Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 11:51 pm BST

PDB ID	:	3WJ4
Title	:	Crystal structure of PPARgamma ligand binding domain in complex with tributyltin
Authors	:	Harada, S.; Hiromori, Y.; Fukakusa, S.; Kawahara, K.; Nakamura, S.; Noda, M.; Uchiyama, S.; Fukui, K.; Nishikawa, J.; Nagase, H.; Kobayashi, Y.; Ohkubo, T.; Yoshida, T.; Nakanishi, T.
Deposited on	:	2013-10-04
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

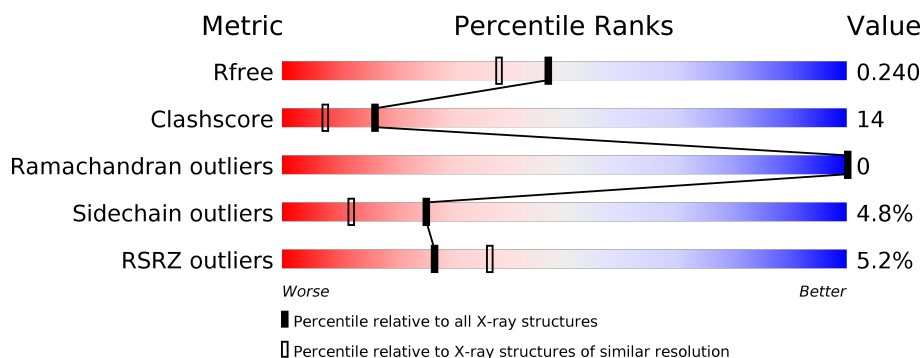|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.240
Clashscore		14
Ramachandran outliers		0
Sidechain outliers		4.8%
RSRZ outliers		5.2%

Worse　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 >=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	276	5%　75%　16%　• 7%
1	B	276	5%　76%　15%　• 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TBY	B	501[A]	-	-	X	-
2	TBY	B	501[B]	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4414 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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2044	1319	334	381	10	0	1	0
1	B	260	Total	C	N	O	S	0	6	0
			2107	1362	346	389	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLY	-	EXPRESSION TAG	UNP P37231
A	203	PRO	-	EXPRESSION TAG	UNP P37231
A	204	LEU	-	EXPRESSION TAG	UNP P37231
A	205	GLY	-	EXPRESSION TAG	UNP P37231
A	206	SER	-	EXPRESSION TAG	UNP P37231
B	202	GLY	-	EXPRESSION TAG	UNP P37231
B	203	PRO	-	EXPRESSION TAG	UNP P37231
B	204	LEU	-	EXPRESSION TAG	UNP P37231
B	205	GLY	-	EXPRESSION TAG	UNP P37231
B	206	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is tributylstannanyl (three-letter code: TBY) (formula: $C_{12}H_{27}Sn$).

TBY
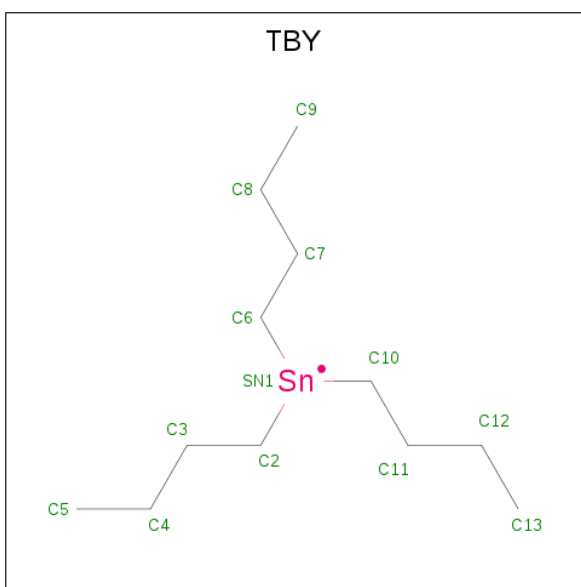
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 12	Sn 1	0	0
2	B	1	Total 26	C 24	Sn 2	0	1

• Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	126	Total 126	O 126	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Peroxisome proliferator-activated receptor gamma

Chain A:

• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:
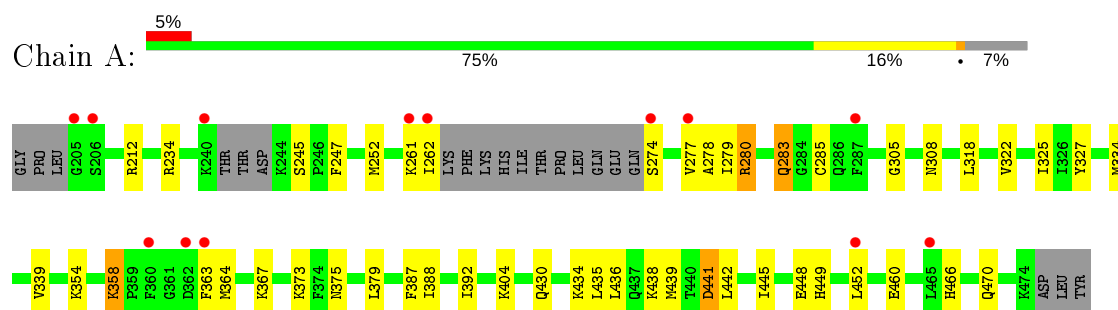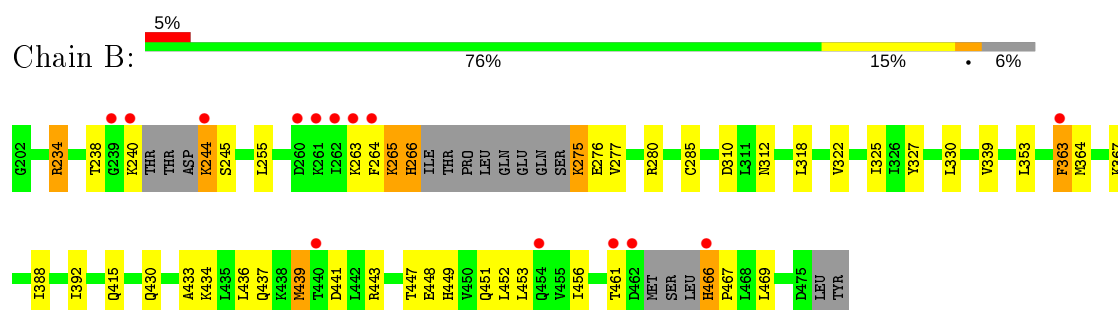
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.34Å 88.29Å 57.51Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	36.44 – 1.95 36.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.44-1.95) 99.9 (36.44-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.27 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.241 0.197 , 0.240	Depositor DCC
R_{free} test set	2088 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.027 for h,-k,-l 0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.80	0/2079	0.75	2/2796 (0.1%)
1	B	0.85	1/2159 (0.0%)	0.79	1/2901 (0.0%)
All	All	0.82	1/4238 (0.0%)	0.77	3/5697 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	MET	CG-SD	-5.30	1.67	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	212	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	439	MET	CB-CG-SD	-5.52	95.85	112.40

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	2044	0	2109	46	0
1	B	2107	0	2180	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	21	3	0
2	B	26	0	42	50	0
3	A	98	0	0	1	0
3	B	126	0	0	0	0
All	All	4414	0	4352	122	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 14.

