



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:39 AM UTC

PDB ID : 4KLX / pdb_00004klx
Title : Crystal structure of dihydrofolate reductase from Mycobacterium tuberculosis in an open conformation.
Authors : Dias, M.V.B.; Tyrakis, P.; Blundell, T.L.
Deposited on : 2013-05-07
Resolution : 1.23 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

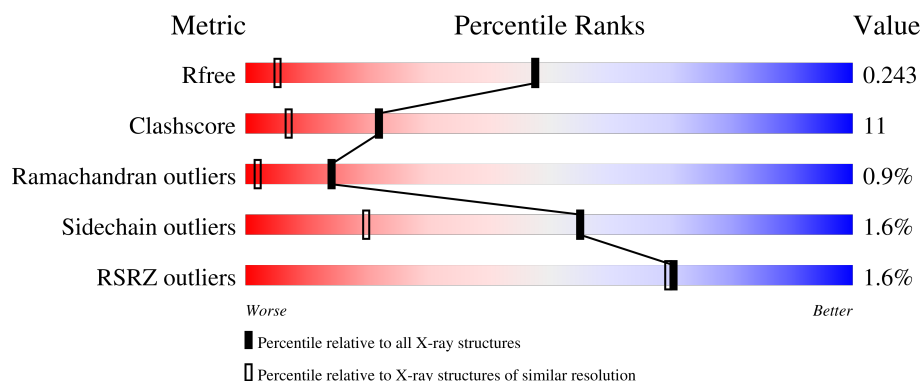
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

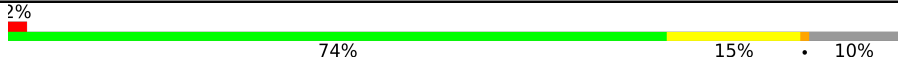
The reported resolution of this entry is 1.23 Å.

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	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

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	179	
1	B	179	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3123 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	3	0
			1268	798	233	232	5			
1	B	160	Total	C	N	O	S	0	3	0
			1256	793	227	231	5			

There are 40 discrepancies between the modelled and reference sequences:

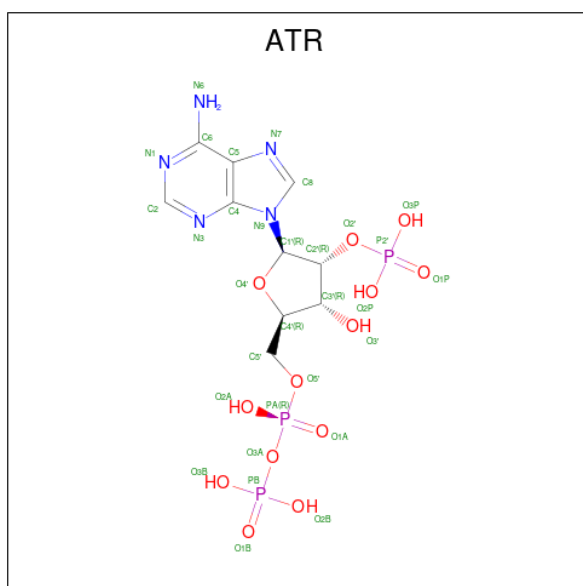
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A546
A	-18	GLY	-	expression tag	UNP P0A546
A	-17	SER	-	expression tag	UNP P0A546
A	-16	SER	-	expression tag	UNP P0A546
A	-15	HIS	-	expression tag	UNP P0A546
A	-14	HIS	-	expression tag	UNP P0A546
A	-13	HIS	-	expression tag	UNP P0A546
A	-12	HIS	-	expression tag	UNP P0A546
A	-11	HIS	-	expression tag	UNP P0A546
A	-10	HIS	-	expression tag	UNP P0A546
A	-9	SER	-	expression tag	UNP P0A546
A	-8	SER	-	expression tag	UNP P0A546
A	-7	GLY	-	expression tag	UNP P0A546
A	-6	LEU	-	expression tag	UNP P0A546
A	-5	VAL	-	expression tag	UNP P0A546
A	-4	PRO	-	expression tag	UNP P0A546
A	-3	ARG	-	expression tag	UNP P0A546
A	-2	GLY	-	expression tag	UNP P0A546
A	-1	SER	-	expression tag	UNP P0A546
A	0	HIS	-	expression tag	UNP P0A546
B	-19	MET	-	expression tag	UNP P0A546
B	-18	GLY	-	expression tag	UNP P0A546
B	-17	SER	-	expression tag	UNP P0A546
B	-16	SER	-	expression tag	UNP P0A546
B	-15	HIS	-	expression tag	UNP P0A546

Continued on next page...

