



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:45 PM UTC

PDB ID : 8OY6 / pdb_00008oy6
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (3 nanosecond pump-probe delay)
Authors : Lane, T.J.; Christou, N.-E.; Melo, D.V.M.; Apostolopoulou, V.; Pateras, A.; Mashhour, A.R.; Galchenkova, M.; Gunther, S.; Reinke, P.; Kremling, V.; Oberthuer, D.; Henkel, A.; Sprenger, J.; Scheer, T.E.S.; Lange, E.; Yefanov, O.N.; Middendorf, P.; Sellberg, J.A.; Schubert, R.; Fadini, A.; Cirelli, C.; Beale, E.V.; Johnson, P.; Dworkowski, F.; Ozerov, D.; Bertrand, Q.; Wranik, M.; Zitter, E.D.; Turk, D.; Bajt, S.; Chapman, H.; Bacellar, C.
Deposited on : 2023-05-03
Resolution : 2.35 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)

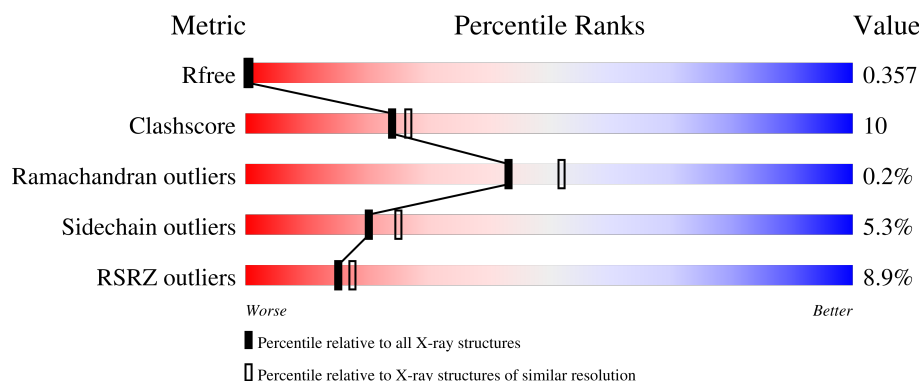
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	498	
1	B	498	

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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

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Mol	Chain	Length	Quality of chain
2	C	14	7% 57% 43%
2	E	14	14% 29% 57% 14%
3	D	14	57% 43%
3	F	14	14% 29% 71%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8638 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 Deoxyribodipyrimidine photo-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3713	2388	626	684	15			
1	B	428	Total	C	N	O	S	0	1	0
			3496	2247	590	644	15			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8PYK9
A	-18	GLY	-	expression tag	UNP Q8PYK9
A	-17	SER	-	expression tag	UNP Q8PYK9
A	-16	SER	-	expression tag	UNP Q8PYK9
A	-15	HIS	-	expression tag	UNP Q8PYK9
A	-14	HIS	-	expression tag	UNP Q8PYK9
A	-13	HIS	-	expression tag	UNP Q8PYK9
A	-12	HIS	-	expression tag	UNP Q8PYK9
A	-11	HIS	-	expression tag	UNP Q8PYK9
A	-10	HIS	-	expression tag	UNP Q8PYK9
A	-9	SER	-	expression tag	UNP Q8PYK9
A	-8	SER	-	expression tag	UNP Q8PYK9
A	-7	GLY	-	expression tag	UNP Q8PYK9
A	-6	LEU	-	expression tag	UNP Q8PYK9
A	-5	VAL	-	expression tag	UNP Q8PYK9
A	-4	PRO	-	expression tag	UNP Q8PYK9
A	-3	ARG	-	expression tag	UNP Q8PYK9
A	-2	GLY	-	expression tag	UNP Q8PYK9
A	-1	SER	-	expression tag	UNP Q8PYK9
A	0	HIS	-	expression tag	UNP Q8PYK9
A	465	ASP	-	expression tag	UNP Q8PYK9
A	466	LYS	-	expression tag	UNP Q8PYK9
A	467	LEU	-	expression tag	UNP Q8PYK9
A	468	ALA	-	expression tag	UNP Q8PYK9
A	469	ALA	-	expression tag	UNP Q8PYK9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	470	ALA	-	expression tag	UNP Q8PYK9
A	471	LEU	-	expression tag	UNP Q8PYK9
A	472	GLU	-	expression tag	UNP Q8PYK9
A	473	HIS	-	expression tag	UNP Q8PYK9
A	474	HIS	-	expression tag	UNP Q8PYK9
A	475	HIS	-	expression tag	UNP Q8PYK9
A	476	HIS	-	expression tag	UNP Q8PYK9
A	477	HIS	-	expression tag	UNP Q8PYK9
A	478	HIS	-	expression tag	UNP Q8PYK9
B	-19	MET	-	initiating methionine	UNP Q8PYK9
B	-18	GLY	-	expression tag	UNP Q8PYK9
B	-17	SER	-	expression tag	UNP Q8PYK9
B	-16	SER	-	expression tag	UNP Q8PYK9
B	-15	HIS	-	expression tag	UNP Q8PYK9
B	-14	HIS	-	expression tag	UNP Q8PYK9
B	-13	HIS	-	expression tag	UNP Q8PYK9
B	-12	HIS	-	expression tag	UNP Q8PYK9
B	-11	HIS	-	expression tag	UNP Q8PYK9
B	-10	HIS	-	expression tag	UNP Q8PYK9
B	-9	SER	-	expression tag	UNP Q8PYK9
B	-8	SER	-	expression tag	UNP Q8PYK9
B	-7	GLY	-	expression tag	UNP Q8PYK9
B	-6	LEU	-	expression tag	UNP Q8PYK9
B	-5	VAL	-	expression tag	UNP Q8PYK9
B	-4	PRO	-	expression tag	UNP Q8PYK9
B	-3	ARG	-	expression tag	UNP Q8PYK9
B	-2	GLY	-	expression tag	UNP Q8PYK9
B	-1	SER	-	expression tag	UNP Q8PYK9
B	0	HIS	-	expression tag	UNP Q8PYK9
B	465	ASP	-	expression tag	UNP Q8PYK9
B	466	LYS	-	expression tag	UNP Q8PYK9
B	467	LEU	-	expression tag	UNP Q8PYK9
B	468	ALA	-	expression tag	UNP Q8PYK9
B	469	ALA	-	expression tag	UNP Q8PYK9
B	470	ALA	-	expression tag	UNP Q8PYK9
B	471	LEU	-	expression tag	UNP Q8PYK9
B	472	GLU	-	expression tag	UNP Q8PYK9
B	473	HIS	-	expression tag	UNP Q8PYK9
B	474	HIS	-	expression tag	UNP Q8PYK9
B	475	HIS	-	expression tag	UNP Q8PYK9
B	476	HIS	-	expression tag	UNP Q8PYK9
B	477	HIS	-	expression tag	UNP Q8PYK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	HIS	-	expression tag	UNP Q8PYK9

