



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:21 pm BST

PDB ID : 5ABM
Title : Sheep aldehyde dehydrogenase 1A1
Authors : Koch, M.F.; Harteis, S.; Blank, I.D.; Pestel, G.; Tietze, L.F.; Ochsenfeld, C.;
Schneider, S.; Sieber, S.A.
Deposited on : 2015-08-07
Resolution : 1.70 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 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 : 2.11
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

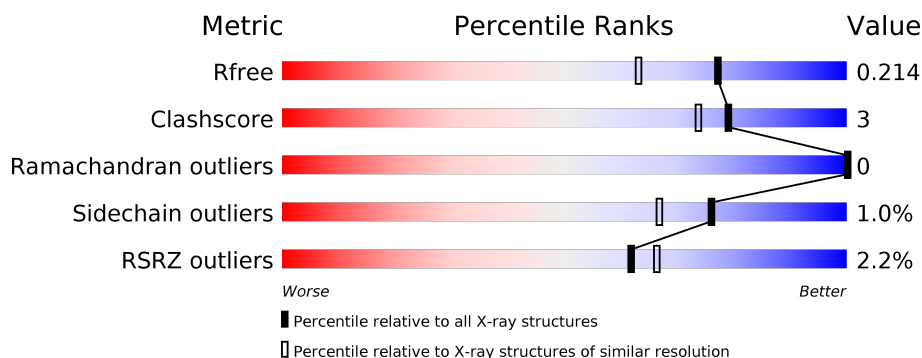
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	500	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	500	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	C	500	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>
1	D	500	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TXE	A	501	X	-	-	-
2	TXE	B	501	X	-	-	-
2	TXE	C	501	X	-	-	-
2	TXE	D	501	X	-	-	-

2 Entry composition ⓘ

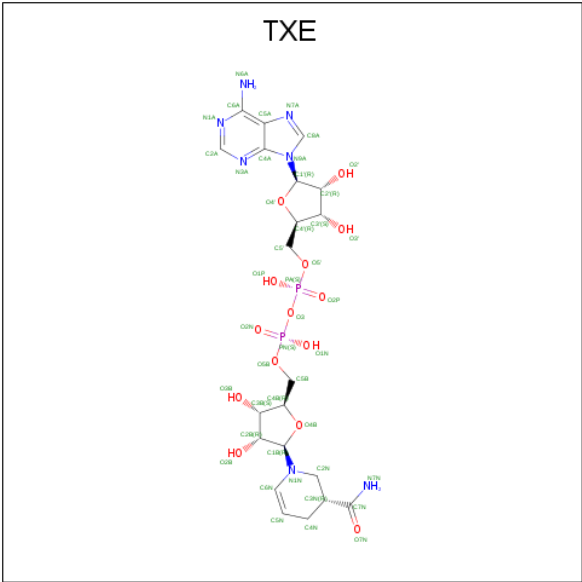
There are 4 unique types of molecules in this entry. The entry contains 16987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINAL DEHYDROGENASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	6	0
			3862	2460	648	731	23			
1	B	494	Total	C	N	O	S	0	8	0
			3870	2465	648	733	24			
1	C	494	Total	C	N	O	S	0	8	0
			3875	2467	649	736	23			
1	D	494	Total	C	N	O	S	0	6	0
			3857	2457	648	729	23			

- Molecule 2 is [[(2R,3S,4R,5R)-5-[(3R)-3-aminocarbonyl-3,4-dihydro-2H-pyridin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanidyl-phosphoryl] [(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphate (three-letter code: TXE) (formula: C₂₁H₃₁N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

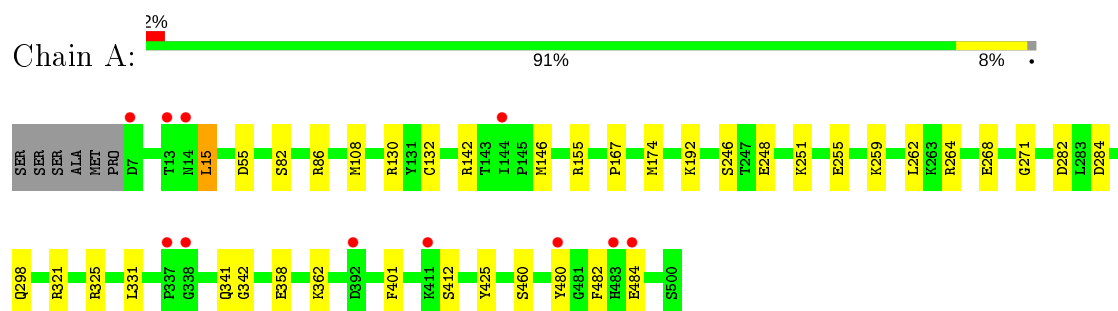
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	363	Total	O	0	1
			364	364		
4	B	332	Total	O	0	1
			333	333		
4	C	355	Total	O	0	1
			356	356		
4	D	290	Total	O	0	0
			290	290		

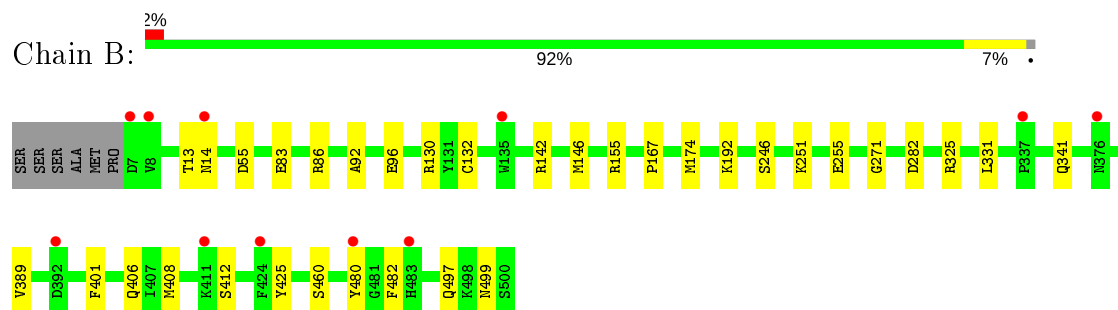
3 Residue-property plots [i](#)

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.