Continued from previous page...

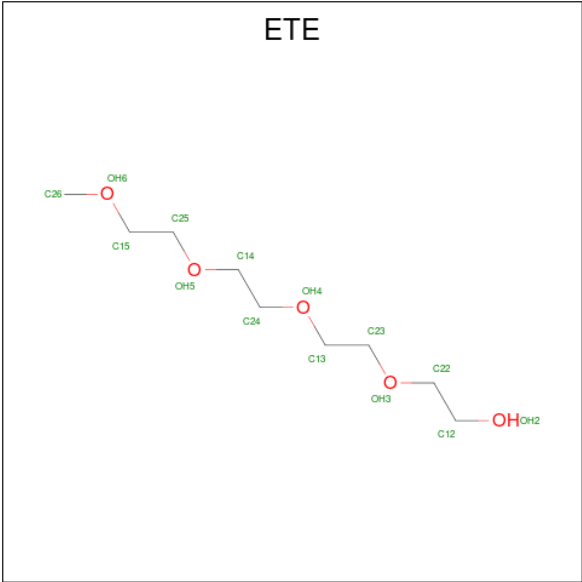
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P0A546
B	-13	HIS	-	expression tag	UNP P0A546
B	-12	HIS	-	expression tag	UNP P0A546
B	-11	HIS	-	expression tag	UNP P0A546
B	-10	HIS	-	expression tag	UNP P0A546
B	-9	SER	-	expression tag	UNP P0A546
B	-8	SER	-	expression tag	UNP P0A546
B	-7	GLY	-	expression tag	UNP P0A546
B	-6	LEU	-	expression tag	UNP P0A546
B	-5	VAL	-	expression tag	UNP P0A546
B	-4	PRO	-	expression tag	UNP P0A546
B	-3	ARG	-	expression tag	UNP P0A546
B	-2	GLY	-	expression tag	UNP P0A546
B	-1	SER	-	expression tag	UNP P0A546
B	0	HIS	-	expression tag	UNP P0A546

- Molecule 2 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (CCD ID: ATR) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	9	5		

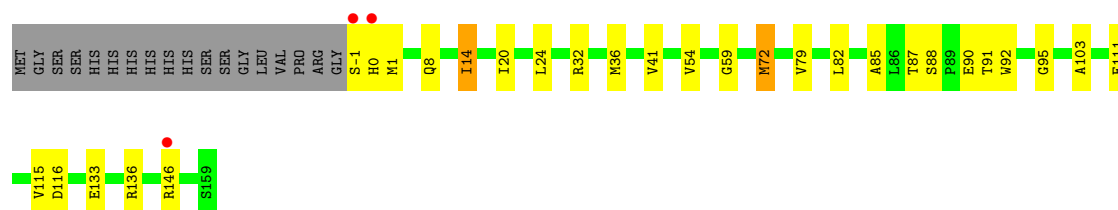
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	248	Total	O	0	0
			248	248		