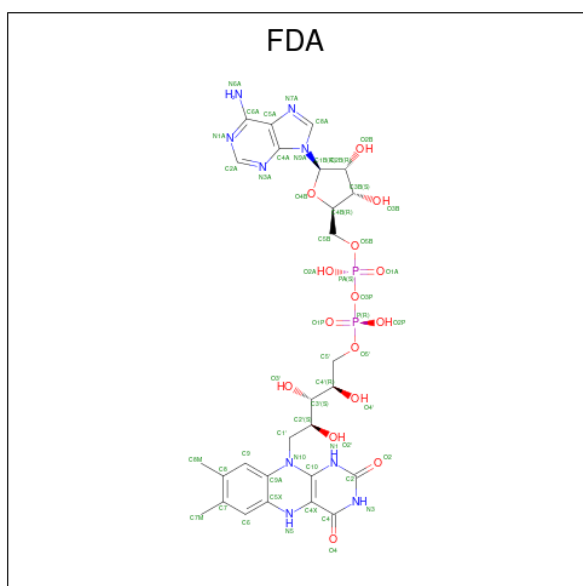
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			282	135	51	83	13			
2	E	12	Total	C	N	O	P	0	0	0
			244	115	44	73	12			

- Molecule 3 is a DNA chain called COUNTERSTRAND-OLIGONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			

- Molecule 4 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

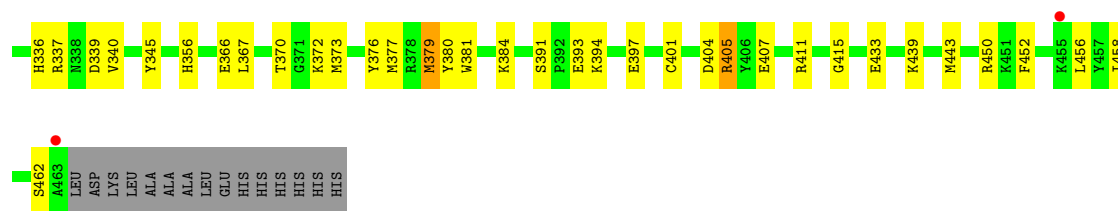
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



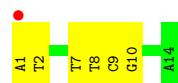
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

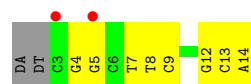
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	B	70	Total	O	0	0
			70	70		
6	C	11	Total	O	0	0
			11	11		
6	D	3	Total	O	0	0
			3	3		
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		



● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.20Å 117.76Å 170.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.29 – 2.35 31.29 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.9 (31.29-2.35) 83.3 (31.29-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.287 , 0.357 0.286 , 0.357	Depositor DCC
R_{free} test set	2576 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8638	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: SO4, FDA

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	0.47	0/3812	0.62	0/5154
1	B	0.42	0/3594	0.60	0/4859
2	C	0.51	0/315	0.65	0/484
2	E	0.50	0/272	0.73	0/417
3	D	0.55	0/321	0.59	0/494
3	F	0.39	0/321	0.50	0/494
All	All	0.45	0/8635	0.61	0/11902

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3713	0	3649	61	0
1	B	3496	0	3399	81	0
2	C	282	0	159	5	0
2	E	244	0	135	11	0
3	D	286	0	158	3	0
3	F	286	0	158	13	0
4	A	53	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	53	0	33	3	0
5	A	5	0	0	0	0
6	A	129	0	0	2	0
6	B	70	0	0	3	0
6	C	11	0	0	0	0
6	D	3	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
All	All	8638	0	7724	161	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 10.