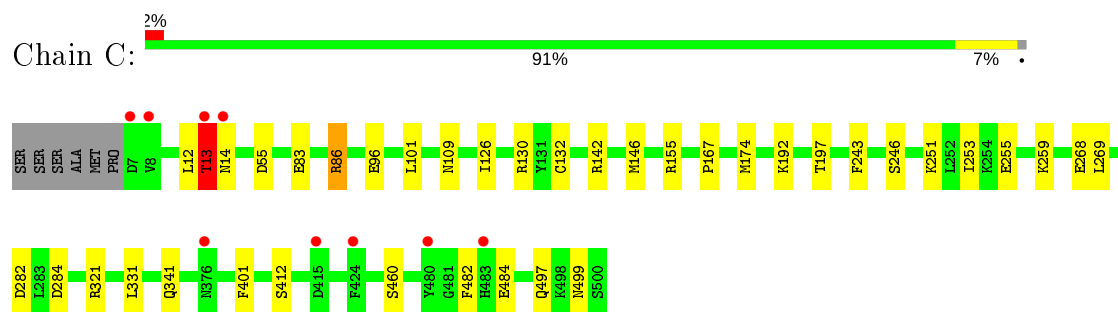
• Molecule 1: RETINAL DEHYDROGENASE 1



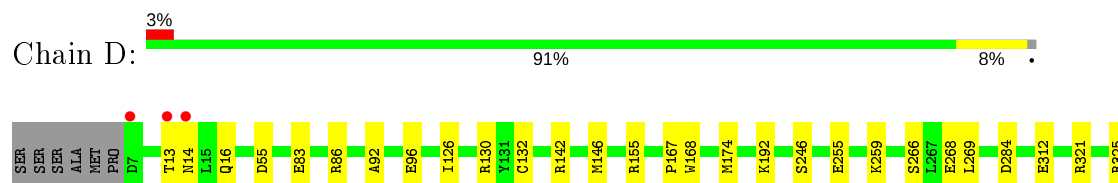
• Molecule 1: RETINAL DEHYDROGENASE 1



• Molecule 1: RETINAL DEHYDROGENASE 1



• Molecule 1: RETINAL DEHYDROGENASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.99Å 80.80Å 171.41Å 90.00° 117.97° 90.00°	Depositor
Resolution (Å)	151.85 – 1.70 48.21 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (151.85-1.70) 99.7 (48.21-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.180 , 0.203 0.194 , 0.214	Depositor DCC
R_{free} test set	12505 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16987	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.97% 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: TXE, MG

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	0.89	2/3946 (0.1%)	0.89	12/5331 (0.2%)
1	B	0.83	0/3960	0.88	9/5350 (0.2%)
1	C	0.87	4/3962 (0.1%)	0.93	19/5353 (0.4%)
1	D	0.83	2/3941 (0.1%)	0.86	9/5325 (0.2%)
All	All	0.86	8/15809 (0.1%)	0.89	49/21359 (0.2%)

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	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	LEU	C-N	-9.20	1.12	1.34
1	C	269	LEU	C-N	-8.58	1.17	1.33
1	C	484	GLU	C-N	-8.20	1.15	1.34
1	C	12	LEU	C-N	-8.16	1.15	1.34
1	C	13	THR	C-N	-7.46	1.16	1.34
1	D	168	TRP	CB-CG	-5.35	1.40	1.50
1	D	266	SER	CB-OG	-5.27	1.35	1.42
1	A	248	GLU	CG-CD	5.04	1.59	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	THR	O-C-N	-11.06	105.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	C	86	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	130	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	15	LEU	O-C-N	9.75	138.30	122.70
1	C	12	LEU	O-C-N	-9.62	107.31	122.70
1	C	86	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	C	130	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	130	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	D	155	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	55	ASP	CB-CG-OD1	8.14	125.62	118.30
1	D	155	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	D	130	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	15	LEU	CA-C-N	-7.83	99.98	117.20
1	C	12	LEU	C-N-CA	7.76	141.11	121.70
1	A	142	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	155	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	C	142	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	142	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	C	155	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	142	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	155	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	130	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	C	12	LEU	CA-C-N	6.98	132.55	117.20
1	D	142	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	142	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	155	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	142	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	C	13	THR	CA-C-N	6.21	130.85	117.20
1	C	269	LEU	O-C-N	-6.20	112.66	123.20
1	B	142	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	155	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	325	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	155	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	55	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	269	LEU	C-N-CA	-5.78	110.15	122.30
1	B	130	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	130	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	484	GLU	O-C-N	-5.39	114.08	122.70
1	C	269	LEU	CA-C-N	5.29	126.78	116.20
1	D	325	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	282	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	264	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	282	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	101	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	282	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	55	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	55	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	13	THR	Mainchain