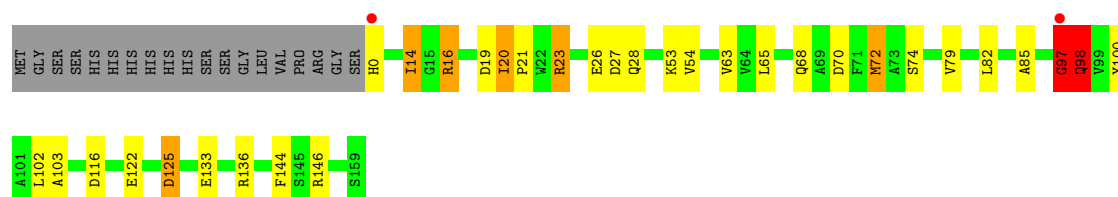
3 Residue-property plots

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: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	32.41Å 63.06Å 78.16Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.87 – 1.23 19.87 – 1.23	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.87-1.23) 99.1 (19.87-1.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.23Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.244 0.179 , 0.243	Depositor DCC
R_{free} test set	4452 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	7.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.59	8/1308 (0.6%)	1.38	3/1777 (0.2%)
1	B	1.54	6/1296 (0.5%)	1.40	10/1762 (0.6%)
All	All	1.56	14/2604 (0.5%)	1.39	13/3539 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ILE	CA-C	8.79	1.61	1.53
1	B	125	ASP	CA-CB	6.06	1.62	1.53
1	A	111	GLU	CA-C	-5.91	1.45	1.52
1	B	98	GLN	N-CA	5.89	1.57	1.46
1	A	116	ASP	N-CA	5.81	1.54	1.46
1	A	8	GLN	CA-C	5.73	1.59	1.52
1	B	63	VAL	N-CA	5.58	1.52	1.46
1	A	14	ILE	C-O	-5.28	1.19	1.24
1	A	115	VAL	N-CA	-5.22	1.39	1.46
1	A	24	LEU	N-CA	5.19	1.52	1.46
1	B	116	ASP	N-CA	5.17	1.53	1.46
1	B	26	GLU	N-CA	-5.17	1.39	1.46
1	B	144	PHE	N-CA	5.08	1.52	1.46
1	A	92	TRP	N-CA	5.06	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ILE	N-CA-C	-9.08	100.05	108.95
1	B	20	ILE	N-CA-C	-7.42	100.87	108.96
1	A	20	ILE	CB-CA-C	-6.78	103.57	110.89
1	A	95	GLY	CA-C-O	-6.57	117.00	122.33
1	B	97	GLY	N-CA-C	6.25	128.00	113.18
1	B	14	ILE	CA-CB-CG1	6.22	120.97	110.40
1	B	54	VAL	CA-C-O	6.12	124.43	119.29
1	B	97	GLY	CA-C-N	5.94	132.39	121.70
1	B	97	GLY	C-N-CA	5.94	132.39	121.70
1	B	14	ILE	CA-CB-CG2	5.54	119.92	110.50
1	B	16	ARG	CG-CD-NE	5.12	123.26	112.00
1	B	19	ASP	N-CA-C	5.06	118.00	109.95
1	B	125	ASP	N-CA-CB	5.00	118.33	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	14	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	GLN	Peptide

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	1268	0	1250	25	0
1	B	1256	0	1236	28	3
2	A	31	0	11	0	0
2	B	31	0	11	0	0
3	A	14	0	20	6	0
4	A	275	0	0	10	0
4	B	248	0	0	6	3
All	All	3123	0	2528	55	3

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 11.

All (55) 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:16:ARG:NH1	1:B:125:ASP:OD1	1.90	1.05
1:B:133:GLU:O	1:B:136:ARG:NH2	1.89	1.04
1:A:146:ARG:HD3	1:A:146:ARG:O	1.76	0.86
1:B:102:LEU:HD12	4:B:490:HOH:O	1.76	0.85
3:A:202:ETE:H261	4:A:495:HOH:O	1.78	0.81
1:B:28:GLN:HG3	4:B:455:HOH:O	1.78	0.81
1:A:14:ILE:HD11	4:A:392:HOH:O	1.80	0.79
1:B:23:ARG:NH1	1:B:23:ARG:HB2	1.97	0.79
1:B:23:ARG:HB2	1:B:23:ARG:HH11	1.49	0.78
3:A:202:ETE:C26	4:A:495:HOH:O	2.36	0.73
1:A:136:ARG:HH12	3:A:202:ETE:H232	1.52	0.72
1:A:32:ARG:O	1:A:36:MET:HG2	1.89	0.72
1:B:97:GLY:HA3	1:B:98:GLN:CB	2.24	0.67
1:B:0:HIS:CB	4:B:442:HOH:O	2.43	0.67
1:A:-1:SER:CB	1:A:87:THR:O	2.44	0.65
1:B:72:MET:HE2	1:B:74:SER:HB2	1.81	0.62
1:A:72:MET:HB2	4:A:433:HOH:O	2.01	0.61
1:A:32:ARG:NH1	4:A:421:HOH:O	1.78	0.60
1:B:79[A]:VAL:HG21	1:B:85:ALA:HB2	1.83	0.59
1:B:16:ARG:NH1	1:B:125:ASP:CG	2.59	0.59
1:B:16:ARG:HH12	1:B:125:ASP:CG	2.11	0.58
1:A:82:LEU:HD21	1:A:103:ALA:HA	1.86	0.57
1:A:146:ARG:HD3	1:A:146:ARG:C	2.28	0.57
1:B:16:ARG:HH11	1:B:16:ARG:HG3	1.72	0.55
1:B:16:ARG:HH12	1:B:122:GLU:HG2	1.73	0.54
1:A:87:THR:HG22	4:A:412:HOH:O	2.07	0.52
1:A:79:VAL:HG21	1:A:85:ALA:HB2	1.90	0.52
1:A:133:GLU:CD	1:A:133:GLU:H	2.17	0.52
1:B:97:GLY:O	1:B:100:TYR:HB2	2.10	0.51
1:A:32:ARG:HG3	1:A:36:MET:CG	2.41	0.50
1:B:97:GLY:HA3	1:B:98:GLN:HB2	1.94	0.50
1:A:136:ARG:HH12	3:A:202:ETE:H221	1.77	0.49
1:A:72:MET:CB	4:A:433:HOH:O	2.57	0.49
1:A:36:MET:HE1	1:A:59:GLY:HA3	1.95	0.49
1:B:23:ARG:HH11	1:B:23:ARG:CB	2.23	0.48
1:A:136:ARG:NH1	3:A:202:ETE:H221	2.30	0.47
1:A:1:MET:N	4:A:409:HOH:O	2.47	0.47
1:A:-1:SER:CB	1:A:87:THR:C	2.89	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD21	1:B:103:ALA:HA	1.98	0.46
1:B:82:LEU:HD22	1:B:102:LEU:HB3	1.98	0.46
1:B:65:LEU:HD23	1:B:79[A]:VAL:HG23	1.98	0.46
1:A:54:VAL:HG13	4:A:487:HOH:O	2.16	0.45
1:A:1:MET:HE3	1:A:90:GLU:HG3	1.98	0.44
1:B:68[B]:GLN:HG2	1:B:70:ASP:OD1	2.17	0.44
1:A:41:VAL:HG23	1:A:91:THR:HG23	1.99	0.44
1:A:14:ILE:HD13	1:A:14:ILE:HG21	1.68	0.43
1:A:136:ARG:NH1	3:A:202:ETE:H232	2.28	0.43
1:B:97:GLY:CA	1:B:98:GLN:CB	2.96	0.43
1:B:72:MET:HE3	4:B:513:HOH:O	2.19	0.42
1:B:97:GLY:HA3	1:B:98:GLN:HB3	1.99	0.42
1:B:20:ILE:HA	1:B:21:PRO:HD3	1.84	0.42
1:B:14:ILE:HG21	1:B:14:ILE:HD12	1.24	0.42
1:B:0:HIS:HA	4:B:531:HOH:O	2.19	0.42
1:B:27:ASP:HA	4:B:419:HOH:O	2.21	0.41
1:A:1:MET:CA	4:A:409:HOH:O	2.70	0.40

