1:B:1369:ARG:HH21	1.42	0.67
1:B:1368:ARG:HH12	1:B:1369:ARG:NH2	1.93	0.66
1:A:255:THR:HG21	1:A:345:GLU:OE2	1.96	0.66
1:B:1372:LYS:CB	1:B:1375:MET:HG2	2.26	0.66
1:B:1191:GLU:O	1:B:1195:LYS:HD3	1.96	0.64
1:B:1372:LYS:HB2	1:B:1375:MET:HG2	1.78	0.63
1:A:372:LYS:CB	1:A:375:MET:HG2	2.27	0.63
1:A:186:LEU:HD12	1:A:363:ILE:HD12	1.81	0.63
1:A:188:ASP:O	1:A:192:LYS:HD3	2.00	0.61
1:B:1273:LEU:O	1:B:1277:THR:HG23	2.01	0.61
1:A:410:PRO:HB2	2:E:689:ILE:HD11	1.83	0.59
1:A:401:LYS:NZ	1:A:413:GLN:HE22	2.00	0.59
1:B:1189:LEU:O	1:B:1193:ILE:HG12	2.03	0.59
1:A:285:THR:HG22	1:A:295:ASN:HA	1.84	0.58
1:A:201:PHE:CD2	1:A:274:ARG:HD3	2.39	0.58
1:B:1242:VAL:O	1:B:1246:LYS:HG3	2.04	0.58
1:B:1397:VAL:HG22	3:B:1501:TTB:H211	1.86	0.58
1:A:355:GLU:HB2	1:A:356:PRO:HD3	1.85	0.57
1:A:321:LEU:HD23	1:A:379:ILE:HG12	1.86	0.57
1:B:1191:GLU:CD	1:B:1194:ARG:HH21	2.08	0.57
1:B:1315:ALA:O	1:B:1319:LEU:HD23	2.05	0.57
1:B:1203:SER:HB3	1:B:1206:GLN:HG3	1.87	0.56
1:B:1416:LEU:N	1:B:1416:LEU:HD22	2.20	0.56
1:A:415:MET:SD	2:E:690:LEU:HD11	2.46	0.56
1:B:1199:GLU:CB	1:B:1247:ARG:HH12	2.19	0.56
1:A:413:GLN:O	1:A:417:GLU:HB2	2.05	0.55
1:A:323:MET:HA	1:A:327:GLU:OE2	2.06	0.55
1:B:1382:LYS:CE	1:B:1382:LYS:HA	2.29	0.55
1:A:334:ILE:HD13	1:A:358:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HD11	1:A:353:LEU:CD1	2.37	0.54
1:A:342:GLN:NE2	1:B:1317:GLN:OE1	2.41	0.54
1:A:387:ARG:HD3	1:A:387:ARG:O	2.07	0.54
1:B:1316:ASN:O	1:B:1320:PRO:HD3	2.07	0.54
1:B:1381:MET:HG3	4:B:1686:HOH:O	2.07	0.54
1:A:194:ARG:O	1:A:198:GLN:HG3	2.06	0.54
1:A:183:THR:HG21	1:A:363:ILE:HD13	1.89	0.54
1:B:1282:GLU:H	1:B:1282:GLU:CD	2.12	0.53
1:A:327:GLU:OE1	1:A:368:ARG:HD3	2.09	0.53
1:B:1411:LEU:O	1:B:1415:MET:HG2	2.09	0.52
1:A:369:ARG:HB3	1:A:372:LYS:CG	2.36	0.52
1:B:1281:PRO:HG2	1:B:1282:GLU:OE2	2.09	0.52
1:B:1368:ARG:NH1	1:B:1369:ARG:HH21	2.08	0.52
1:B:1369:ARG:N	1:B:1370:PRO:HD3	2.25	0.52
1:B:1199:GLU:HB2	1:B:1247:ARG:NH1	2.24	0.52
1:A:254:LEU:HD11	1:A:353:LEU:HD11	1.91	0.51
1:B:1299:MET:HA	1:B:1299:MET:CE	2.37	0.51
1:A:397:VAL:CG2	3:A:501:TTB:H241	2.40	0.51
1:A:189:LEU:O	1:A:193:ILE:HG12	2.11	0.51
1:A:375:MET:O	1:A:379:ILE:HG13	2.11	0.51
1:A:399:THR:O	1:A:403:GLU:HG3	2.11	0.50
1:A:256:ILE:HD12	1:A:256:ILE:N	2.27	0.50
1:A:295:ASN:HB2	4:A:668:HOH:O	2.12	0.49
1:B:1194:ARG:O	1:B:1198:GLN:HG3	2.13	0.49
1:A:365:ILE:CD1	1:A:379:ILE:HD12	2.42	0.49
1:A:201:PHE:CZ	1:A:274:ARG:HB3	2.48	0.48
1:B:1397:VAL:O	1:B:1401:LYS:HG3	2.13	0.48
1:A:273:LEU:O	1:A:277:THR:HG23	2.14	0.48
1:A:412:ILE:O	1:A:416:LEU:HD23	2.14	0.48
1:A:346:GLU:OE2	1:A:349:LYS:HD3	2.14	0.47
1:A:194:ARG:NH1	1:A:198:GLN:OE1	2.47	0.47
1:B:1355:GLU:HB2	1:B:1356:PRO:HD3	1.95	0.47
1:A:255:THR:HG22	1:A:258:ASP:HB2	1.96	0.47
1:A:361:LEU:O	1:A:365:ILE:HG13	2.14	0.47