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	3862	0	3825	26	0
1	B	3870	0	3838	23	0
1	C	3875	0	3832	20	0
1	D	3857	0	3823	24	0
2	A	44	0	28	3	0
2	B	44	0	28	3	0
2	C	44	0	28	3	0
2	D	44	0	28	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	364	0	0	6	0
4	B	333	0	0	4	1
4	C	356	0	0	2	0
4	D	290	0	0	5	0
All	All	16987	0	15430	88	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (88) 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:255[B]:GLU:HG3	1:D:255[B]:GLU:HG3	1.50	0.92
2:D:501:TXE:H5N	4:D:2154:HOH:O	1.84	0.78
1:A:15:LEU:CD1	1:A:15:LEU:H	1.97	0.78
1:A:15:LEU:HD12	1:A:15:LEU:H	1.50	0.77
2:A:501:TXE:C5N	4:A:2170:HOH:O	2.33	0.77
1:A:167:PRO:HG2	1:A:174[B]:MET:SD	2.25	0.76
2:A:501:TXE:H5N	4:A:2170:HOH:O	1.85	0.75
1:A:255[A]:GLU:HG3	1:B:255:GLU:HG3	1.69	0.75
1:C:13:THR:O	1:C:14:ASN:CB	2.33	0.73
1:D:268:GLU:OE1	4:D:2198:HOH:O	2.11	0.68
1:A:259:LYS:HE3	4:A:2226:HOH:O	1.92	0.68
1:A:15:LEU:HD12	1:A:15:LEU:N	2.10	0.67
1:D:284:ASP:OD1	1:D:321:ARG:NH2	2.29	0.66
1:C:167:PRO:HG2	1:C:174[B]:MET:SD	2.34	0.65
1:D:167:PRO:HG2	1:D:174[B]:MET:SD	2.37	0.65
1:B:406:GLN:HB3	1:B:408[A]:MET:HE2	1.80	0.64
1:C:331:LEU:HD22	1:C:341:GLN:HB3	1.78	0.63
2:D:501:TXE:C5N	4:D:2154:HOH:O	2.44	0.63
1:A:480:TYR:CD2	4:A:2345:HOH:O	2.50	0.63
1:B:331:LEU:HD22	1:B:341:GLN:HB3	1.81	0.63
1:A:284:ASP:OD1	1:A:321:ARG:NH1	2.32	0.63
1:C:13:THR:O	1:C:14:ASN:HB3	1.98	0.62
1:B:480[A]:TYR:CD2	4:B:2323:HOH:O	2.51	0.61
1:D:331:LEU:HD22	1:D:341:GLN:HB3	1.83	0.61
1:D:132:CYS:HG	1:D:482:PHE:HZ	1.50	0.60
1:C:109:ASN:HD21	1:C:197:THR:HA	1.65	0.60
1:A:331:LEU:HD22	1:A:341:GLN:HB3	1.83	0.60
1:D:480[A]:TYR:CD2	4:D:2279:HOH:O	2.52	0.59
2:C:501:TXE:H5N	4:C:2171:HOH:O	2.02	0.58
1:B:167:PRO:HG2	1:B:174[B]:MET:SD	2.44	0.58
2:B:501:TXE:C5N	4:B:2168:HOH:O	2.53	0.57
1:C:255[B]:GLU:CG	1:D:255[B]:GLU:HG3	2.31	0.56
2:C:501:TXE:C5N	4:C:2171:HOH:O	2.53	0.55
1:A:146:MET:CE	1:B:460:SER:HB2	2.37	0.55
1:A:132:CYS:HG	1:A:482:PHE:HZ	1.55	0.54
1:D:13:THR:O	1:D:14:ASN:HB3	2.08	0.54
1:C:146:MET:HE1	1:D:460:SER:HB2	1.90	0.53
1:C:132:CYS:HG	1:C:482:PHE:HZ	1.57	0.52
2:B:501:TXE:H5N	4:B:2168:HOH:O	2.08	0.52
1:A:460:SER:HB2	1:B:146:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLN:NE2	4:D:2005:HOH:O	2.42	0.52
1:B:497[B]:GLN:NE2	1:B:499:ASN:HD21	2.08	0.51
1:C:83:GLU:OE1	1:C:86:ARG:NH2	2.44	0.50
1:C:146:MET:CE	1:D:460:SER:HB2	2.41	0.50
1:D:255[B]:GLU:HG2	1:D:259:LYS:HE2	1.93	0.50
1:C:251:LYS:O	1:C:255[A]:GLU:HG3	2.12	0.49
1:A:146:MET:HE1	1:B:460:SER:HB2	1.94	0.49
1:D:312:GLU:HG2	1:D:409:LYS:HD3	1.95	0.49
1:D:246:SER:HB3	2:D:501:TXE:O4B	2.13	0.49
1:B:132:CYS:HG	1:B:482:PHE:HZ	1.60	0.48
1:A:480:TYR:HD2	4:A:2345:HOH:O	1.91	0.48
1:A:460:SER:HB2	1:B:146:MET:CE	2.43	0.48
1:A:271:GLY:HA2	1:A:425:TYR:CD1	2.48	0.48
1:C:96[B]:GLU:HG2	1:C:126:ILE:HD13	1.97	0.47
1:C:460:SER:HB2	1:D:146:MET:CE	2.45	0.47
1:C:109:ASN:ND2	1:C:197:THR:HA	2.28	0.47
1:B:271:GLY:HA2	1:B:425:TYR:CD1	2.49	0.46
1:A:167:PRO:CG	1:A:174[B]:MET:SD	3.00	0.46
1:A:246:SER:HB3	2:A:501:TXE:O4B	2.15	0.46
1:D:497[A]:GLN:HG3	1:D:497[A]:GLN:O	2.16	0.46
1:B:389:VAL:HG11	1:B:408[A]:MET:HE2	1.98	0.46
1:C:243:PHE:CD1	1:C:253:ILE:CD1	2.99	0.46
1:D:497[A]:GLN:NE2	1:D:499:ASN:HD21	2.14	0.46
1:D:92:ALA:O	1:D:96[A]:GLU:HG3	2.16	0.46
1:C:497[B]:GLN:NE2	1:C:499:ASN:HD21	2.15	0.45
1:C:284:ASP:OD1	1:C:321:ARG:NH2	2.28	0.45
1:B:13:THR:O	1:B:14:ASN:HB3	2.17	0.44
1:C:460:SER:HB2	1:D:146:MET:HE1	2.00	0.44
1:B:497[B]:GLN:O	1:B:497[B]:GLN:HG3	2.16	0.44
1:A:484[B]:GLU:O	1:A:484[B]:GLU:HG3	2.16	0.44
1:A:358:GLU:HG3	1:A:362:LYS:HE2	2.00	0.44
1:D:96[A]:GLU:HG2	1:D:126:ILE:HD13	1.99	0.44
1:A:15:LEU:HD13	1:A:108:MET:SD	2.58	0.43
1:D:83:GLU:OE1	1:D:86:ARG:NE	2.52	0.43
1:A:298:GLN:NE2	1:A:342:GLY:H	2.17	0.43
1:B:406:GLN:HB3	1:B:408[A]:MET:CE	2.47	0.42
1:C:246:SER:HB3	2:C:501:TXE:O4B	2.19	0.42
1:B:83:GLU:OE1	1:B:86:ARG:NH2	2.51	0.42
4:A:2224:HOH:O	1:B:251:LYS:NZ	2.39	0.42
1:B:246:SER:HB3	2:B:501:TXE:O4B	2.20	0.41
1:D:481:GLY:O	1:D:484:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLU:OE1	1:D:86:ARG:NH2	2.53	0.41
1:A:262:LEU:HD21	1:B:251:LYS:HA	2.03	0.41
1:A:251:LYS:O	1:A:255[B]:GLU:HG3	2.20	0.41
1:B:480[A]:TYR:HD2	4:B:2323:HOH:O	1.98	0.41
1:B:92:ALA:O	1:B:96[A]:GLU:HG3	2.21	0.40
1:A:146:MET:HE3	1:B:460:SER:HB2	2.02	0.40
1:A:82:SER:O	1:A:86:ARG:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2111:HOH:O	4:B:2111:HOH:O[2_656]	1.84	0.36

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	498/500 (100%)	487 (98%)	11 (2%)	0	100	100
1	B	500/500 (100%)	492 (98%)	8 (2%)	0	100	100
1	C	500/500 (100%)	490 (98%)	10 (2%)	0	100	100
1	D	498/500 (100%)	485 (97%)	13 (3%)	0	100	100
All	All	1996/2000 (100%)	1954 (98%)	42 (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	415/414 (100%)	411 (99%)	4 (1%)	76	67
1	B	417/414 (101%)	414 (99%)	3 (1%)	84	77
1	C	417/414 (101%)	412 (99%)	5 (1%)	71	59
1	D	414/414 (100%)	409 (99%)	5 (1%)	71	59
All	All	1663/1656 (100%)	1646 (99%)	17 (1%)	76	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	268	GLU
1	A	401	PHE
1	A	412	SER
1	B	192	LYS
1	B	401	PHE
1	B	412	SER
1	C	192	LYS
1	C	259	LYS
1	C	268	GLU
1	C	401	PHE
1	C	412	SER
1	D	192	LYS
1	D	401	PHE
1	D	412	SER
1	D	497[A]	GLN
1	D	497[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	298	GLN
1	A	473	ASN
1	B	109	ASN
1	B	292	GLN
1	B	499	ASN

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Mol	Chain	Res	Type
1	C	109	ASN
1	C	499	ASN
1	D	16	GLN
1	D	109	ASN
1	D	292	GLN
1	D	298	GLN
1	D	499	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	TXE	B	501	3	41,48,48	2.70	11 (26%)	44,73,73	2.01	10 (22%)
2	TXE	D	501	3	41,48,48	2.17	6 (14%)	44,73,73	1.60	5 (11%)
2	TXE	A	501	3	41,48,48	2.30	8 (19%)	44,73,73	1.61	7 (15%)
2	TXE	C	501	3	41,48,48	2.41	9 (21%)	44,73,73	1.78	8 (18%)