All (122) 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:363:PHE:CE1	2:B:501[A]:TBY:H13A	1.73	1.22
2:B:501[B]:TBY:C6	2:B:501[B]:TBY:H13B	1.70	1.21
1:B:364:MET:SD	2:B:501[A]:TBY:H5B	1.86	1.16
1:B:327:TYR:OH	2:B:501[A]:TBY:H11A	1.46	1.13
1:A:439:MET:HA	1:A:439:MET:HE2	1.30	1.09
1:B:364:MET:HG3	2:B:501[A]:TBY:H5	1.37	1.05
1:B:364:MET:CE	2:B:501[A]:TBY:H5B	1.86	1.05
1:B:364:MET:CE	2:B:501[A]:TBY:C5	2.38	1.01
1:A:439:MET:CE	1:A:439:MET:HA	1.90	0.98
1:B:363:PHE:CE1	2:B:501[A]:TBY:C13	2.47	0.97
1:A:439:MET:CE	1:A:442:LEU:HD12	1.94	0.96
1:B:364:MET:HG3	2:B:501[A]:TBY:C5	1.95	0.94
1:B:285[B]:CYS:SG	2:B:501[B]:TBY:C6	2.56	0.93
1:B:363:PHE:HE1	2:B:501[A]:TBY:C13	1.83	0.91
1:B:364:MET:HE1	2:B:501[B]:TBY:C13	2.03	0.88
1:B:265:LYS:HB3	1:B:265:LYS:NZ	1.92	0.85
1:A:439:MET:HE2	1:A:442:LEU:HD12	1.58	0.84
1:B:364:MET:HE1	2:B:501[B]:TBY:H13	1.59	0.83
1:B:364:MET:SD	2:B:501[A]:TBY:C6	2.69	0.80
1:B:364:MET:HE1	2:B:501[A]:TBY:C5	2.11	0.79
1:A:439:MET:HE1	1:A:442:LEU:HD12	1.63	0.79
1:A:327:TYR:OH	1:A:449:HIS:HD2	1.66	0.78
1:B:364:MET:HE1	2:B:501[B]:TBY:C12	2.13	0.78
1:B:364:MET:SD	2:B:501[B]:TBY:H12	2.23	0.78
2:B:501[A]:TBY:C6	2:B:501[A]:TBY:H4	2.17	0.75
1:B:364:MET:CG	2:B:501[A]:TBY:C5	2.65	0.75
1:A:448:GLU:O	1:A:452:LEU:HD13	1.87	0.75
1:B:364:MET:CE	2:B:501[B]:TBY:H12A	2.16	0.75
1:B:265:LYS:HB3	1:B:265:LYS:HZ2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:MET:SD	2:B:501[B]:TBY:C12	2.76	0.74
1:A:358:LYS:H	1:A:358:LYS:HE3	1.52	0.73
1:B:449:HIS:HE1	2:B:501[A]:TBY:H13B	1.51	0.73
1:B:265:LYS:CB	1:B:265:LYS:NZ	2.52	0.73
1:B:436:LEU:O	1:B:439:MET:HB3	1.89	0.72
1:A:439:MET:CE	1:A:439:MET:CA	2.67	0.72
1:B:449:HIS:CE1	2:B:501[A]:TBY:H13B	2.25	0.71
1:B:364:MET:HE2	2:B:501[A]:TBY:C5	2.21	0.71
1:B:364:MET:HE1	2:B:501[B]:TBY:H12A	1.70	0.71
1:B:364:MET:CE	2:B:501[B]:TBY:C12	2.68	0.70
1:B:364:MET:CG	2:B:501[A]:TBY:H5B	2.22	0.70
1:B:363:PHE:HD1	2:B:501[A]:TBY:H8	1.57	0.68
1:A:363:PHE:CZ	1:A:452:LEU:HB3	2.28	0.68
2:B:501[B]:TBY:C13	2:B:501[B]:TBY:C6	2.62	0.68
1:A:327:TYR:OH	1:A:449:HIS:CD2	2.46	0.67
1:B:364:MET:CG	2:B:501[A]:TBY:C6	2.73	0.67
1:B:364:MET:CE	2:B:501[B]:TBY:H13	2.25	0.67
1:A:325:ILE:HG12	1:A:388:ILE:HG23	1.76	0.66
1:B:364:MET:CE	2:B:501[A]:TBY:H5A	2.25	0.66
2:B:501[A]:TBY:C4	2:B:501[A]:TBY:C6	2.73	0.66
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.77	0.65
1:B:353:LEU:HD13	2:B:501[A]:TBY:H5	1.78	0.65
1:B:449:HIS:HE1	2:B:501[A]:TBY:C13	2.08	0.65
1:B:364:MET:HE1	2:B:501[A]:TBY:H5A	1.78	0.65
1:B:363:PHE:HE1	2:B:501[A]:TBY:H13	1.63	0.64
1:A:327:TYR:HE1	1:A:367:LYS:HG2	1.63	0.64
1:B:466:HIS:CD2	1:B:467:PRO:HD3	2.34	0.63
1:A:358:LYS:H	1:A:358:LYS:CE	2.11	0.63
1:A:327:TYR:CE1	1:A:367:LYS:HG2	2.33	0.62
1:B:266:HIS:N	1:B:266:HIS:ND1	2.45	0.62
1:A:234:ARG:HH22	1:A:375:ASN:ND2	1.96	0.62
1:B:364:MET:HE1	2:B:501[A]:TBY:H5B	1.70	0.60
1:A:285:CYS:SG	2:A:501:TBY:H3A	2.41	0.59
1:B:327:TYR:HH	2:B:501[A]:TBY:H11A	1.65	0.59
1:A:339:VAL:HG11	2:A:501:TBY:H8A	1.85	0.58