All (3) 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:B:53:LYS:CE	4:B:441:HOH:O[2_656]	1.94	0.26
1:B:23:ARG:NH2	4:B:395:HOH:O[2_656]	2.04	0.16
1:B:146:ARG:CB	4:B:514:HOH:O[1_655]	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	162/179 (90%)	159 (98%)	2 (1%)	1 (1%)	21 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	161/179 (90%)	158 (98%)	1 (1%)	2 (1%)	10	1
All	All	323/358 (90%)	317 (98%)	3 (1%)	3 (1%)	14	2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	B	98	GLN
1	B	97	GLY

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	130/144 (90%)	127 (98%)	3 (2%)	44	10
1	B	129/144 (90%)	127 (98%)	2 (2%)	55	20
All	All	259/288 (90%)	254 (98%)	5 (2%)	55	14

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	MET
1	A	88[A]	SER
1	A	88[B]	SER
1	B	23	ARG
1	B	72	MET

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

Mol	Chain	Res	Type
1	A	68	GLN
1	A	157	HIS
1	B	157	HIS

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 oligosaccharides 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	ATR	A	201	-	32,33,33	1.56	7 (21%)	50,52,52	1.42	8 (16%)
2	ATR	B	200	-	32,33,33	1.34	4 (12%)	50,52,52	2.04	13 (26%)
3	ETE	A	202	-	13,13,13	0.58	0	12,12,12	1.61	2 (16%)