1:B:1307:LEU:CD1	1:B:1393:GLY:HA2	2.45	0.47
1:B:1399:THR:HA	1:B:1402:MET:CE	2.45	0.46
1:A:331:LEU:HD11	1:A:383:ILE:HG13	1.97	0.46
1:A:416:LEU:N	1:A:416:LEU:HD22	2.30	0.46
1:B:1307:LEU:HD11	1:B:1393:GLY:HA2	1.98	0.46
1:B:1199:GLU:HB2	1:B:1247:ARG:HH12	1.79	0.46
1:B:1307:LEU:HD21	1:B:1392:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE2	1:A:249:PRO:HG2	1.98	0.45
1:A:408:MET:O	1:A:409:PRO:C	2.53	0.45
1:A:214:SER:O	1:A:215:SER:C	2.53	0.45
1:A:387:ARG:HB2	1:B:1384:THR:HG23	1.98	0.45
1:B:1299:MET:CA	1:B:1299:MET:HE2	2.44	0.45
1:A:193:ILE:HD12	1:A:248:LEU:CD2	2.47	0.45
1:B:1220:VAL:HG22	1:B:1301:ASN:CG	2.38	0.45
1:A:399:THR:HA	1:A:402:MET:HE2	1.99	0.44
1:A:193:ILE:HD12	1:A:248:LEU:HD22	1.99	0.44
1:A:267:CYS:HB2	1:A:415:MET:CE	2.48	0.44
1:A:365:ILE:HD13	1:A:379:ILE:HD12	1.99	0.44
1:B:1321:LEU:N	1:B:1321:LEU:HD12	2.33	0.43
1:B:1319:LEU:N	1:B:1320:PRO:CD	2.82	0.43
1:A:365:ILE:HG23	1:A:369:ARG:HH11	1.83	0.43
1:B:1372:LYS:HB3	1:B:1375:MET:HG2	1.99	0.43
1:B:1278:ARG:HH11	1:B:1278:ARG:HG3	1.83	0.43
1:B:1399:THR:HA	1:B:1402:MET:HE3	2.01	0.43
1:A:409:PRO:HA	1:A:410:PRO:HD2	1.88	0.43
1:B:1246:LYS:HE2	4:B:1655:HOH:O	2.17	0.43
1:A:338:CYS:O	1:A:341:ARG:HG2	2.19	0.42
1:B:1412:ILE:O	1:B:1416:LEU:CD2	2.58	0.42
1:A:256:ILE:HD12	1:A:256:ILE:H	1.84	0.42
1:A:397:VAL:HG21	1:A:416:LEU:HG	2.01	0.42
1:B:1246:LYS:HD2	4:F:901:HOH:O	2.20	0.42
1:B:1278:ARG:NH1	1:B:1278:ARG:HG3	2.35	0.42
1:A:186:LEU:CD1	1:A:363:ILE:HD12	2.49	0.41
1:A:387:ARG:HD2	1:B:1388:SER:HB2	2.02	0.41
1:B:1416:LEU:CD2	1:B:1416:LEU:N	2.83	0.41
1:A:205:CYS:SG	1:A:206:GLN:N	2.93	0.41
1:B:1288:PHE:CE1	1:B:1299:MET:HE3	2.55	0.41
1:A:270:ILE:O	1:A:274:ARG:HG3	2.21	0.41
1:B:1316:ASN:O	1:B:1320:PRO:CD	2.68	0.41
1:A:321:LEU:O	1:A:369:ARG:NH2	2.53	0.41
1:A:374:HIS:H	1:A:374:HIS:CD2	2.38	0.41
1:A:218:HIS:H	1:A:218:HIS:CD2	2.37	0.41
1:B:1353:LEU:O	1:B:1356:PRO:HD2	2.21	0.41
1:A:384:THR:HG22	1:B:1384:THR:OG1	2.21	0.41
1:B:1283:GLN:O	1:B:1285:THR:HG23	2.21	0.41
1:B:1271:LEU:C	3:B:1501:TTB:H3A	2.41	0.41
1:B:1243:GLU:OE2	1:B:1247:ARG:NH2	2.54	0.41
1:B:1363:ILE:CG2	1:B:1367:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1202:PRO:HG2	1:B:1278:ARG:NH2	2.36	0.40
1:B:1399:THR:O	1:B:1403:GLU:HG3	2.21	0.40
1:B:1201:PHE:CZ	1:B:1274:ARG:HB3	2.56	0.40
1:B:1412:ILE:HG23	3:B:1501:TTB:H191	2.04	0.40
1:A:191:GLU:O	1:A:195:LYS:HG3	2.21	0.40
1:A:217:ASP:CG	1:A:218:HIS:H	2.25	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	238/267 (89%)	227 (95%)	10 (4%)	1 (0%)	34	24
1	B	237/267 (89%)	231 (98%)	5 (2%)	1 (0%)	34	24
2	E	9/25 (36%)	8 (89%)	1 (11%)	0	100	100
2	F	10/25 (40%)	9 (90%)	1 (10%)	0	100	100
All	All	494/584 (85%)	475 (96%)	17 (3%)	2 (0%)	34	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1215	SER
1	A	215	SER