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.32	0.58
1:A:441:ASP:O	1:A:445:ILE:HG12	2.04	0.57
2:B:501[A]:TBY:H5B	2:B:501[A]:TBY:C6	2.34	0.57
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.88	0.56
1:B:363:PHE:CD1	2:B:501[A]:TBY:H13A	2.37	0.56
1:A:279:ILE:HD11	1:A:460:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PHE:HZ	1:A:439:MET:HE3	1.71	0.55
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.72	0.55
1:B:275:LYS:HE3	1:B:276:GLU:H	1.72	0.54
1:A:252:MET:SD	1:A:277:VAL:HG21	2.48	0.53
1:B:244:LYS:NZ	1:B:244:LYS:HB2	2.23	0.53
1:A:439:MET:HE1	1:A:442:LEU:CD1	2.38	0.53
1:B:433:ALA:O	1:B:437:GLN:HG3	2.09	0.53
1:B:439:MET:O	1:B:439:MET:CE	2.57	0.52
2:B:501[A]:TBY:C5	2:B:501[A]:TBY:C6	2.88	0.52
1:A:274:SER:O	1:A:280:ARG:HG3	2.10	0.52
1:B:318:LEU:O	1:B:322:VAL:HG13	2.10	0.52
1:A:448:GLU:O	1:A:452:LEU:CD1	2.57	0.52
1:A:334:MET:CE	1:A:364:MET:CE	2.88	0.52
1:B:364:MET:HG2	2:B:501[A]:TBY:C6	2.40	0.51
1:B:453:LEU:O	1:B:456:ILE:HG13	2.09	0.51
1:A:436:LEU:O	1:A:439:MET:HB2	2.09	0.51
1:B:466:HIS:CG	1:B:467:PRO:HD3	2.46	0.51
1:A:387:PHE:HZ	1:A:439:MET:CE	2.24	0.51
1:B:325:ILE:HG12	1:B:388:ILE:HG23	1.93	0.51
1:A:279:ILE:O	1:A:283:GLN:HG2	2.11	0.51
1:A:363:PHE:HB2	2:A:501:TBY:H4A	1.93	0.50
1:A:466:HIS:O	1:A:470:GLN:HG3	2.12	0.49
1:B:275:LYS:N	1:B:280:ARG:HD3	2.28	0.49
1:B:443:ARG:O	1:B:447:THR:HG23	2.13	0.48
1:A:438:LYS:HE2	3:A:1021:HOH:O	2.13	0.48
1:B:449:HIS:CE1	2:B:501[A]:TBY:C13	2.91	0.48
1:A:430:GLN:O	1:A:434:LYS:HG3	2.14	0.48
1:B:364:MET:HG2	2:B:501[A]:TBY:H7A	1.96	0.47
1:A:318:LEU:O	1:A:322:VAL:HG13	2.15	0.47
1:A:387:PHE:CZ	1:A:439:MET:CE	2.98	0.47
1:B:310:ASP:OD1	1:B:312:ASN:HB2	2.14	0.47
1:B:330:LEU:HD21	2:B:501[B]:TBY:C13	2.45	0.46
1:A:234:ARG:NH2	1:A:375:ASN:ND2	2.64	0.46
1:B:264:PHE:HB3	1:B:266:HIS:NE2	2.31	0.46
1:A:334:MET:HE1	1:A:364:MET:CE	2.46	0.46
1:B:364:MET:SD	2:B:501[B]:TBY:H13	2.56	0.46
1:B:363:PHE:O	1:B:367:LYS:NZ	2.45	0.45
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.46	0.45
1:A:277:VAL:HG13	1:A:278:ALA:H	1.81	0.44
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.00	0.44
1:B:339:VAL:HG11	2:B:501[A]:TBY:H5A	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HD23	1:B:277:VAL:CG1	2.49	0.43
1:B:448:GLU:HA	1:B:451:GLN:HE21	1.83	0.43
1:B:285[A]:CYS:HB3	2:B:501[A]:TBY:C12	2.49	0.42
1:A:247:PHE:HB3	1:A:262:ILE:HD11	2.01	0.42
1:A:373:LYS:HE2	1:A:373:LYS:HB2	1.88	0.42
1:B:234:ARG:O	1:B:238:THR:HG23	2.19	0.42
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.54	0.41
1:A:387:PHE:CZ	1:A:439:MET:HE3	2.52	0.41
1:B:364:MET:SD	2:B:501[B]:TBY:C13	3.09	0.41
1:B:430:GLN:O	1:B:434:LYS:HG3	2.21	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	251/276 (91%)	250 (100%)	1 (0%)	0	100	100
1	B	258/276 (94%)	252 (98%)	6 (2%)	0	100	100
All	All	509/552 (92%)	502 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	229/247 (93%)	221 (96%)	8 (4%)	36	24
1	B	237/247 (96%)	223 (94%)	14 (6%)	19	8
All	All	466/494 (94%)	444 (95%)	22 (5%)	25	13