All (161) 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:A:59:ASP:OD1	1:A:94:ARG:NH2	2.11	0.83
1:B:48:ASN:ND2	6:B:601:HOH:O	2.14	0.79
1:B:377:MET:HA	1:B:377:MET:HE2	1.66	0.78
1:A:117:PHE:HA	1:A:123:LYS:HZ1	1.47	0.77
1:A:445:TYR:OH	1:A:455:LYS:NZ	2.22	0.72
1:B:305:TRP:CE3	2:E:7:DT:H72	2.26	0.70
1:B:336:HIS:ND1	1:B:339:ASP:OD2	2.23	0.69
1:B:57:LEU:HD11	1:B:62:LEU:HG	1.74	0.69
1:A:218:LEU:HD12	1:A:222:ASP:HB3	1.73	0.69
1:A:21:VAL:HG21	1:A:43:ILE:HG13	1.75	0.69
1:B:157:GLU:HG3	1:B:163:PHE:HD1	1.59	0.68
1:A:142:ASP:OD2	1:A:148:PRO:HA	1.93	0.68
1:A:305:TRP:CE3	2:C:7:DT:H72	2.32	0.65
1:B:41:ARG:NH2	1:B:183:PRO:O	2.29	0.65
1:A:9:ARG:NH1	1:A:314:TYR:OH	2.29	0.64
1:A:305:TRP:CZ3	2:C:7:DT:H72	2.34	0.63
1:A:334:ASN:HA	1:A:337:ARG:HG3	1.81	0.63
1:A:89:PRO:HG3	1:A:188:PRO:HG3	1.81	0.63
1:B:157:GLU:HG3	1:B:163:PHE:CD1	2.34	0.63
1:A:218:LEU:HD22	1:A:467:LEU:HB3	1.83	0.60
1:B:244:PHE:CD1	1:B:265:SER:HA	2.36	0.60
1:B:439:LYS:NZ	3:F:10:DG:OP1	2.26	0.60
3:F:1:DT:H6	3:F:1:DT:H5'	1.67	0.60
1:B:9:ARG:NH1	1:B:314:TYR:OH	2.35	0.60
1:B:376:TYR:HD2	1:B:377:MET:HE3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:131:ILE:HG23	2.02	0.59
1:B:305:TRP:CD2	2:E:7:DT:H72	2.38	0.59
1:B:103:ARG:NH2	1:B:107:ASP:OD2	2.36	0.59
1:B:3:MET:HE1	1:B:39:PHE:HB2	1.83	0.58
2:C:9:DC:H2'	2:C:10:DG:C8	2.38	0.58
1:B:3:MET:HE3	1:B:8:ILE:HD11	1.85	0.58
2:E:9:DC:H42	3:F:7:DG:H1	1.49	0.58
1:B:86:LYS:HD2	1:B:181:LEU:HD23	1.85	0.58
1:B:450:ARG:NH2	2:E:12:DG:N7	2.52	0.58
1:B:241:MET:O	1:B:245:ILE:HG13	2.03	0.57
1:B:58:THR:HB	1:B:61:PHE:HB2	1.86	0.57
1:A:244:PHE:CD1	1:A:265:SER:HA	2.40	0.57
1:A:204:LEU:O	1:A:208:VAL:HG23	2.05	0.56
1:B:325:PHE:O	1:B:330:LYS:HE2	2.06	0.56
1:A:200:LEU:HA	1:A:203:VAL:HB	1.90	0.54
1:B:379:MET:HE3	1:B:443:MET:SD	2.48	0.54
1:A:45:LYS:NZ	1:A:182:GLU:OE1	2.42	0.53
3:F:12:DC:H2''	3:F:13:DG:C8	2.45	0.52
1:A:379:MET:SD	2:C:8:DT:C6	3.02	0.52
1:B:41:ARG:NH1	1:B:45:LYS:HB2	2.25	0.51
1:B:144:HIS:O	1:B:306:LYS:NZ	2.42	0.51
1:A:5:PRO:HA	1:A:8:ILE:HD12	1.93	0.51
3:F:3:DG:H2''	3:F:4:DC:OP2	2.10	0.51
1:B:379:MET:SD	2:E:8:DT:C6	3.04	0.50
1:A:387:GLU:OE2	1:A:442:TYR:HE1	1.95	0.50
1:B:380:TYR:CE1	1:B:384:LYS:HE2	2.47	0.50
1:A:268:SER:HB3	4:A:501:FDA:O2P	2.12	0.50
2:E:9:DC:N4	3:F:7:DG:H1	2.11	0.49
1:A:389:SER:OG	1:A:395:ALA:HB2	2.12	0.49
1:B:301:GLU:HB3	4:B:501:FDA:C8A	2.41	0.49
1:A:167:LEU:HD23	1:A:304:ILE:HD13	1.95	0.49
1:B:377:MET:HA	1:B:377:MET:CE	2.41	0.49
1:B:255:LEU:HD23	1:B:261:LYS:HG3	1.95	0.49
1:B:164:ARG:NH2	6:B:607:HOH:O	2.46	0.48
1:A:460:LYS:HD3	1:A:461:TYR:CZ	2.48	0.48
2:C:1:DA:H2'	2:C:2:DT:C6	2.48	0.48
1:A:168:TYR:HE1	1:A:304:ILE:HD11	1.78	0.48
1:A:153:SER:OG	1:A:157:GLU:OE2	2.29	0.48
1:A:347:LEU:HD13	1:A:398:ILE:HG23	1.94	0.48
1:B:74:LYS:HB3	1:B:232:PRO:HG2	1.96	0.48
1:B:373:MET:HE1	1:B:381:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DG:H4'	2:E:5:DG:OP1	2.13	0.48
1:A:37:LEU:HD12	1:A:37:LEU:O	2.14	0.48
1:A:177:GLU:OE2	1:A:280:ARG:NH1	2.44	0.48
1:A:384:LYS:HB3	1:A:388:TRP:CZ3	2.49	0.48
1:B:71:PHE:CD1	1:B:232:PRO:HB3	2.48	0.48
1:A:67:ARG:NH2	1:A:225:PHE:HB2	2.29	0.47
3:F:1:DT:H5'	3:F:1:DT:C6	2.47	0.47
1:B:15:LYS:O	1:B:137:PRO:HD3	2.15	0.47
1:A:58:THR:OG1	1:A:60:GLU:OE2	2.30	0.47
1:B:305:TRP:CZ3	2:E:7:DT:H72	2.50	0.47
1:B:303:LEU:HA	1:B:303:LEU:HD12	1.63	0.47
2:E:4:DG:H2''	2:E:5:DG:C8	2.50	0.47
3:F:7:DG:H8	3:F:7:DG:H5''	1.80	0.47
1:A:237:ALA:HB2	1:A:270:TYR:CD1	2.50	0.47
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.50	0.46
1:B:112:THR:HG23	1:B:137:PRO:HB2	1.96	0.46
1:B:255:LEU:HB2	1:B:263:MET:HG3	1.97	0.46