### 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	213/238 (90%)	207 (97%)	6 (3%)	43	36
1	B	213/238 (90%)	208 (98%)	5 (2%)	50	45
2	E	9/24 (38%)	9 (100%)	0	100	100
2	F	10/24 (42%)	9 (90%)	1 (10%)	7	3
All	All	445/524 (85%)	433 (97%)	12 (3%)	44	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	MET
1	A	187	ASP
1	A	218	HIS
1	A	316	ASN
1	A	369	ARG
1	A	374	HIS
1	B	1186	LEU
1	B	1187	ASP
1	B	1214	SER
1	B	1381	MET
1	B	1395	GLU
2	F	796	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	316	ASN
1	A	342	GLN
1	B	1206	GLN
1	B	1218	HIS

### 5.3.3 RNA ⓘ

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](#)

2 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	TTB	B	1501	-	26,28,28	6.65	19 (73%)	39,43,43	1.00	2 (5%)
3	TTB	A	501	-	26,28,28	7.13	21 (80%)	39,43,43	1.00	2 (5%)

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	TTB	B	1501	-	-	0/8/31/31	0/3/3/3
3	TTB	A	501	-	-	0/8/31/31	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	TTB	C12-C11	17.28	1.68	1.39
3	B	1501	TTB	C13-C14	14.66	1.59	1.39
3	A	501	TTB	C15-C14	13.90	1.64	1.40
3	B	1501	TTB	C12-C11	11.70	1.59	1.39
3	B	1501	TTB	C16-C11	11.48	1.56	1.39
3	A	501	TTB	C13-C14	10.81	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	TTB	C15-C14	10.11	1.58	1.40
3	A	501	TTB	C9-C7	9.76	1.60	1.39
3	A	501	TTB	C4-C3	-9.75	1.28	1.46
3	A	501	TTB	C10-C4	9.51	1.57	1.39