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	SER
1	A	261	LYS
1	A	280	ARG
1	A	283	GLN
1	A	354	LYS
1	A	358	LYS
1	A	404	LYS
1	A	441	ASP
1	B	234	ARG
1	B	240	LYS
1	B	244	LYS
1	B	245	SER
1	B	263	LYS
1	B	265	LYS
1	B	266	HIS
1	B	275	LYS
1	B	363	PHE
1	B	441	ASP
1	B	452	LEU
1	B	461	THR
1	B	466	HIS
1	B	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	A	314	GLN
1	A	345	GLN
1	A	375	ASN
1	A	430	GLN
1	A	449	HIS
1	B	412	ASN
1	B	451	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

3 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	TBY	B	501[B]	-	9,12,12	0.30	0	6,12,12	0.67	0
2	TBY	A	501	-	9,12,12	0.47	0	6,12,12	0.18	0
2	TBY	B	501[A]	-	9,12,12	0.32	0	6,12,12	0.46	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
2	TBY	B	501[B]	-	-	1/3/12/12	-
2	TBY	A	501	-	-	2/3/12/12	-
2	TBY	B	501[A]	-	-	1/3/12/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501[B]	TBY	C10-C11-C12-C13
2	A	501	TBY	C6-C7-C8-C9
2	B	501[A]	TBY	C2-C3-C4-C5
2	A	501	TBY	C10-C11-C12-C13