1:B:401:CYS:O	1:B:405:ARG:HB3	2.16	0.46
1:A:341:ARG:O	1:B:129:LYS:NZ	2.49	0.46
3:F:6:DC:H2'	3:F:7:DG:C8	2.51	0.46
1:A:261:LYS:HE3	6:A:601:HOH:O	2.15	0.46
1:B:30:ARG:HD3	1:B:274:GLY:O	2.16	0.46
1:A:43:ILE:HD12	1:A:112:THR:HG21	1.98	0.46
1:A:220:ASN:ND2	1:A:222:ASP:HB2	2.31	0.45
1:B:17:GLY:HA3	1:B:111:GLY:HA2	1.98	0.45
1:B:345:TYR:OH	1:B:356:HIS:ND1	2.40	0.45
3:D:1:DT:C6	3:D:2:DT:H72	2.52	0.45
1:B:366:GLU:O	1:B:370:THR:OG1	2.35	0.44
1:A:168:TYR:CE1	1:A:304:ILE:HD11	2.52	0.44
1:B:254:ALA:HB3	1:B:255:LEU:HD12	2.00	0.44
1:B:41:ARG:HH12	1:B:45:LYS:HB2	1.83	0.44
1:A:73:LEU:HD13	1:A:73:LEU:HA	1.73	0.44
1:B:259:PRO:HD2	1:B:452:PHE:CD2	2.53	0.44
1:A:255:LEU:HD12	1:A:263:MET:HG2	2.00	0.44
1:B:4:ASN:OD1	1:B:5:PRO:HD2	2.18	0.44
1:B:31:ALA:H	1:B:234:GLU:CD	2.26	0.44
3:D:7:DG:H2''	3:D:8:DA:C8	2.52	0.44
1:B:72:MET:HB3	1:B:72:MET:HE2	1.75	0.43
1:B:266:ASN:HA	1:B:372:LYS:HE3	1.99	0.43
1:B:15:LYS:HD3	1:B:15:LYS:HA	1.69	0.43
1:A:11:LEU:HD11	1:A:140:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:MET:O	1:A:245:ILE:HG13	2.19	0.43
1:B:10:ALA:HB2	1:B:139:PHE:CE1	2.53	0.43
2:E:13:DC:H2''	2:E:14:DA:O4'	2.18	0.43
1:B:299:LEU:O	1:B:303:LEU:HB2	2.18	0.43
2:E:9:DC:N3	3:F:7:DG:N2	2.59	0.43
1:A:341:ARG:CZ	1:A:436:VAL:HG13	2.48	0.43
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.73	0.43
1:A:75:GLY:O	1:A:79:LEU:N	2.40	0.42
3:F:8:DA:OP2	3:F:8:DA:H8	2.02	0.42
1:B:16[B]:GLN:H	1:B:16[B]:GLN:HG3	1.59	0.42
1:B:26:SER:OG	1:B:27:ARG:N	2.52	0.42
1:B:308:ILE:HA	1:B:311:ASN:HB3	2.01	0.42
1:B:394:LYS:HD3	1:B:397:GLU:OE1	2.19	0.42
1:B:39:PHE:CE1	1:B:43:ILE:HD11	2.54	0.42
1:B:415:GLY:HA2	4:B:501:FDA:C4X	2.50	0.42
1:B:23:TYR:HD2	1:B:53:VAL:HG22	1.83	0.42
1:B:391:SER:OG	1:B:394:LYS:HG2	2.19	0.42
1:B:458:ILE:O	1:B:462:SER:HB2	2.19	0.42
1:A:145:ASN:HB3	1:A:307:GLU:CD	2.44	0.42
1:A:332:SER:O	1:A:336:HIS:HD2	2.03	0.42
1:B:71:PHE:CE1	1:B:232:PRO:HB3	2.55	0.42
1:B:244:PHE:HB2	1:B:248:ARG:NH2	2.34	0.42
1:B:306:LYS:NZ	6:B:613:HOH:O	2.50	0.42
1:B:301:GLU:HB3	4:B:501:FDA:H8A	2.01	0.42
1:B:404:ASP:HB3	1:B:411:ARG:HG2	2.02	0.42
1:A:212:LEU:N	1:A:213:PRO:HD2	2.35	0.42
1:B:116:ASP:HB3	1:B:117:PHE:H	1.66	0.42
1:B:164:ARG:HA	1:B:304:ILE:HD12	2.01	0.42
1:B:367:LEU:HD11	1:B:407:GLU:HG2	2.01	0.42
1:B:337:ARG:HH22	1:B:393:GLU:CD	2.28	0.41
1:B:87:LYS:HB2	1:B:184:ASN:HB2	2.02	0.41
1:B:167:LEU:HD13	1:B:167:LEU:O	2.20	0.41
1:A:102:SER:HA	1:A:134:ILE:HD11	2.02	0.41
3:F:12:DC:H4'	3:F:13:DG:OP1	2.21	0.41
1:A:73:LEU:CD1	1:A:200:LEU:HD22	2.51	0.41
3:D:4:DC:H2''	3:D:5:DG:C8	2.56	0.41
1:A:7:ARG:O	1:A:141:VAL:HA	2.20	0.41
1:A:120:LEU:HA	1:A:120:LEU:HD23	1.76	0.41
1:B:52:VAL:HG22	1:B:89:PRO:HG2	2.03	0.41
1:B:79:LEU:HA	1:B:82:SER:HB3	2.03	0.41
1:B:336:HIS:NE2	1:B:433:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:N	1:A:114:VAL:O	2.44	0.41
1:B:53:VAL:O	1:B:90:SER:HA	2.21	0.41
1:A:73:LEU:HD11	1:A:200:LEU:HD22	2.03	0.40
1:B:314:TYR:HD2	1:B:315:TYR:CZ	2.39	0.40
1:A:266:ASN:HD22	1:A:372:LYS:HE3	1.85	0.40
1:B:305:TRP:HA	1:B:308:ILE:HG22	2.02	0.40
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.87	0.40
1:A:415:GLY:HA3	6:A:681:HOH:O	2.21	0.40
3:F:1:DT:H2'	3:F:2:DT:H72	2.03	0.40
1:A:106:LYS:HD3	1:A:106:LYS:HA	1.77	0.40
1:A:235:LYS:O	1:A:239:LYS:HG3	2.21	0.40
1:A:244:PHE:CD1	1:A:248:ARG:HB2	2.56	0.40
1:A:266:ASN:HA	1:A:372:LYS:HE3	2.04	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	454/498 (91%)	435 (96%)	18 (4%)	1 (0%)	43	52
1	B	425/498 (85%)	399 (94%)	25 (6%)	1 (0%)	43	52
All	All	879/996 (88%)	834 (95%)	43 (5%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASP
1	A	16	GLN