3	B	1501	TTB	C16-C15	9.51	1.53	1.39
3	A	501	TTB	C16-C15	9.29	1.53	1.39
3	B	1501	TTB	C10-C4	8.07	1.55	1.39
3	B	1501	TTB	C4-C3	-7.65	1.32	1.46
3	A	501	TTB	C5-C4	7.45	1.53	1.39
3	B	1501	TTB	C6-C7	7.19	1.54	1.39
3	A	501	TTB	C6-C7	7.15	1.54	1.39
3	B	1501	TTB	C9-C7	6.71	1.53	1.39
3	B	1501	TTB	C6-C5	6.55	1.50	1.38
3	B	1501	TTB	C17-C15	6.49	1.62	1.53
3	B	1501	TTB	C22-C14	6.33	1.62	1.53
3	A	501	TTB	C16-C11	5.86	1.48	1.39
3	B	1501	TTB	C5-C4	5.86	1.50	1.39
3	A	501	TTB	C22-C14	5.75	1.61	1.53
3	A	501	TTB	C-C2	5.48	1.61	1.50
3	A	501	TTB	C17-C15	5.40	1.61	1.53
3	B	1501	TTB	C19-C17	4.67	1.66	1.53
3	B	1501	TTB	C21-C20	4.64	1.67	1.53
3	A	501	TTB	C6-C5	4.59	1.47	1.38
3	A	501	TTB	C21-C22	4.51	1.65	1.53
3	B	1501	TTB	C20-C17	4.11	1.64	1.53
3	A	501	TTB	C20-C17	4.02	1.64	1.53
3	A	501	TTB	C21-C20	3.77	1.64	1.53
3	A	501	TTB	C23-C22	3.67	1.64	1.53
3	B	1501	TTB	C10-C9	3.46	1.45	1.38
3	A	501	TTB	C7-C8	-3.44	1.44	1.47
3	A	501	TTB	C18-C17	3.04	1.62	1.53
3	B	1501	TTB	C21-C22	2.93	1.61	1.53
3	B	1501	TTB	C-C2	2.46	1.55	1.50
3	A	501	TTB	C24-C22	2.07	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	TTB	C21-C22-C14	3.13	115.21	110.16
3	A	501	TTB	C21-C22-C14	2.71	114.53	110.16
3	A	501	TTB	C4-C3-C2	2.56	139.80	129.34
3	B	1501	TTB	C20-C17-C15	2.15	113.63	110.16

There are no chirality outliers.

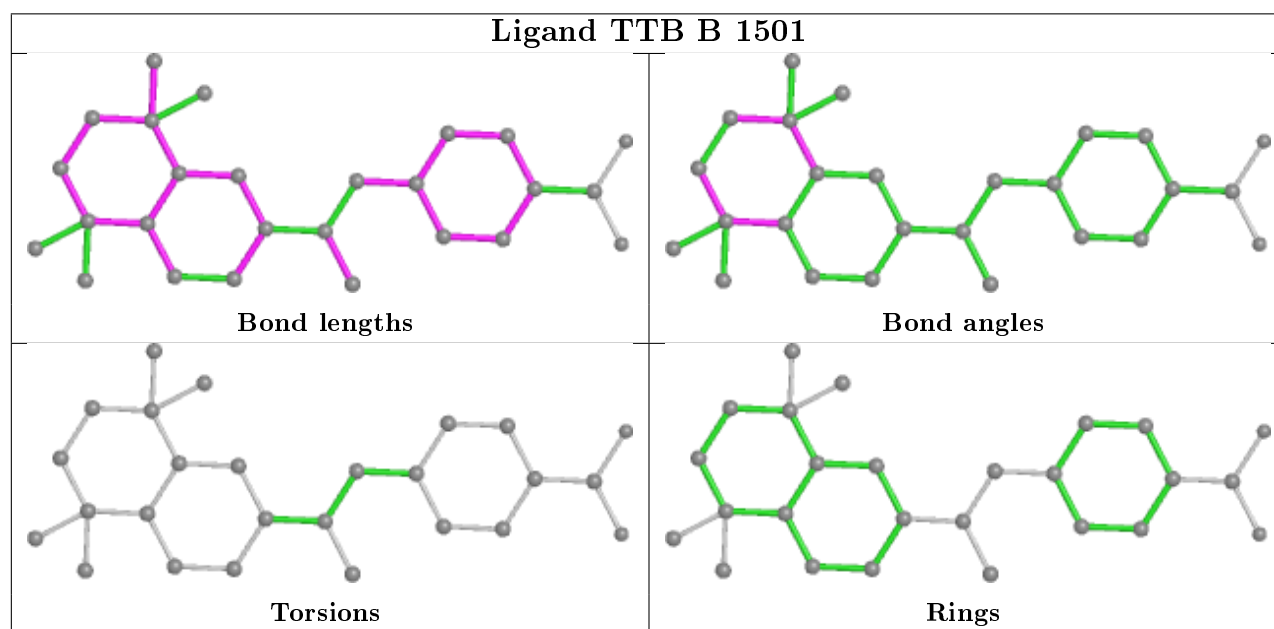
There are no torsion outliers.