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	TXE	B	501	3	1/1/13/15	6/26/72/72	0/5/5/5
2	TXE	D	501	3	1/1/13/15	6/26/72/72	0/5/5/5
2	TXE	A	501	3	1/1/13/15	4/26/72/72	0/5/5/5
2	TXE	C	501	3	1/1/13/15	5/26/72/72	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TXE	C2N-C3N	-11.17	1.35	1.53
2	C	501	TXE	C2N-C3N	-9.73	1.37	1.53
2	A	501	TXE	C2N-C3N	-9.61	1.38	1.53
2	D	501	TXE	C2N-C3N	-8.73	1.39	1.53
2	B	501	TXE	C2N-N1N	-8.60	1.31	1.47
2	C	501	TXE	C2N-N1N	-8.30	1.31	1.47
2	A	501	TXE	C2N-N1N	-7.20	1.33	1.47
2	D	501	TXE	C2N-N1N	-6.95	1.34	1.47
2	D	501	TXE	C4N-C5N	-4.67	1.39	1.49
2	B	501	TXE	C4N-C5N	-4.16	1.40	1.49
2	D	501	TXE	C4N-C3N	-3.68	1.39	1.52
2	A	501	TXE	C5A-C4A	3.63	1.50	1.40
2	C	501	TXE	C4N-C3N	-3.04	1.41	1.52
2	C	501	TXE	C6N-C5N	3.03	1.38	1.33
2	A	501	TXE	C4N-C5N	-2.89	1.43	1.49
2	D	501	TXE	C6N-C5N	2.89	1.38	1.33
2	C	501	TXE	C4N-C5N	-2.87	1.43	1.49
2	A	501	TXE	C2A-N1A	2.83	1.39	1.33
2	B	501	TXE	C2A-N1A	2.80	1.39	1.33
2	B	501	TXE	C4N-C3N	-2.79	1.42	1.52
2	B	501	TXE	PN-O2N	2.74	1.60	1.50
2	C	501	TXE	C5A-C4A	2.74	1.48	1.40
2	B	501	TXE	C8A-N7A	2.71	1.39	1.34
2	A	501	TXE	C6N-C5N	2.71	1.38	1.33
2	B	501	TXE	C5A-C4A	2.65	1.48	1.40
2	B	501	TXE	C2A-N3A	2.63	1.36	1.32
2	B	501	TXE	C6N-C5N	2.61	1.38	1.33
2	C	501	TXE	O3'-C3'	-2.60	1.36	1.43
2	A	501	TXE	C4N-C3N	-2.55	1.43	1.52
2	B	501	TXE	O7N-C7N	-2.46	1.19	1.23
2	C	501	TXE	C5A-N7A	-2.46	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TXE	O3B-C3B	2.42	1.48	1.43
2	C	501	TXE	C4A-N3A	-2.31	1.32	1.35
2	D	501	TXE	C5A-C4A	2.16	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TXE	N3A-C2A-N1A	-7.28	117.29	128.68
2	D	501	TXE	C2N-C3N-C7N	6.81	122.85	110.07
2	C	501	TXE	C2N-C3N-C7N	5.72	120.80	110.07
2	B	501	TXE	C2N-C3N-C7N	5.34	120.09	110.07
2	A	501	TXE	C2N-C3N-C7N	5.21	119.85	110.07
2	C	501	TXE	N3A-C2A-N1A	-5.06	120.77	128.68
2	A	501	TXE	N3A-C2A-N1A	-4.74	121.26	128.68
2	D	501	TXE	N3A-C2A-N1A	-3.78	122.77	128.68
2	B	501	TXE	C1'-N9A-C4A	-3.73	120.09	126.64
2	B	501	TXE	C5A-C6A-N6A	-3.26	115.39	120.35
2	B	501	TXE	C2A-N1A-C6A	3.25	124.31	118.75
2	A	501	TXE	C3B-C2B-C1B	3.11	107.33	101.43
2	C	501	TXE	C4A-C5A-N7A	-2.86	106.42	109.40
2	B	501	TXE	C2B-C3B-C4B	-2.83	97.14	102.64
2	C	501	TXE	C2'-C3'-C4'	-2.80	97.20	102.64
2	C	501	TXE	C2B-C3B-C4B	-2.72	97.36	102.64
2	C	501	TXE	O4B-C4B-C3B	2.71	110.48	105.11
2	C	501	TXE	C1'-N9A-C4A	-2.65	121.98	126.64
2	D	501	TXE	C4A-C5A-N7A	-2.59	106.70	109.40
2	D	501	TXE	C2A-N1A-C6A	2.56	123.13	118.75
2	A	501	TXE	O4B-C1B-N1N	2.45	112.65	109.35
2	C	501	TXE	O5'-C5'-C4'	2.40	117.26	108.99
2	D	501	TXE	O7N-C7N-N7N	-2.40	118.83	123.00
2	B	501	TXE	N6A-C6A-N1A	2.32	123.39	118.57
2	B	501	TXE	C3B-C2B-C1B	2.24	105.68	101.43
2	A	501	TXE	C2B-C3B-C4B	-2.24	98.30	102.64
2	A	501	TXE	C4A-C5A-N7A	-2.13	107.18	109.40
2	B	501	TXE	O4B-C1B-C2B	-2.10	102.06	106.64
2	A	501	TXE	O4B-C1B-C2B	-2.07	102.13	106.64
2	B	501	TXE	C2'-C3'-C4'	-2.01	98.73	102.64

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	TXE	C3N

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Mol	Chain	Res	Type	Atom
2	D	501	TXE	C3N
2	A	501	TXE	C3N
2	C	501	TXE	C3N

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	TXE	O4B-C1B-N1N-C2N
2	B	501	TXE	C4N-C3N-C7N-N7N
2	D	501	TXE	C5'-O5'-PA-O1P
2	D	501	TXE	O4B-C1B-N1N-C2N
2	A	501	TXE	O4B-C1B-N1N-C2N
2	C	501	TXE	O4B-C1B-N1N-C2N
2	B	501	TXE	C4N-C3N-C7N-O7N
2	A	501	TXE	C4N-C3N-C7N-N7N
2	A	501	TXE	C4N-C3N-C7N-O7N
2	C	501	TXE	C4N-C3N-C7N-N7N
2	C	501	TXE	C4N-C3N-C7N-O7N
2	D	501	TXE	C4N-C3N-C7N-N7N
2	D	501	TXE	C4N-C3N-C7N-O7N
2	B	501	TXE	C5'-O5'-PA-O3
2	D	501	TXE	C5'-O5'-PA-O3
2	A	501	TXE	C5'-O5'-PA-O3
2	C	501	TXE	C5'-O5'-PA-O3
2	B	501	TXE	C5'-O5'-PA-O2P
2	D	501	TXE	C5'-O5'-PA-O2P
2	C	501	TXE	C5'-O5'-PA-O2P
2	B	501	TXE	C5B-O5B-PN-O3