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	397/429 (92%)	374 (94%)	23 (6%)	18	22
1	B	373/429 (87%)	355 (95%)	18 (5%)	23	29
All	All	770/858 (90%)	729 (95%)	41 (5%)	20	25

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	SER
1	A	62	LEU
1	A	85	ARG
1	A	90	SER
1	A	134	ILE
1	A	186	VAL
1	A	203	VAL
1	A	204	LEU
1	A	222	ASP
1	A	224	LEU
1	A	243	SER
1	A	250	ASP
1	A	256	ARG
1	A	263	MET
1	A	300	ASP
1	A	302	ILE
1	A	349	GLU
1	A	355	THR
1	A	387	GLU
1	A	403	ASN
1	A	419	ILE
1	A	456	LEU
1	B	13	SER
1	B	15	LYS
1	B	26	SER
1	B	48	ASN

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Mol	Chain	Res	Type
1	B	58	THR
1	B	61	PHE
1	B	66	ILE
1	B	73	LEU
1	B	90	SER
1	B	131	ILE
1	B	234	GLU
1	B	261	LYS
1	B	290	SER
1	B	310	ASP
1	B	340	VAL
1	B	379	MET
1	B	405	ARG
1	B	456	LEU

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

Mol	Chain	Res	Type
1	A	161	HIS
1	A	262	ASN
1	A	266	ASN
1	B	29	GLN
1	B	374	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	FDA	A	501	-	57,58,58	0.61	0	78,89,89	0.76	2 (2%)
5	SO4	A	502	-	4,4,4	0.47	0	6,6,6	0.10	0
4	FDA	B	501	-	57,58,58	0.52	0	78,89,89	0.67	3 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FDA	A	501	-	-	2/34/50/50	0/6/6/6
4	FDA	B	501	-	-	6/34/50/50	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	FDA	C2'-C1'-N10	2.64	122.67	110.20
4	A	501	FDA	C2'-C1'-N10	2.50	122.00	110.20
4	A	501	FDA	N3-C2-N1	2.36	119.45	115.74
4	B	501	FDA	N3-C2-N1	2.26	119.29	115.74
4	B	501	FDA	O2-C2-N3	-2.07	118.18	121.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	FDA	C5B-O5B-PA-O1A
4	B	501	FDA	C5B-O5B-PA-O3P
4	A	501	FDA	O4'-C4'-C5'-O5'
4	B	501	FDA	C5B-O5B-PA-O2A
4	B	501	FDA	C4'-C5'-O5'-P