There are no ring outliers.
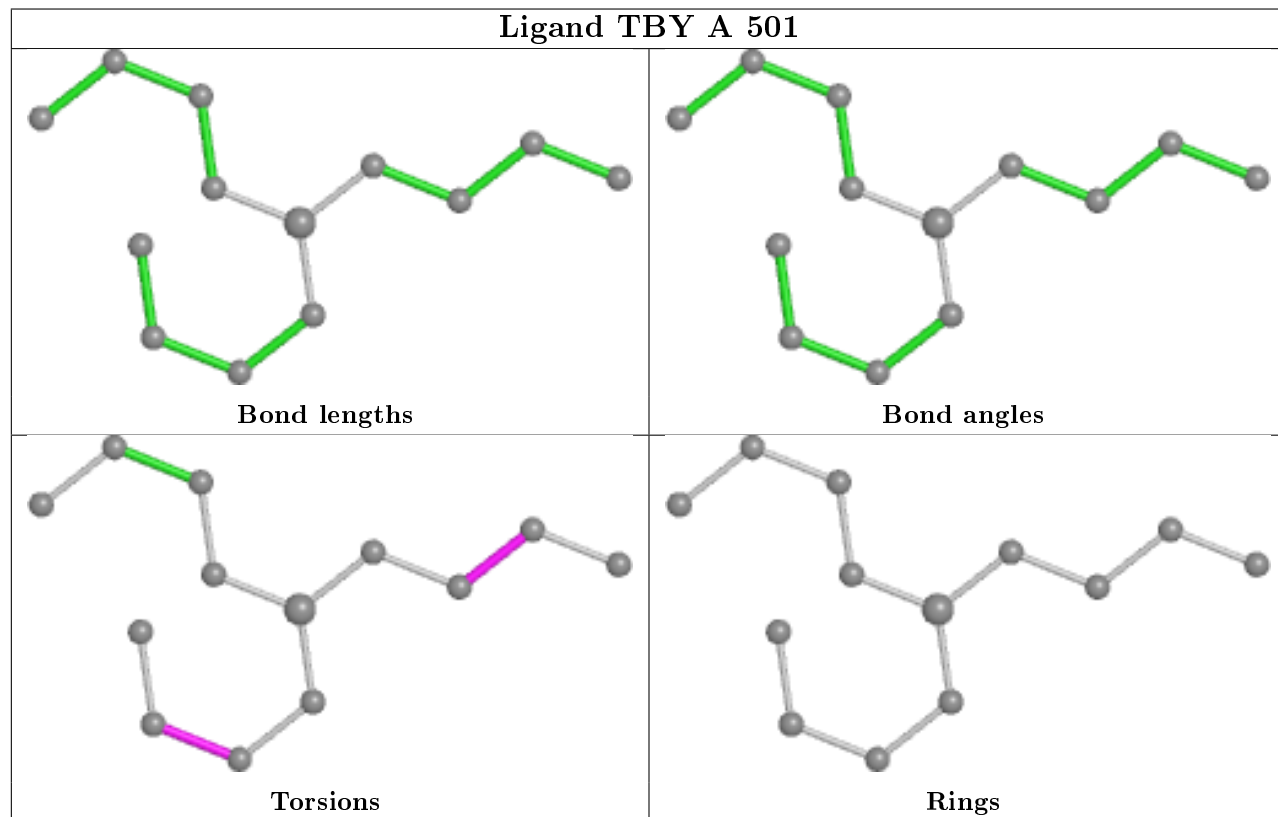
3 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501[B]	TBY	15	0
2	A	501	TBY	3	0
2	B	501[A]	TBY	35	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.
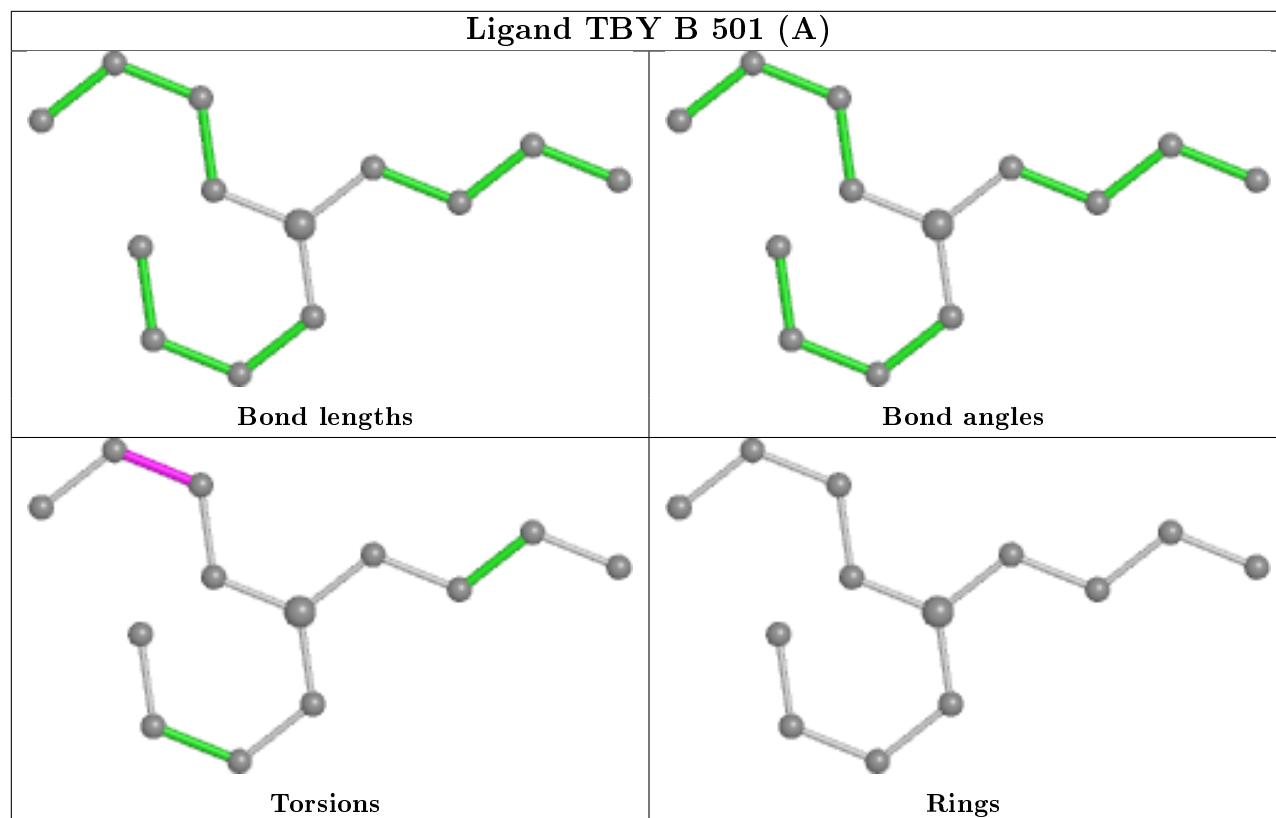
Ligand TBY B 501 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand TBY A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand TBY B 501 (A)