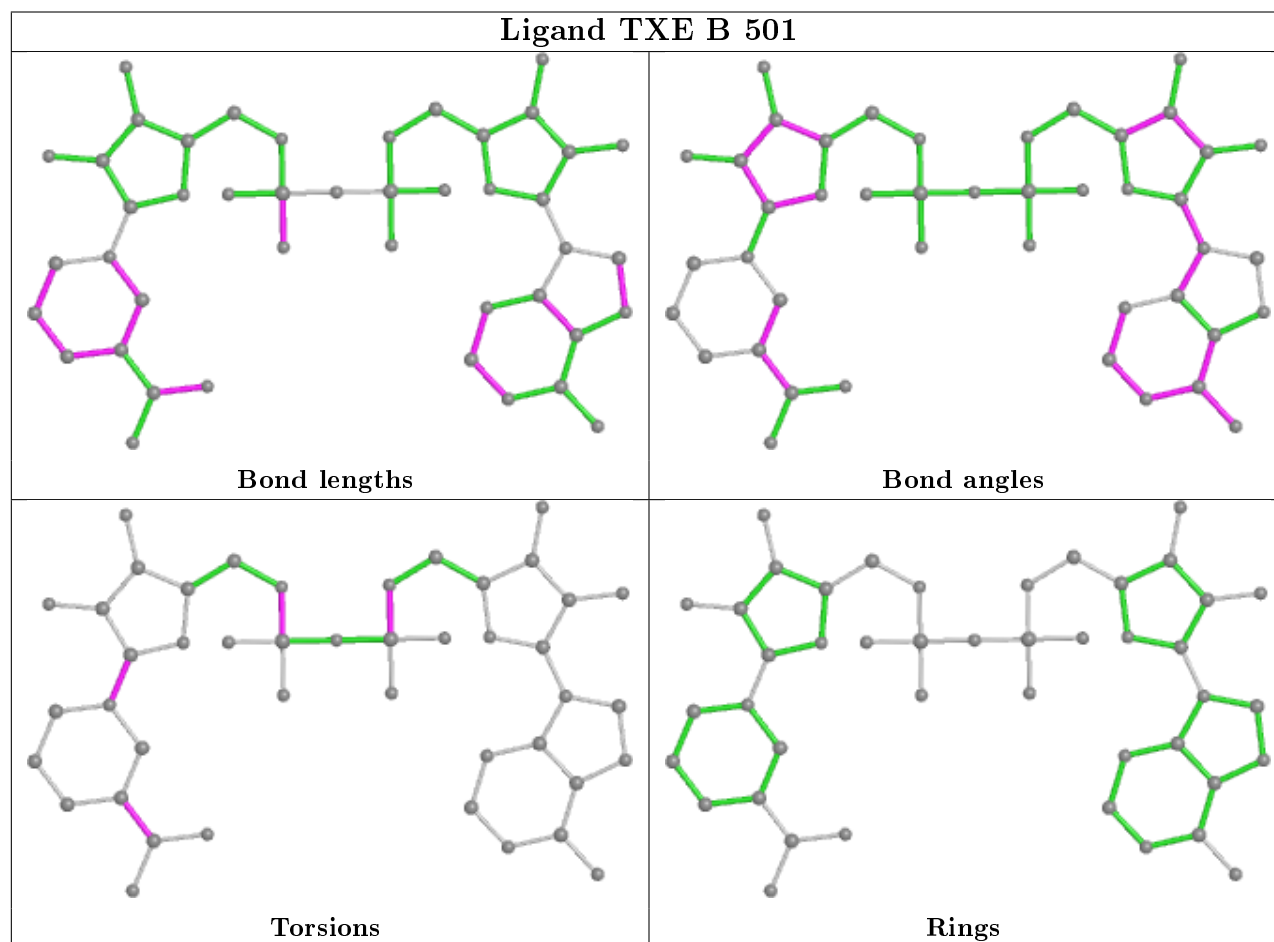
There are no ring outliers.

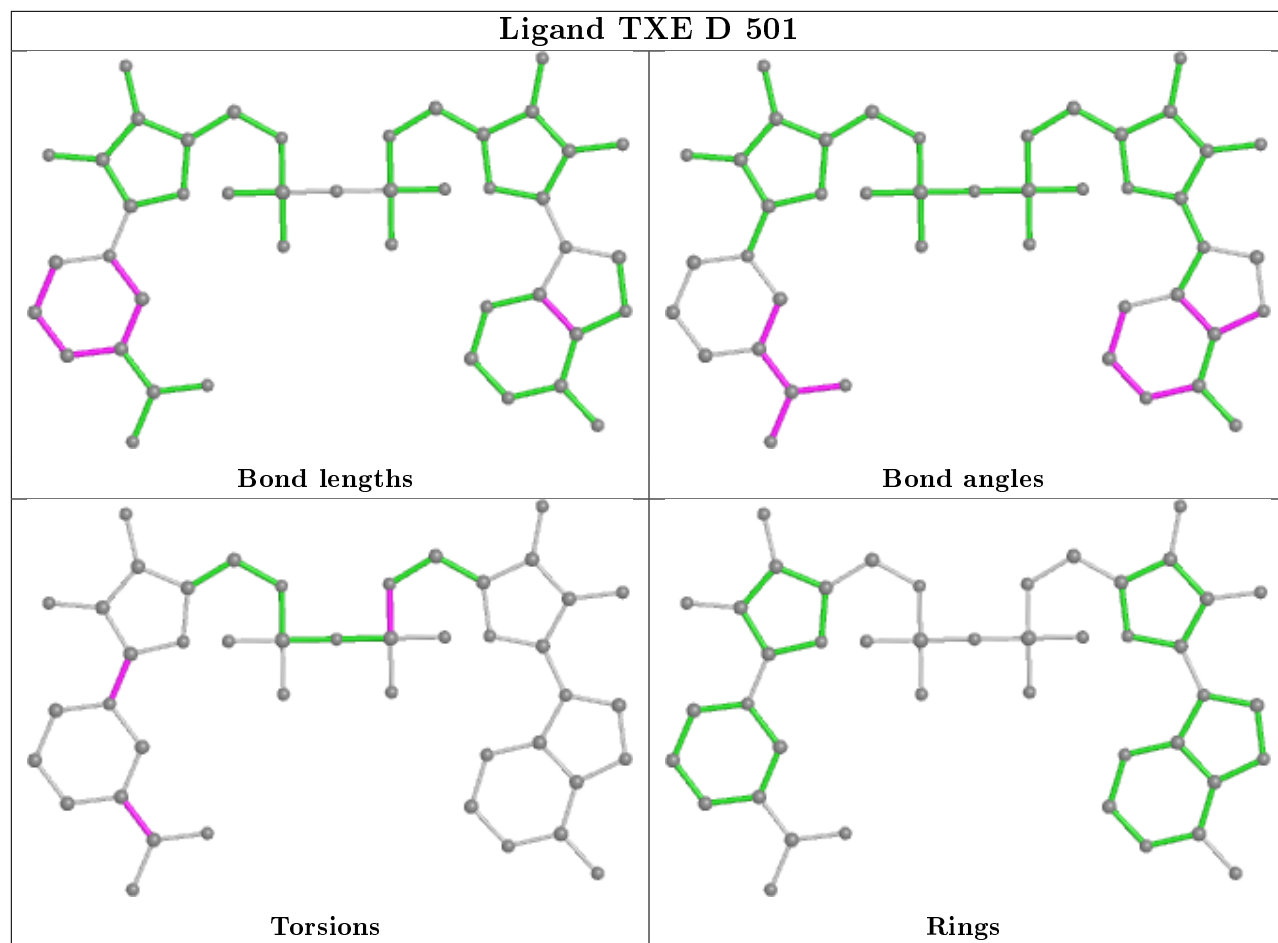
4 monomers are involved in 12 short contacts:

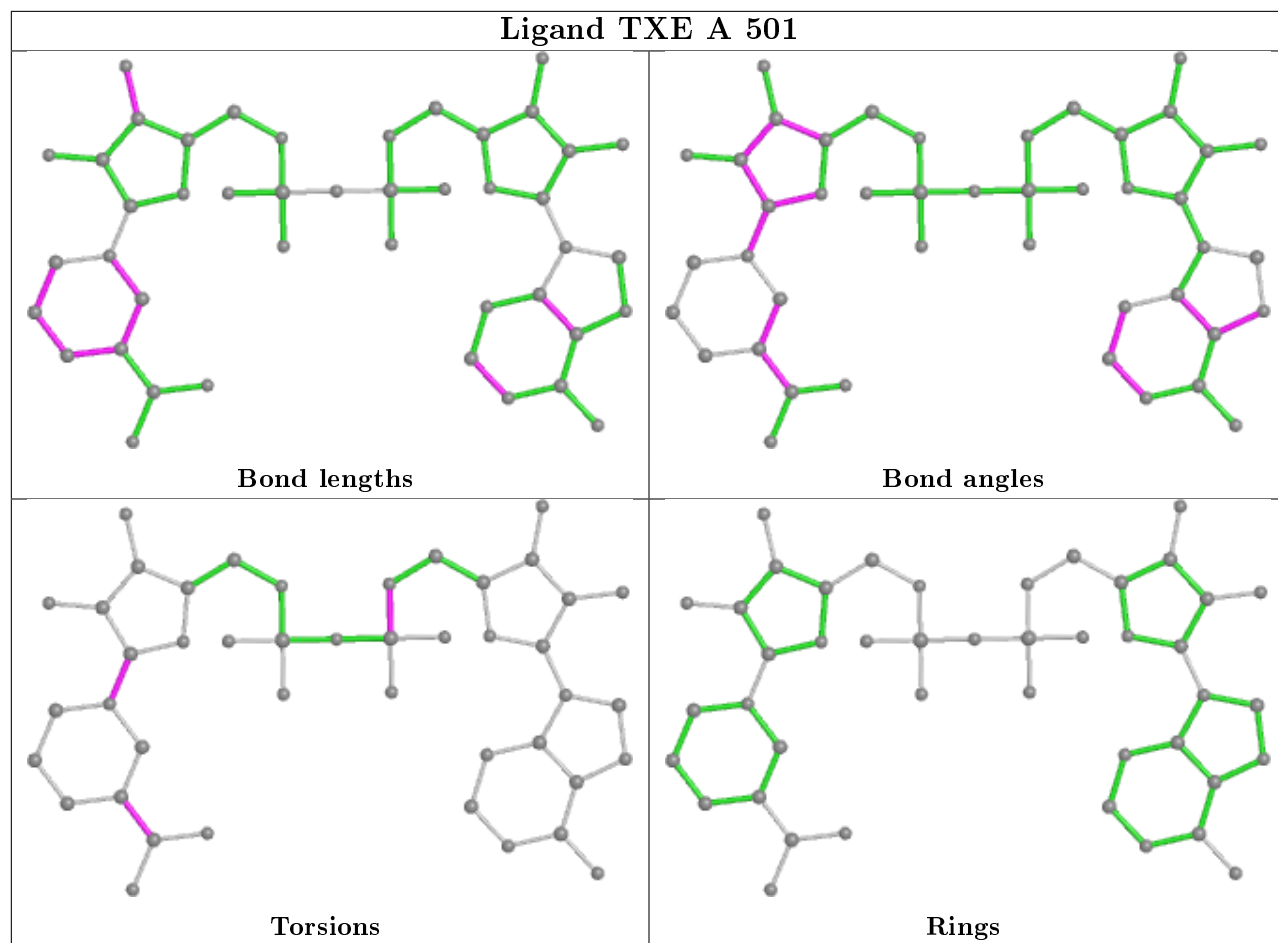
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	TXE	3	0
2	D	501	TXE	3	0
2	A	501	TXE	3	0
2	C	501	TXE	3	0

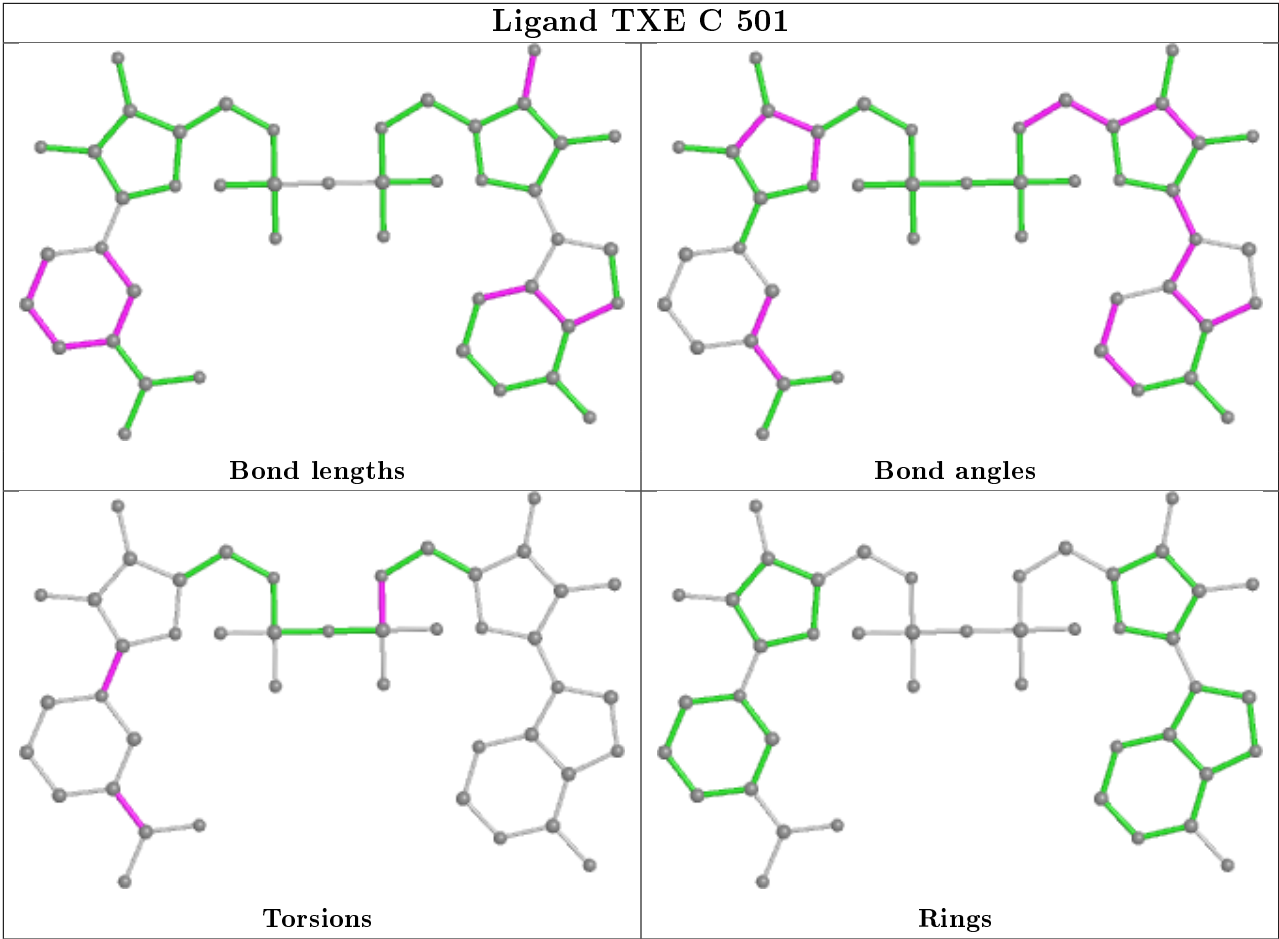
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	269:LEU	C	270:GLY	N	1.17
1	C	13:THR	C	14:ASN	N	1.16
1	C	12:LEU	C	13:THR	N	1.15
1	C	484:GLU	C	485:TYR	N	1.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	15:LEU	C	16:GLN	N	1.12