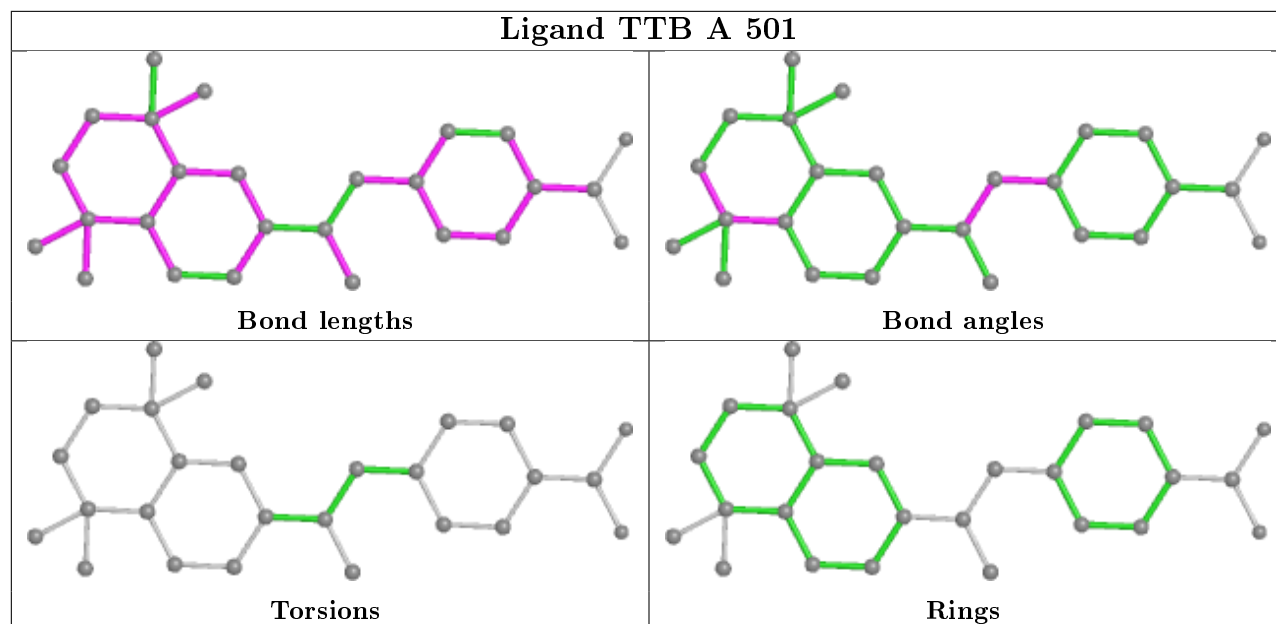
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	TTB	3	0
3	A	501	TTB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	240/267 (89%)	0.52	24 (10%) 7 8	19, 33, 63, 72	2 (0%)
1	B	239/267 (89%)	0.23	10 (4%) 36 39	16, 27, 49, 62	1 (0%)
2	E	11/25 (44%)	1.00	4 (36%) 0 0	34, 39, 59, 62	2 (18%)
2	F	12/25 (48%)	0.52	1 (8%) 11 13	24, 34, 49, 51	2 (16%)
All	All	502/584 (85%)	0.39	39 (7%) 13 14	16, 31, 56, 72	7 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	CYS	7.7
1	B	1205	CYS	7.2
1	A	371	SER	7.0
1	A	207	LEU	6.8
1	A	370	PRO	6.4
1	A	372	LYS	5.5
1	B	1180	TYR	5.5
1	B	1418	ASN	4.5
1	B	1319	LEU	4.0
1	A	374	HIS	3.6
1	A	217	ASP	3.5
2	E	691	HIS	3.4
2	F	797	GLY	3.3
1	A	206	GLN	3.3
1	B	1373	PRO	3.1
1	A	203	SER	3.0
1	A	180	TYR	2.9
1	A	185	GLU	2.8
1	B	1282	GLU	2.8
1	A	204	LEU	2.7
2	E	696	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	2.6
1	A	373	PRO	2.6
2	E	686	ARG	2.5
1	A	179	SER	2.5
1	A	182	MET	2.5
1	A	417	GLU	2.5
1	A	218	HIS	2.5
1	A	342	GLN	2.5
1	B	1371	SER	2.5
1	A	343	ASP	2.3
1	B	1366	ARG	2.3
1	A	369	ARG	2.3
1	A	186	LEU	2.1
1	B	1221	ARG	2.1
1	A	359	GLU	2.1
1	B	1206	GLN	2.1
1	A	340	ASP	2.0
2	E	688	LYS	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<sup>th</sup> 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.