Bond lengths

Bond angles

Torsions

Rings
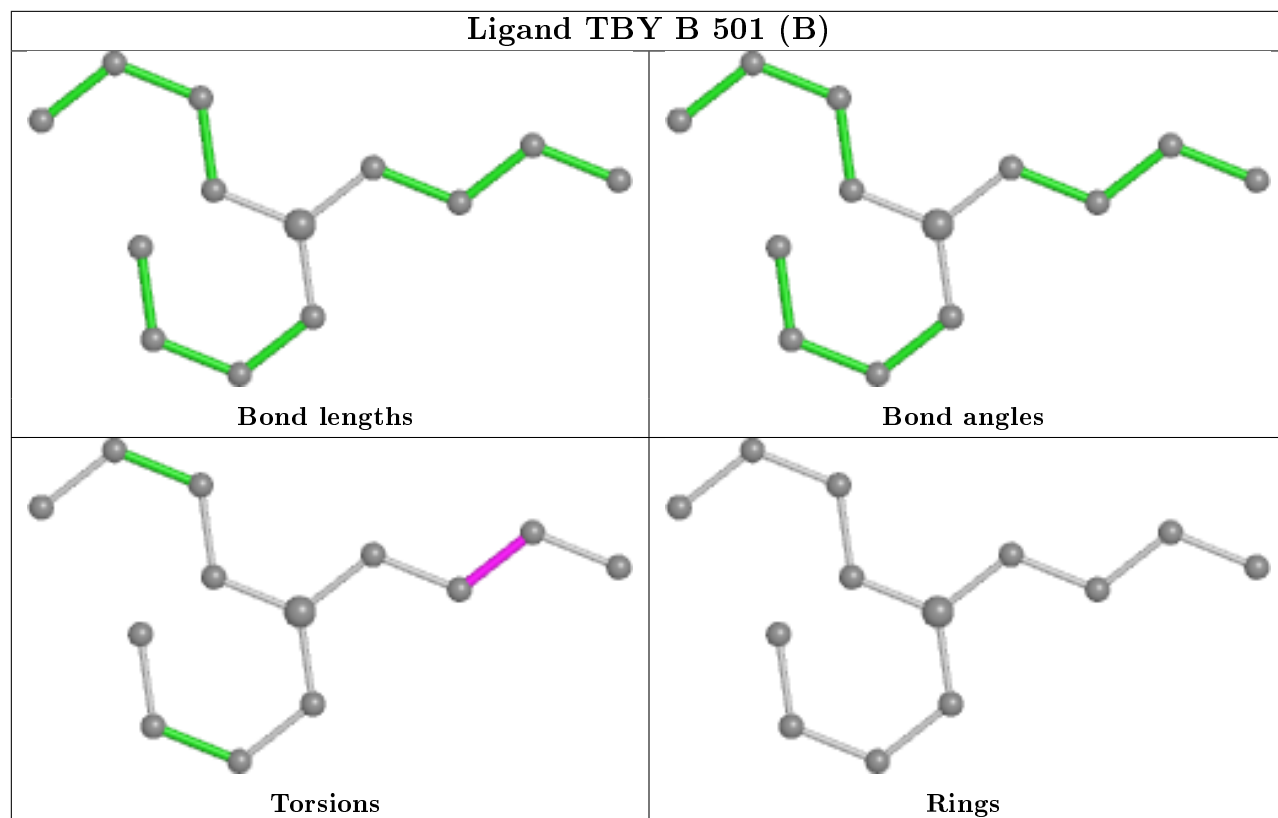
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	256/276 (92%)	0.20	13 (5%)	28	37	11, 22, 45, 57	0
1	B	260/276 (94%)	0.23	14 (5%)	25	34	10, 21, 52, 63	0
All	All	516/552 (93%)	0.22	27 (5%)	27	37	10, 22, 47, 63	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	461	THR	6.2
1	B	264	PHE	5.4
1	A	206	SER	4.4
1	B	261	LYS	4.1
1	B	363	PHE	4.0
1	A	274	SER	3.9
1	A	205	GLY	3.9
1	B	260	ASP	3.9
1	B	244	LYS	3.9
1	A	262	ILE	3.4
1	A	363	PHE	3.2
1	A	360	PHE	3.1
1	A	287	PHE	3.1
1	B	263	LYS	3.0
1	B	454	GLN	2.8
1	A	261	LYS	2.7
1	B	240	LYS	2.7
1	A	362	ASP	2.5
1	B	239	GLY	2.5
1	B	262	ILE	2.4
1	A	240	LYS	2.4
1	B	440	THR	2.4
1	B	462	ASP	2.3
1	A	465	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	277	VAL	2.2
1	A	452	LEU	2.1
1	B	466	HIS	2.1