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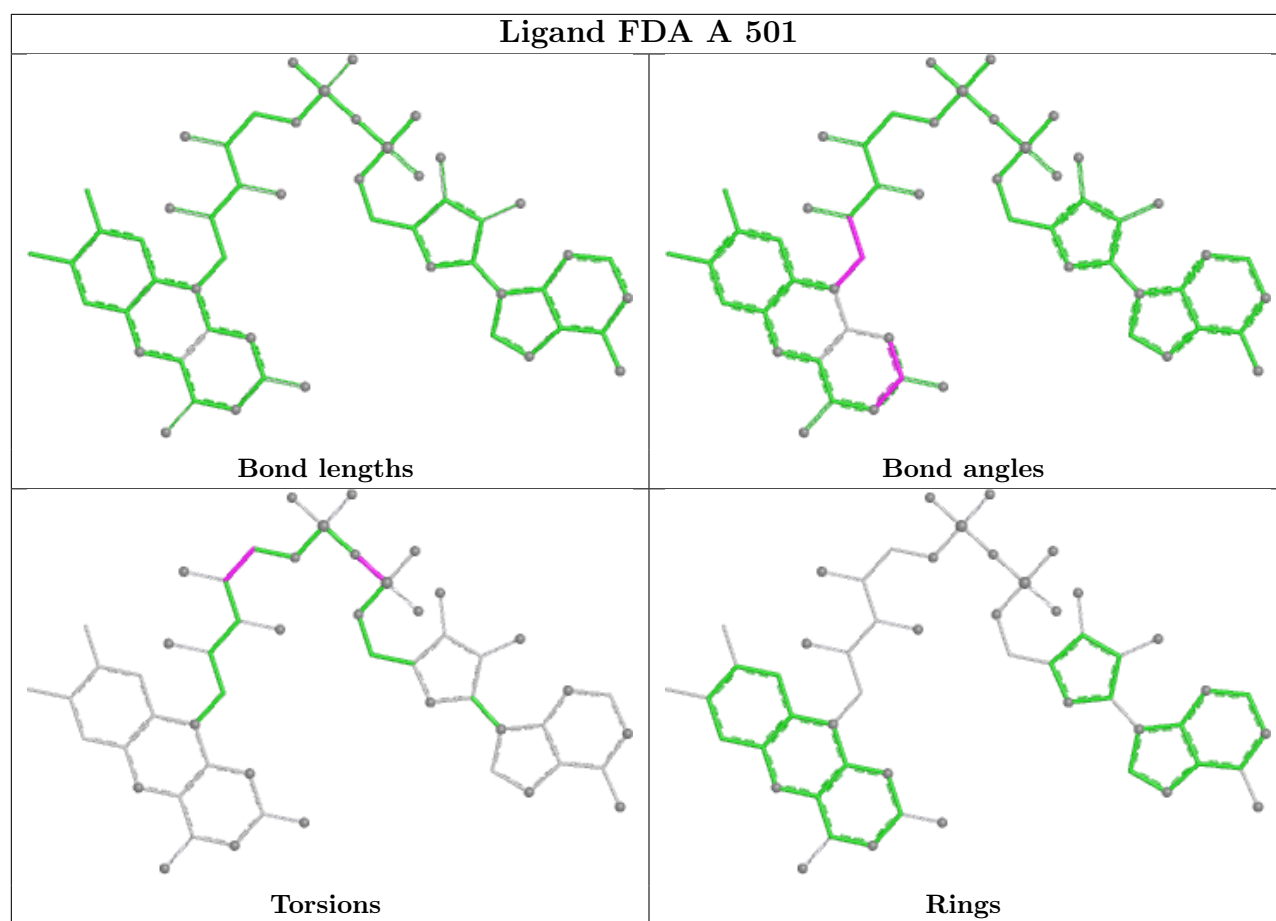
Mol	Chain	Res	Type	Atoms
4	B	501	FDA	P-O3P-PA-O1A
4	B	501	FDA	P-O3P-PA-O2A
4	A	501	FDA	P-O3P-PA-O2A