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	ATR	A	201	-	-	0/21/37/37	0/3/3/3
2	ATR	B	200	-	-	0/21/37/37	0/3/3/3
3	ETE	A	202	-	-	9/11/11/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	ATR	C5-C4	5.16	1.48	1.39
2	B	200	ATR	C5-C4	2.94	1.44	1.39
2	B	200	ATR	P2'-O2'	2.72	1.64	1.59
2	A	201	ATR	C4-N9	-2.64	1.32	1.37
2	A	201	ATR	P2'-O2'	2.52	1.63	1.59
2	A	201	ATR	C5-N7	-2.25	1.35	1.39
2	A	201	ATR	C2-N1	2.23	1.37	1.33
2	A	201	ATR	PA-O2A	-2.21	1.45	1.55
2	B	200	ATR	O4'-C1'	2.10	1.46	1.42
2	B	200	ATR	PB-O3B	-2.09	1.47	1.54
2	A	201	ATR	PA-O3A	2.06	1.61	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	ATR	C4-N9-C8	6.84	112.92	105.74
2	B	200	ATR	N9-C8-N7	-5.16	106.62	113.94
2	B	200	ATR	C4-C5-N7	-4.07	105.92	110.58
3	A	202	ETE	C25-OH5-C14	-3.90	96.21	113.26
2	B	200	ATR	C5-N7-C8	3.84	109.48	103.45
2	A	201	ATR	C4-C5-N7	-3.76	106.28	110.58
2	B	200	ATR	C2'-C1'-N9	3.38	119.31	113.75
2	B	200	ATR	O2B-PB-O3A	3.13	115.12	104.64
2	B	200	ATR	C6-C5-N7	3.09	138.05	132.09
2	A	201	ATR	N3-C2-N1	-3.07	123.93	128.58
2	B	200	ATR	N3-C2-N1	-2.91	124.18	128.58
2	A	201	ATR	C6-C5-N7	2.59	137.08	132.09
2	B	200	ATR	N3-C4-N9	2.58	131.55	127.17
2	B	200	ATR	C3'-C2'-C1'	-2.53	97.96	102.81
2	A	201	ATR	C5-N7-C8	2.52	107.41	103.45
2	B	200	ATR	O2'-C2'-C1'	-2.45	101.42	110.05
2	A	201	ATR	C2-N1-C6	2.45	122.75	118.73
2	B	200	ATR	C5-C4-N3	-2.41	123.39	126.72
2	A	201	ATR	C4-N9-C8	2.35	108.21	105.74
2	A	201	ATR	O4'-C1'-N9	2.22	112.34	108.09
2	A	201	ATR	C2'-C1'-N9	-2.10	110.30	113.75
2	B	200	ATR	O2'-P2'-O1P	-2.08	101.91	109.33
3	A	202	ETE	OH4-C13-C23	-2.04	101.07	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	ETE	OH4-C13-C23-OH3
3	A	202	ETE	OH2-C12-C22-OH3
3	A	202	ETE	OH6-C15-C25-OH5
3	A	202	ETE	C25-C15-OH6-C26
3	A	202	ETE	OH5-C14-C24-OH4
3	A	202	ETE	C23-C13-OH4-C24
3	A	202	ETE	C14-C24-OH4-C13
3	A	202	ETE	C24-C14-OH5-C25
3	A	202	ETE	C12-C22-OH3-C23

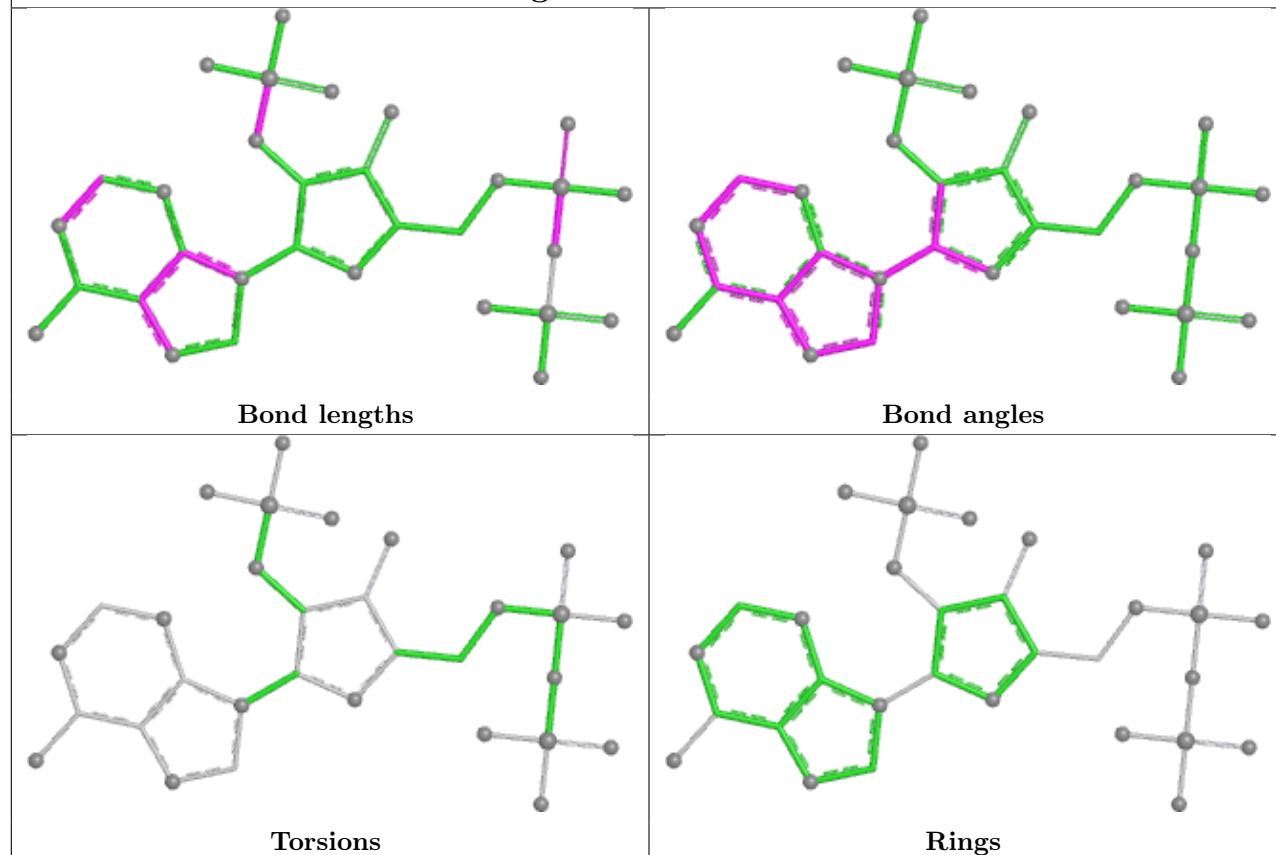
There are no ring outliers.