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 carbohydrates 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
2	TBY	B	501[B]	13/13	0.90	0.35	5,20,24,28	13
2	TBY	B	501[A]	13/13	0.90	0.35	7,21,27,29	13
2	TBY	A	501	13/13	0.98	0.13	41,44,45,46	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.
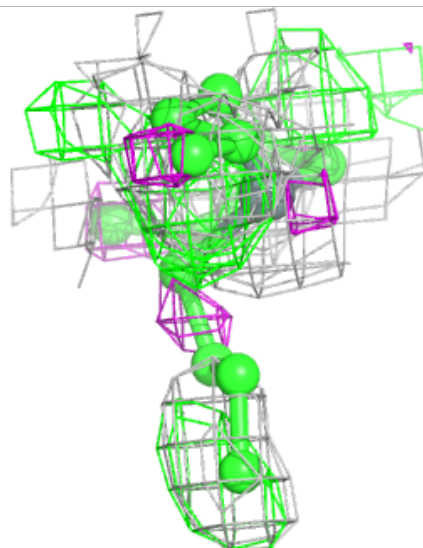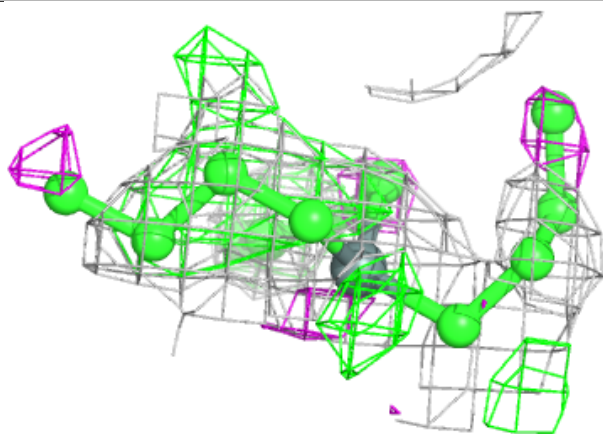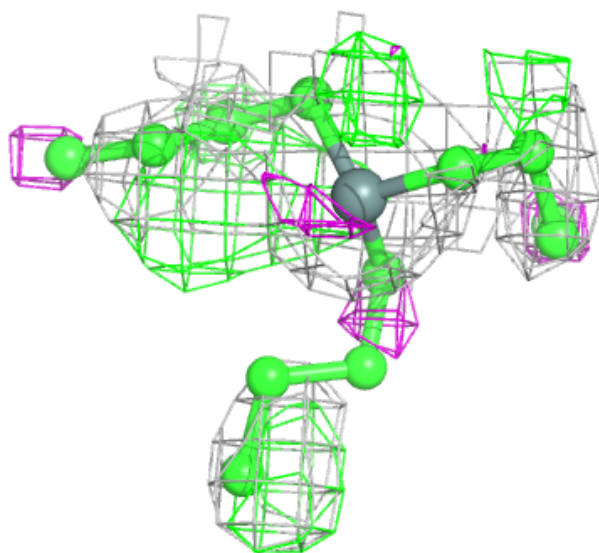
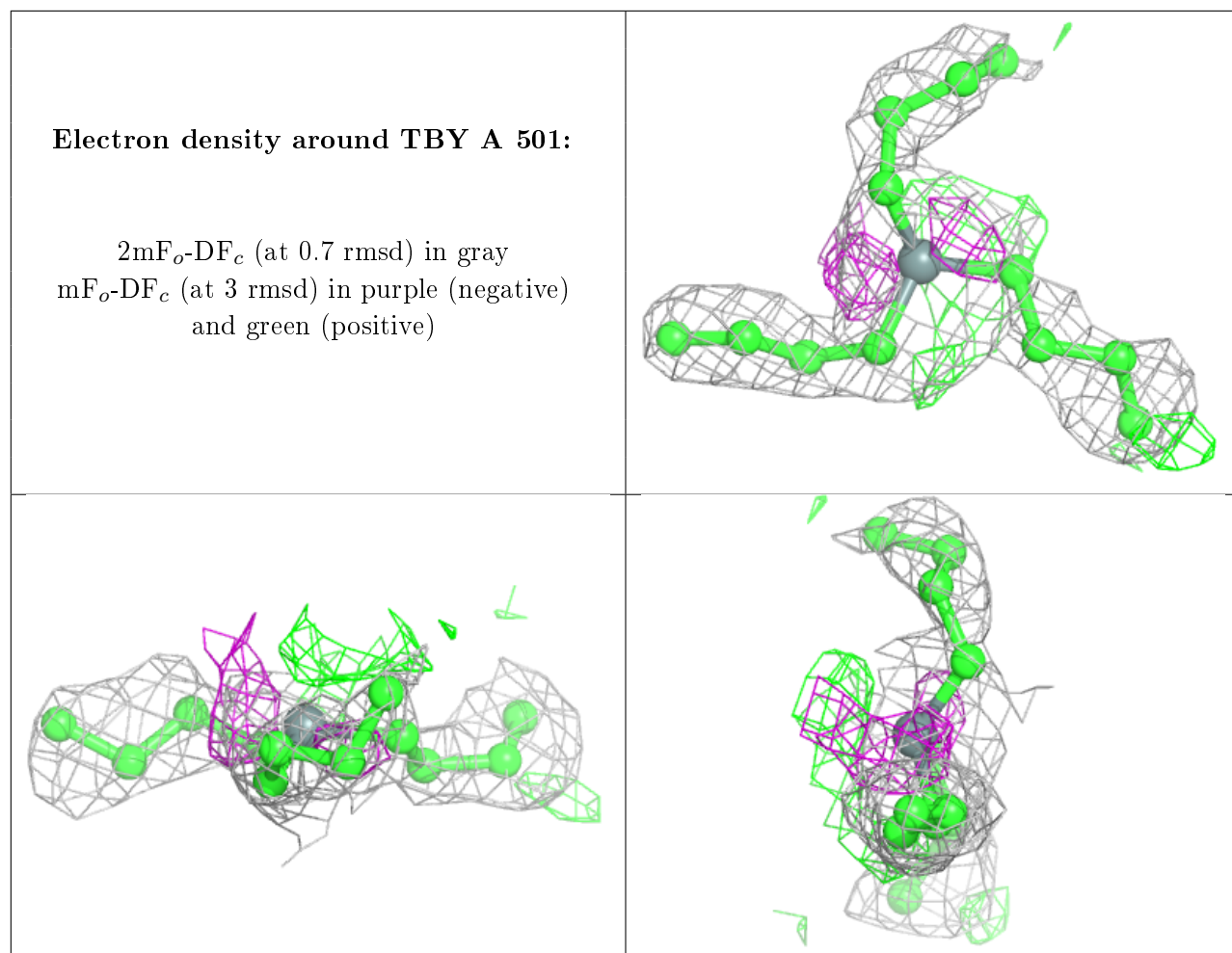**Electron density around TBY B 501 (B):**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
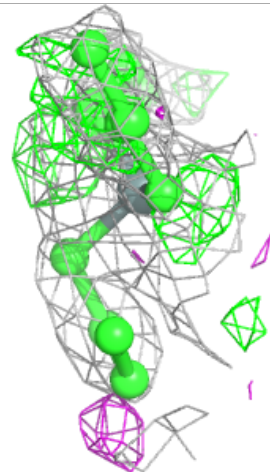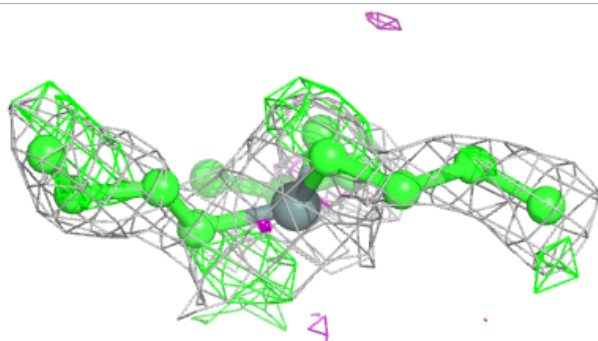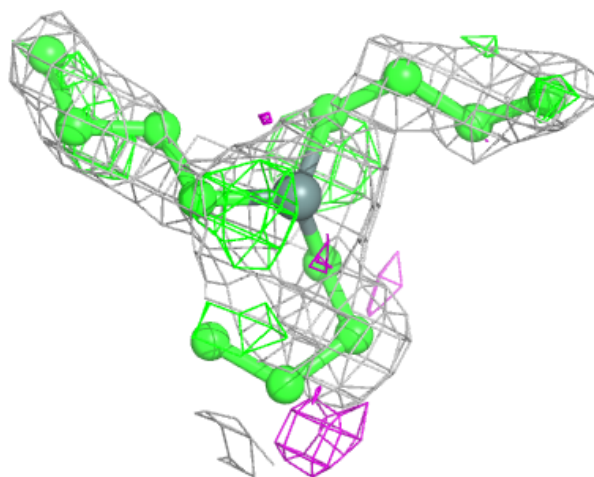
Electron density around TBY B 501 (A):

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

Electron density around TBY 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 (i)

There are no such residues in this entry.