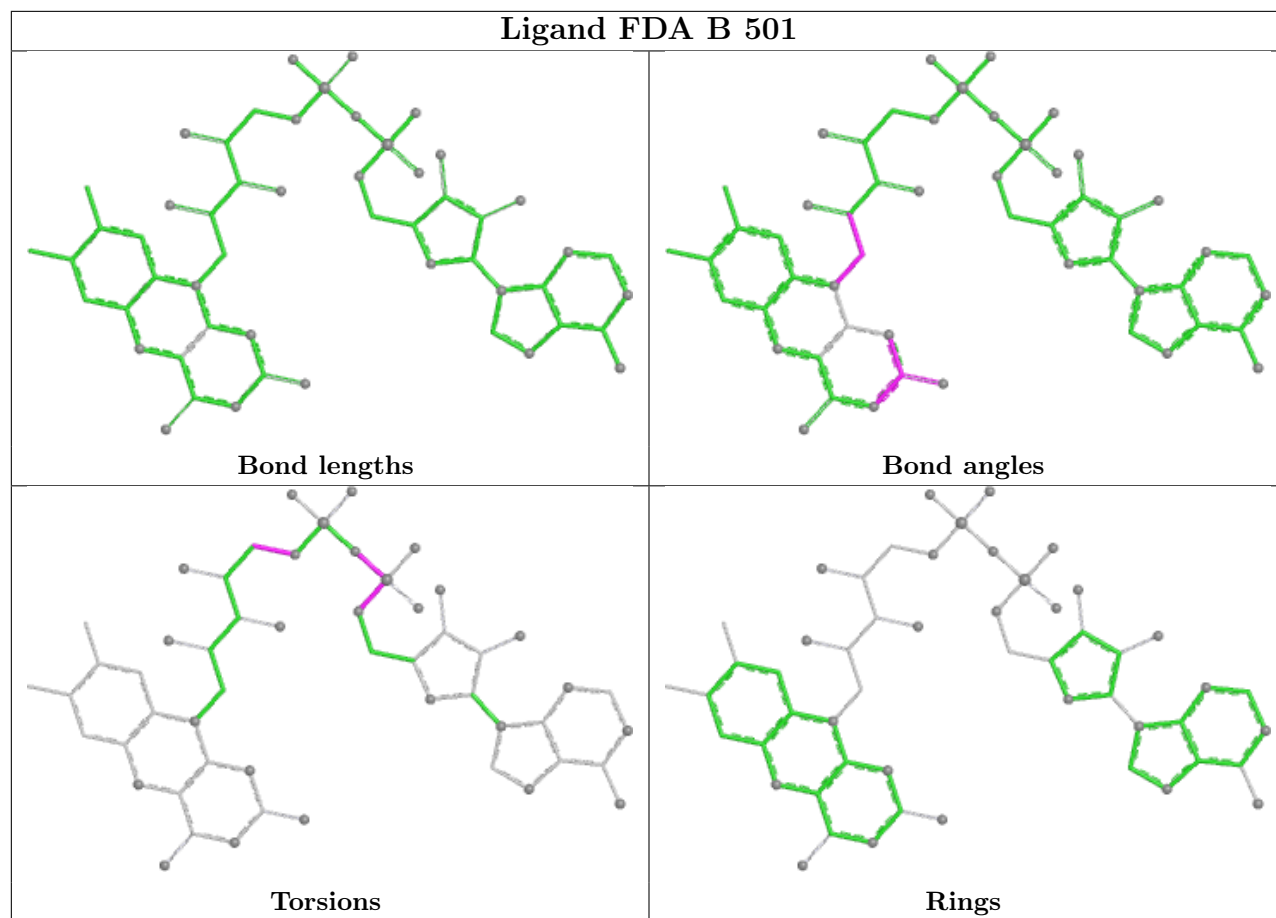
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	FDA	1	0
4	B	501	FDA	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/498 (91%)	0.62	28 (6%) 27 31	23, 37, 69, 85	0
1	B	428/498 (85%)	1.05	51 (11%) 9 10	28, 53, 78, 120	1 (0%)
2	C	14/14 (100%)	0.47	1 (7%) 22 25	34, 56, 90, 90	0
2	E	12/14 (85%)	0.80	2 (16%) 4 4	45, 65, 107, 119	0
3	D	14/14 (100%)	0.78	0 100 100	43, 59, 73, 80	0
3	F	14/14 (100%)	1.16	2 (14%) 6 7	62, 74, 108, 123	0
All	All	940/1052 (89%)	0.83	84 (8%) 15 17	23, 45, 76, 123	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	ASP	6.0
1	A	2	ILE	5.1
1	B	61	PHE	4.7
1	B	463	ALA	3.9
1	B	62	LEU	3.6
1	B	55	PHE	3.5
1	A	105	VAL	3.5
1	B	64	ALA	3.5
1	B	253	GLY	3.3
1	B	39	PHE	3.3
1	B	108	TYR	3.3
1	B	177	GLU	3.2
1	B	159	ALA	3.2
1	B	60	GLU	3.1
1	A	203	VAL	3.1
1	A	221	LYS	3.1
1	A	218	LEU	3.0
1	B	49	VAL	3.0
1	A	468	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	69	TYR	2.9
1	B	45	LYS	2.8
1	B	14	GLY	2.8
1	B	48	ASN	2.8
1	A	469	ALA	2.8
1	A	91	PHE	2.8
1	B	455	LYS	2.7
1	A	108	TYR	2.7
1	B	135	SER	2.7
1	B	57	LEU	2.7
1	B	113	LEU	2.7
1	A	14	GLY	2.7
1	B	175	LEU	2.7
1	A	463	ALA	2.6
1	B	186	VAL	2.6
1	B	160	ALA	2.6
1	B	237	ALA	2.6
1	A	18	ASP	2.6
1	B	93	LEU	2.6
1	B	35	TRP	2.6
1	B	257	ASN	2.6
1	B	136	ILE	2.6
1	B	42	ALA	2.5
1	A	95	GLY	2.5
1	A	106	LYS	2.5
1	B	16[A]	GLN	2.5
1	B	302	ILE	2.5
1	A	464	LEU	2.5
1	B	127	ILE	2.5
1	B	188	PRO	2.5
1	B	94	ARG	2.4
1	B	169	ALA	2.4
1	A	199	THR	2.4
1	B	47	ALA	2.4
1	B	3	MET	2.4
1	A	17	GLY	2.3
1	B	58	THR	2.3
1	B	90	SER	2.3
1	B	131	ILE	2.3
1	B	104	PHE	2.3
1	B	224	LEU	2.3
3	F	5	DG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLU	2.3
1	B	101	ILE	2.3
2	E	3	DC	2.3
2	E	5	DG	2.3
1	A	187	THR	2.3
1	B	222	ASP	2.2
1	B	116	ASP	2.2
1	A	62	LEU	2.2
1	A	136	ILE	2.2
1	B	66	ILE	2.2
1	B	138	PHE	2.2
1	B	141	VAL	2.1
1	A	467	LEU	2.1
1	A	186	VAL	2.1
1	A	104	PHE	2.1
1	B	181	LEU	2.1
2	C	1	DA	2.1
1	A	219	LYS	2.1
3	F	4	DC	2.1
1	B	282	VAL	2.1
1	A	109	ASN	2.0
1	A	214	GLU	2.0
1	A	134	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