1 monomer is involved in 6 short contacts:

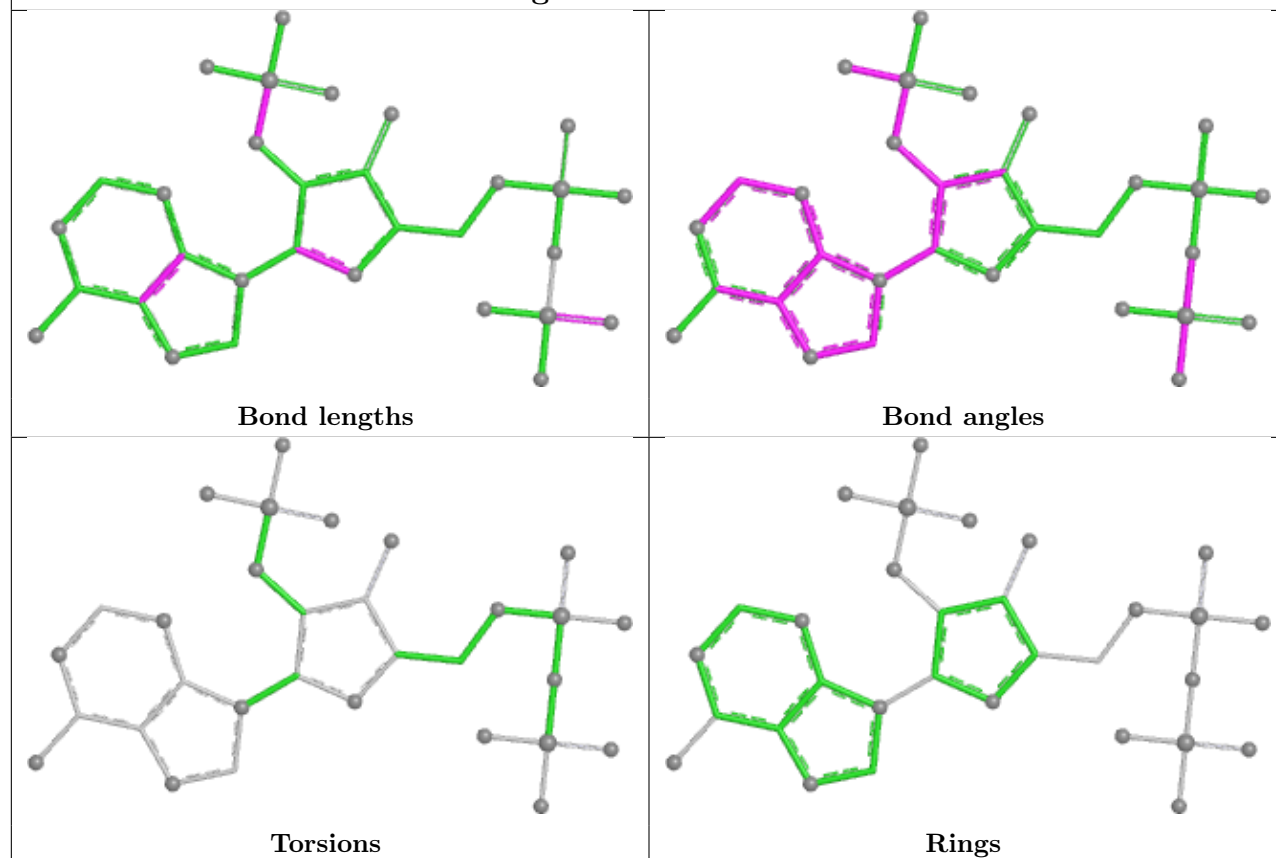
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	ETE	6	0

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.