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	494/500 (98%)	-0.09	11 (2%) 62 66	12, 19, 39, 61	0
1	B	494/500 (98%)	-0.07	11 (2%) 62 66	12, 19, 33, 55	0
1	C	494/500 (98%)	-0.11	9 (1%) 68 72	12, 19, 34, 63	0
1	D	494/500 (98%)	-0.04	13 (2%) 56 60	13, 20, 37, 56	0
All	All	1976/2000 (98%)	-0.08	44 (2%) 62 66	12, 19, 36, 63	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	480[A]	TYR	11.0
1	B	480[A]	TYR	9.7
1	C	480[A]	TYR	7.5
1	D	483	HIS	6.6
1	C	483	HIS	5.7
1	A	14	ASN	5.3
1	A	483	HIS	4.6
1	B	7	ASP	4.4
1	C	7	ASP	3.9
1	A	7	ASP	3.8
1	C	14	ASN	3.7
1	B	8	VAL	3.6
1	A	480	TYR	3.6
1	D	14	ASN	3.5
1	B	14	ASN	3.4
1	B	424	PHE	3.4
1	A	337	PRO	3.3
1	A	411	LYS	3.3
1	C	13	THR	3.2
1	A	13	THR	3.1
1	D	337	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	484[A]	GLU	2.7
1	D	484	GLU	2.7
1	C	376	ASN	2.7
1	B	337	PRO	2.6
1	D	7	ASP	2.6
1	D	485	TYR	2.5
1	D	482	PHE	2.4
1	B	411	LYS	2.4
1	C	415	ASP	2.4
1	B	376	ASN	2.4
1	B	135	TRP	2.3
1	A	392	ASP	2.3
1	D	338	GLY	2.3
1	C	8	VAL	2.3
1	D	376	ASN	2.2
1	A	144	ILE	2.2
1	D	13	THR	2.2
1	A	338	GLY	2.2
1	D	392	ASP	2.2
1	B	483	HIS	2.2
1	B	392	ASP	2.1
1	D	362	LYS	2.1
1	C	424	PHE	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](#)

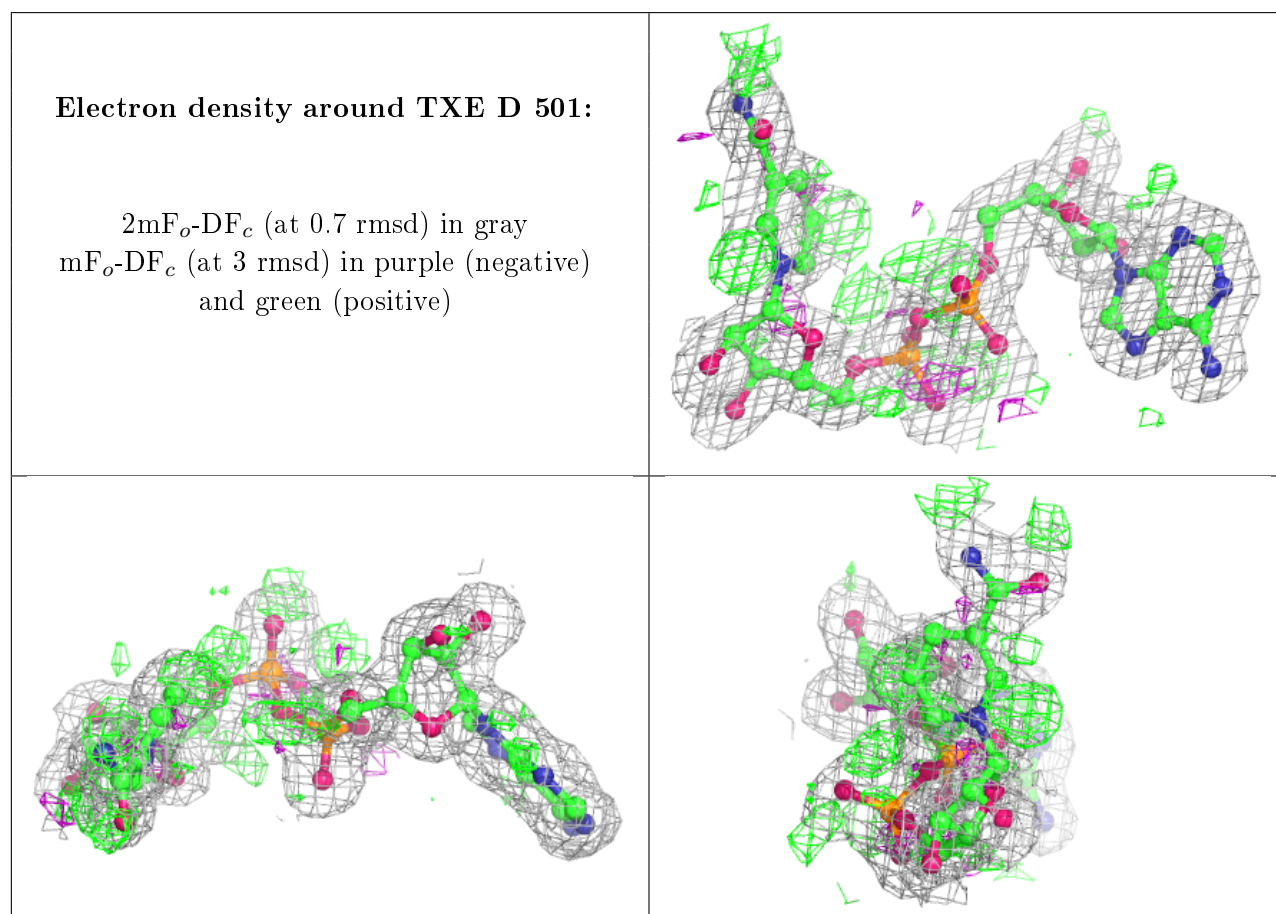
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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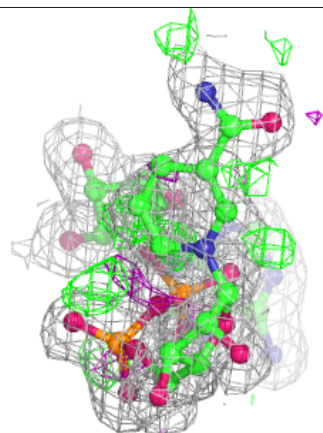
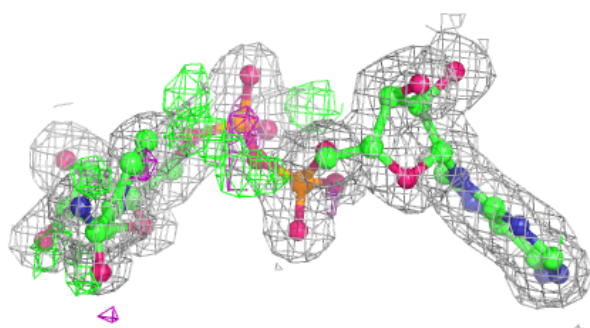
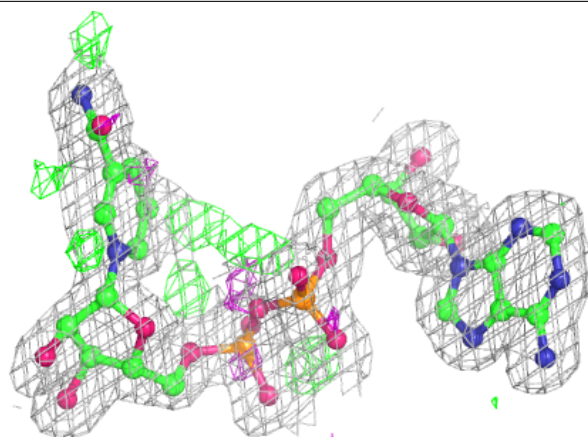
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	D	502	1/1	0.88	0.21	36,36,36,36	0
2	TXE	D	501	44/44	0.89	0.10	14,23,31,36	0
3	MG	B	502	1/1	0.89	0.18	29,29,29,29	0
3	MG	A	502	1/1	0.89	0.08	32,32,32,32	0
2	TXE	B	501	44/44	0.93	0.09	13,22,29,33	0
2	TXE	A	501	44/44	0.93	0.09	13,22,29,31	0
2	TXE	C	501	44/44	0.93	0.09	13,20,25,29	0
3	MG	C	502	1/1	0.97	0.12	24,24,24,24	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.