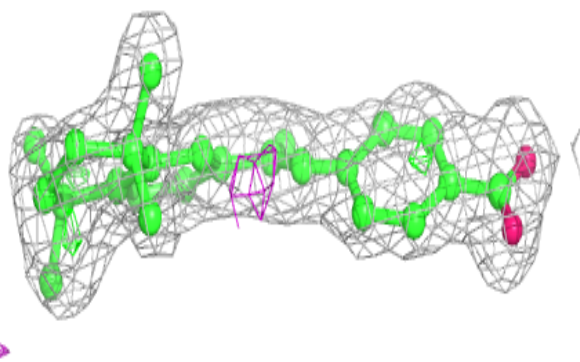
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TTB	B	1501	26/26	0.88	0.17	25,30,34,35	0
3	TTB	A	501	26/26	0.91	0.16	30,36,43,44	0

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.

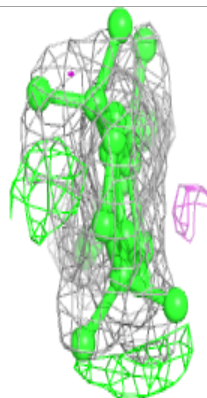
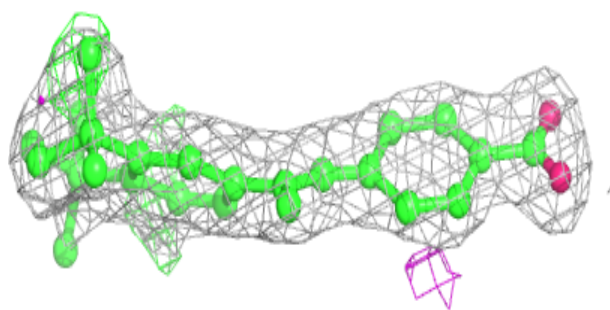
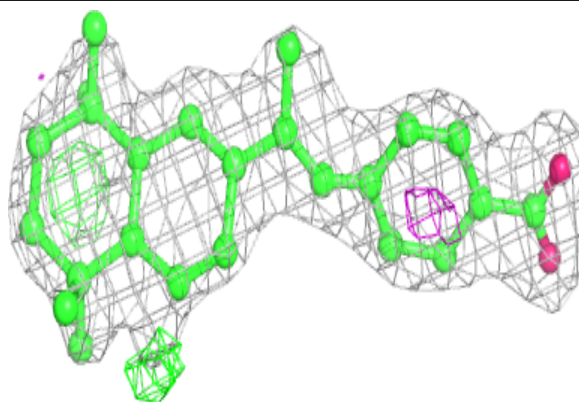
**Electron density around TTB B 1501:**

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



**Electron density around TTB A 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

There are no such residues in this entry.