Ligand ATR A 201



Ligand ATR B 200



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	161/179 (89%)	-0.32	3 (1%) 66 66	3, 8, 18, 40	3 (1%)
1	B	160/179 (89%)	-0.23	2 (1%) 75 74	4, 8, 21, 26	3 (1%)
All	All	321/358 (89%)	-0.28	5 (1%) 70 69	3, 8, 20, 40	6 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	SER	4.5
1	A	0	HIS	3.2
1	B	0	HIS	2.4
1	A	146	ARG	2.3
1	B	97	GLY	2.2

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](#)

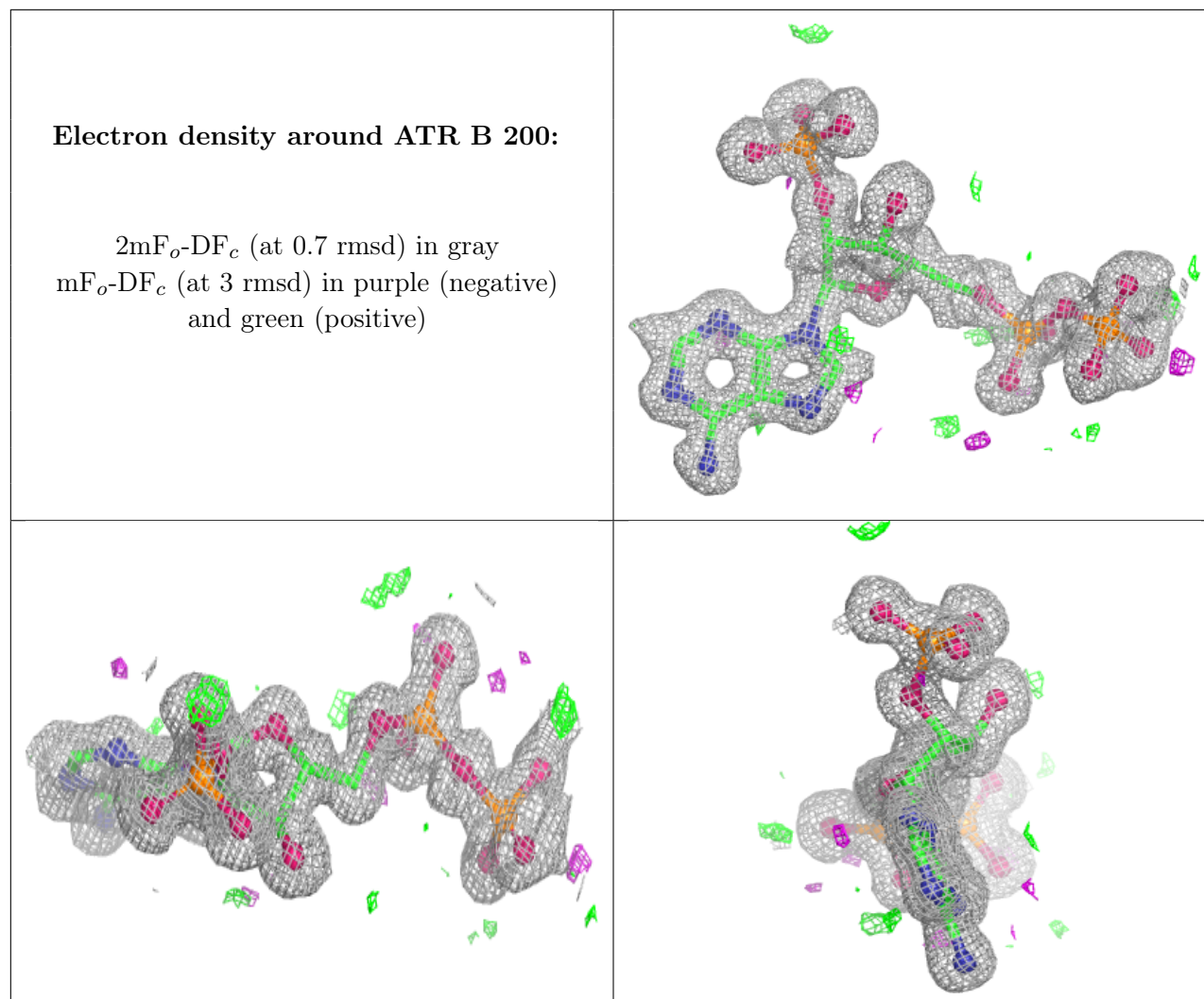
There are no oligosaccharides in this entry.