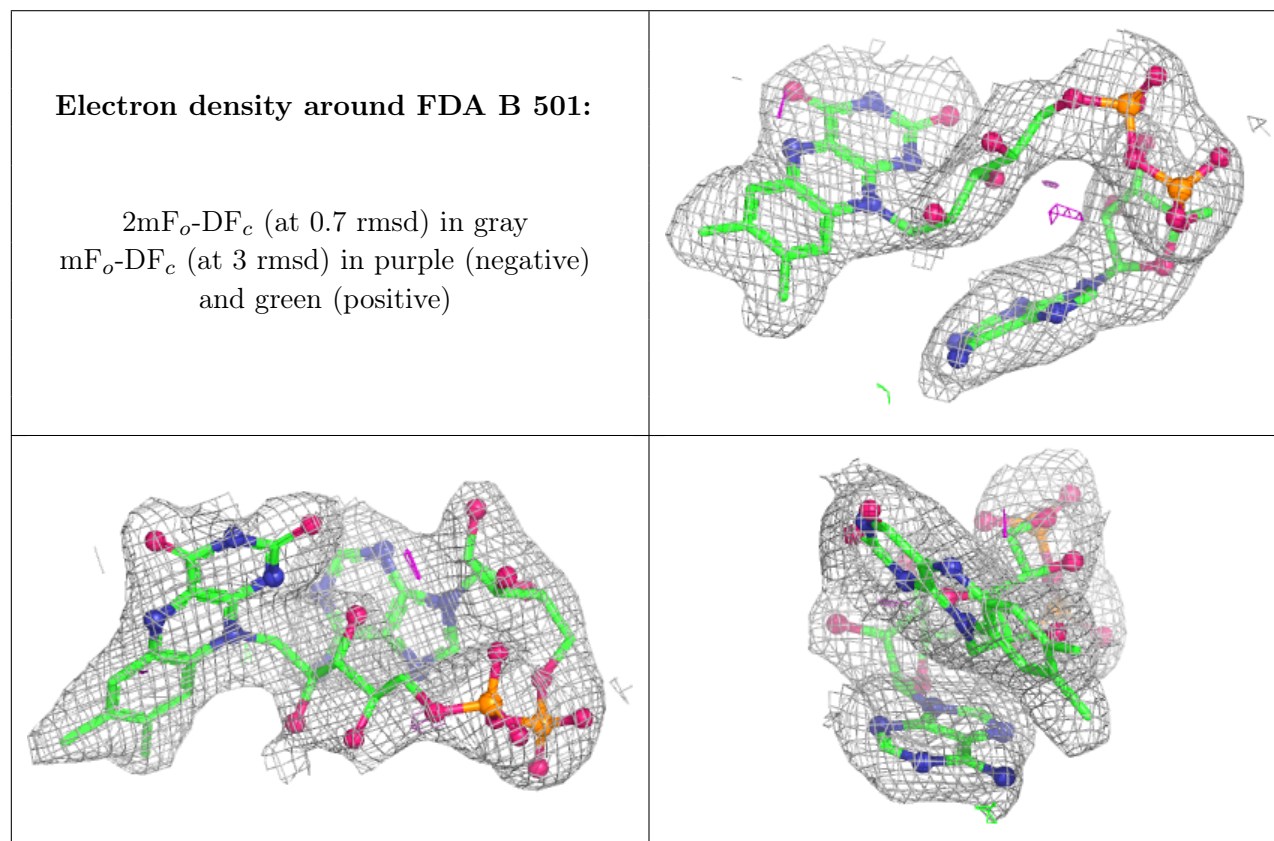
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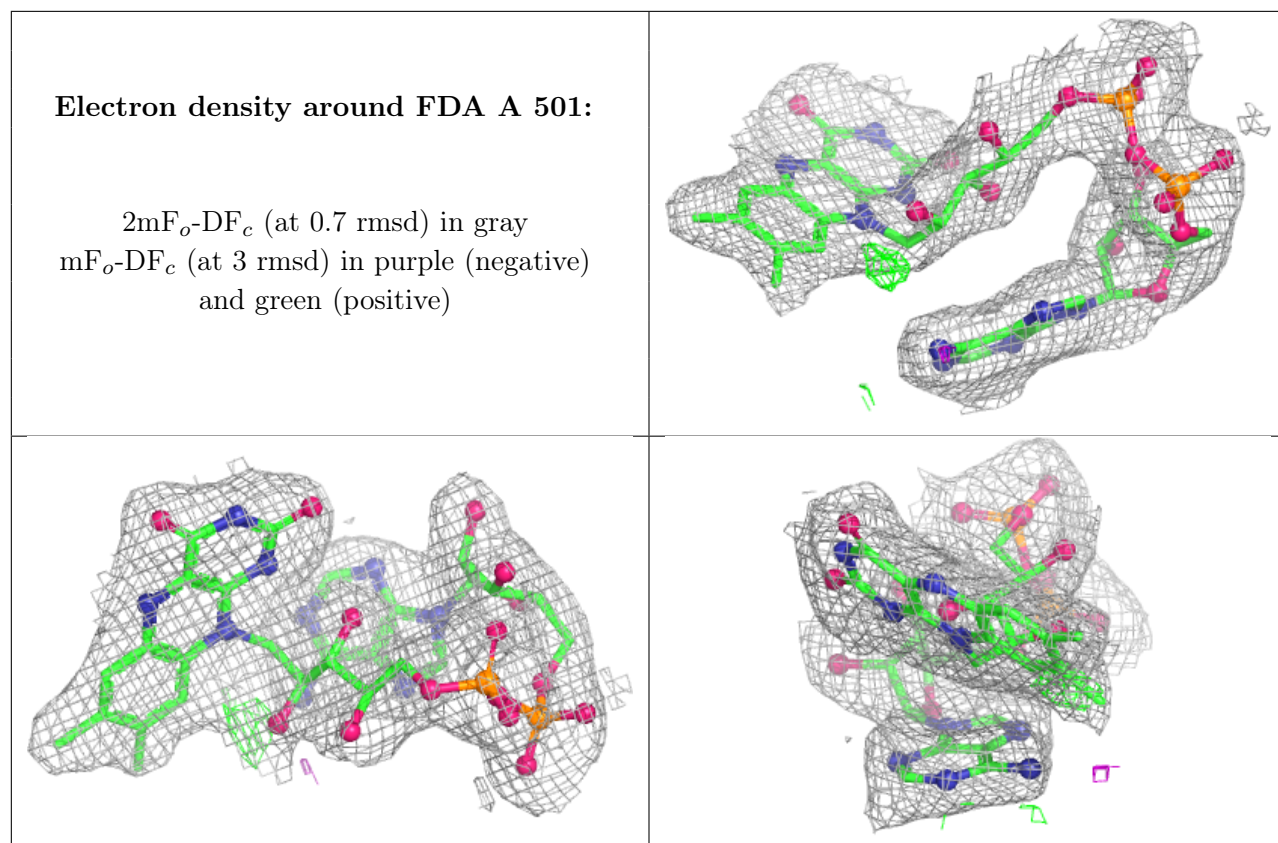
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FDA	B	501	53/53	0.94	0.09	29,38,45,50	0
4	FDA	A	501	53/53	0.96	0.08	18,27,32,36	0
5	SO4	A	502	5/5	0.96	0.10	37,39,40,41	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 [i](#)

There are no such residues in this entry.