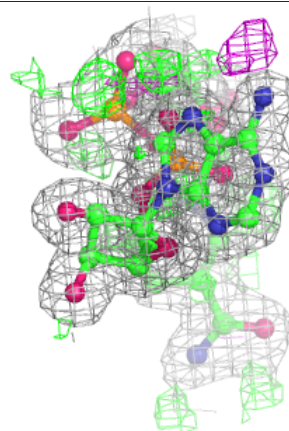
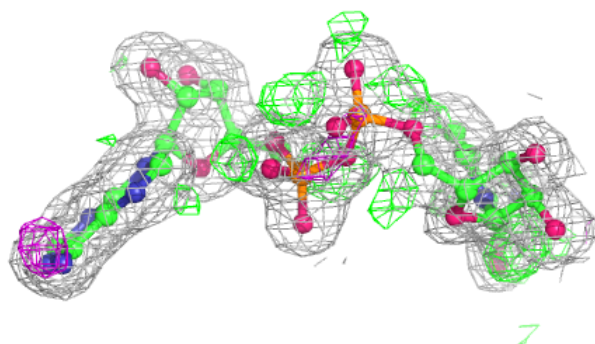
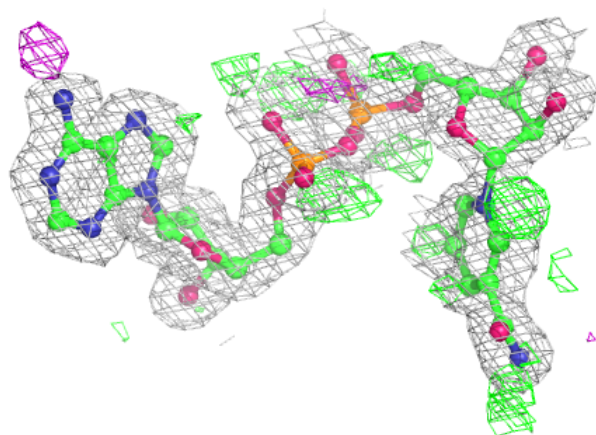
Electron density around TXE B 501:

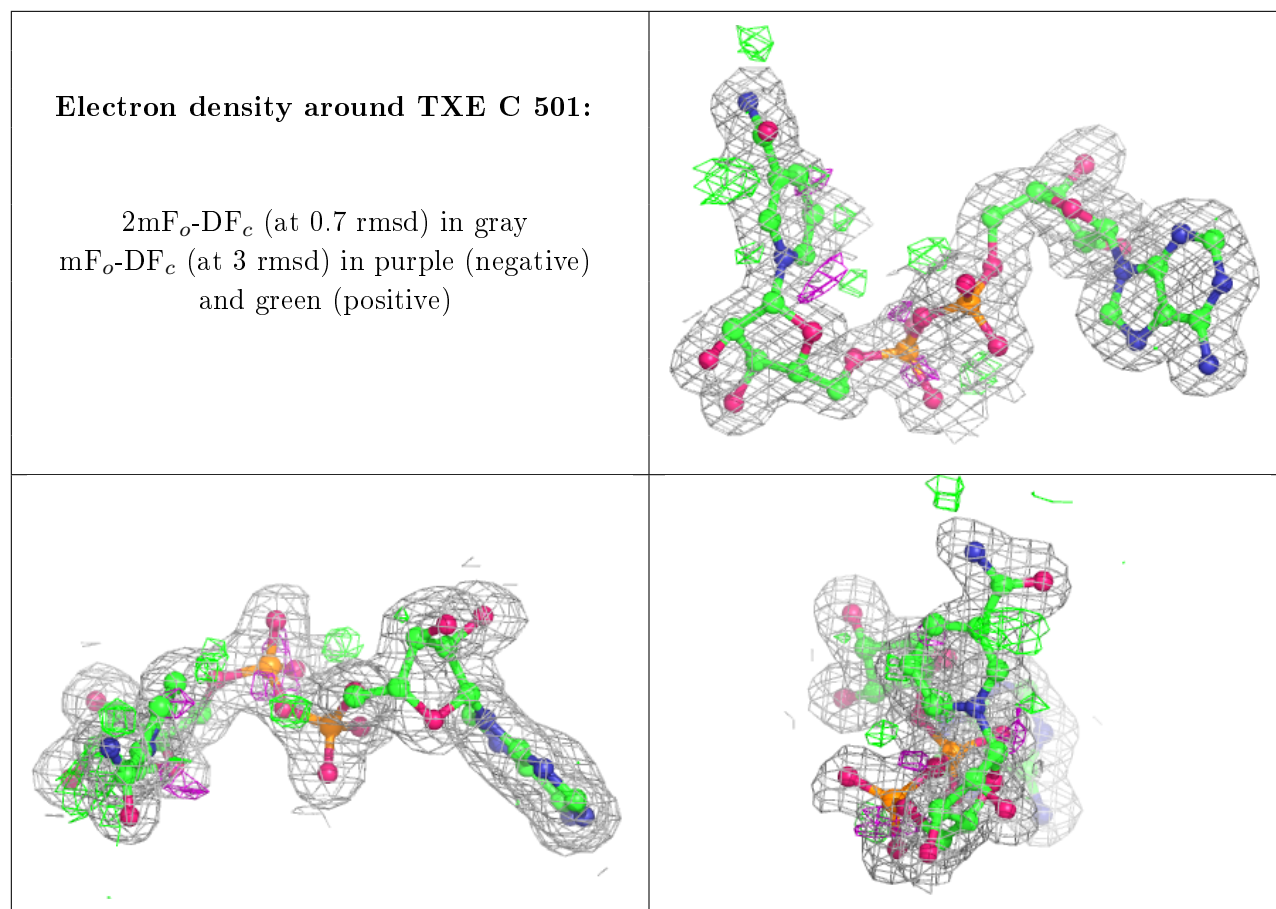
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TXE 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.