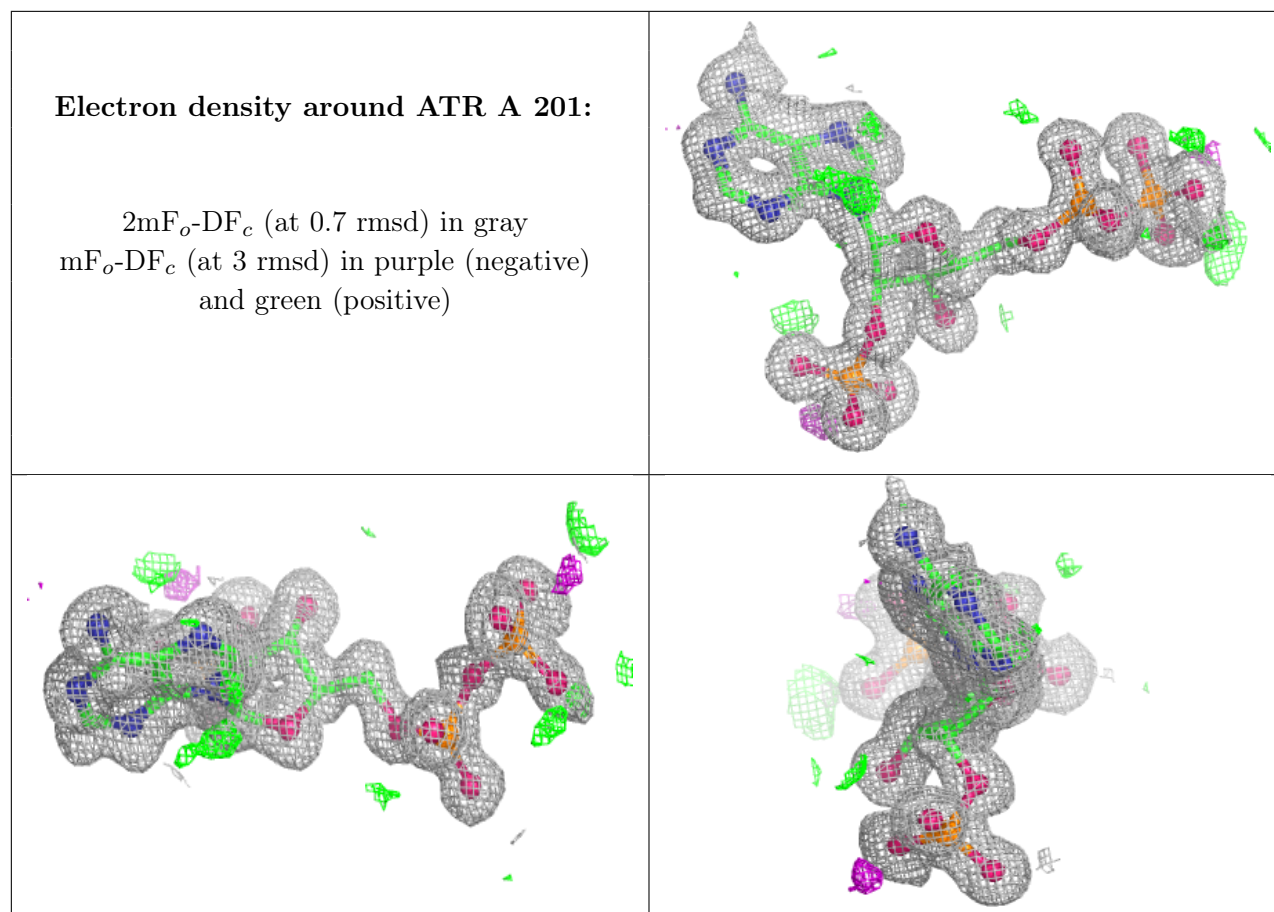
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	ETE	A	202	14/14	0.91	0.10	14,22,30,33	0
2	ATR	B	200	31/31	0.99	0.04	5,7,16,22	0
2	ATR	A	201	31/31	0.99	0.04	5,7,13,16	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.