



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:23 am GMT

PDB ID : 8OY8
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (30 nanosecond timepoint)
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 : 2.39 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158

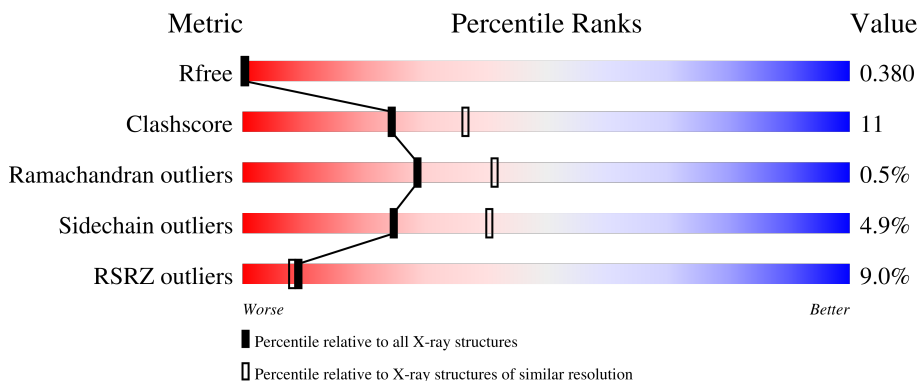
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

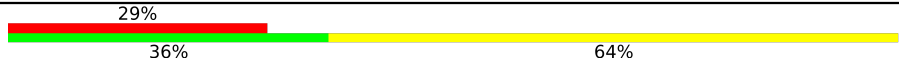

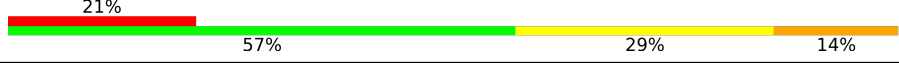
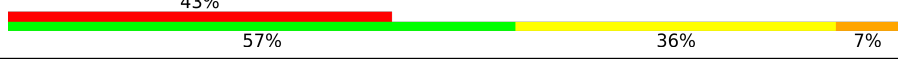
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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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CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	C	14	
2	E	14	
3	D	14	
3	F	14	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8594 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
			Total	C	N	O	S			
1	A	460	3738	2404	630	689	15	0	1	0
1	B	429	3496	2248	590	643	15	0	0	0

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

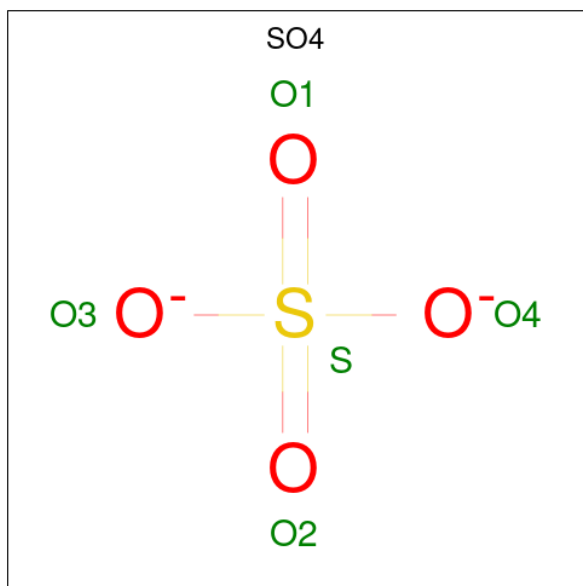
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

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

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

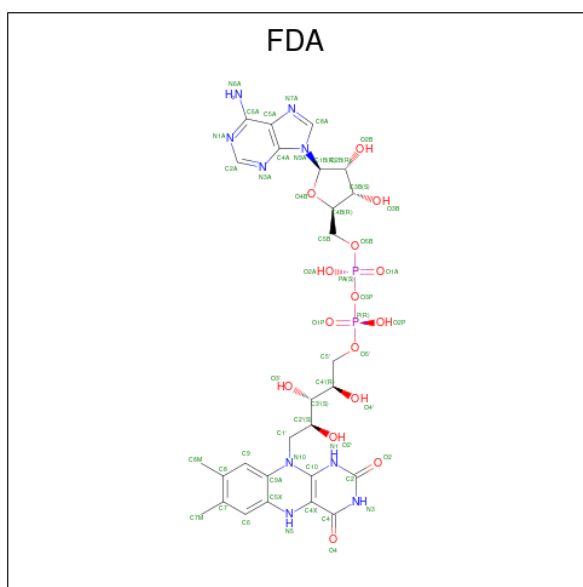
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	286	136	56	81	13	0	0	0
3	F	14	286	136	56	81	13	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

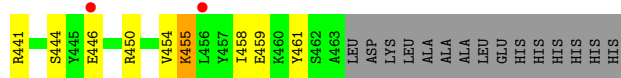
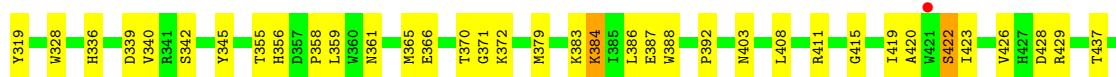
- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



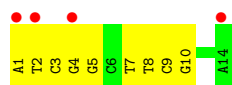
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is water.

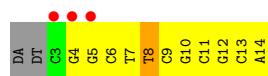
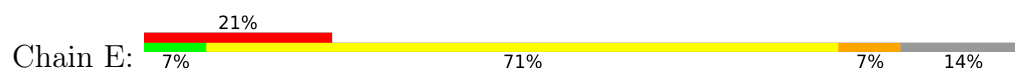
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	39	Total	O	0	0
			39	39		
6	C	8	Total	O	0	0
			8	8		
6	D	6	Total	O	0	0
			6	6		
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		



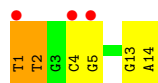
- Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



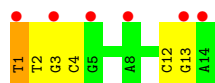
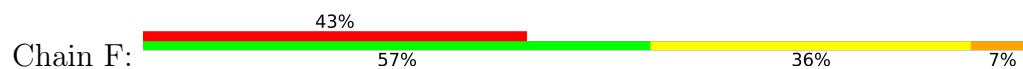
- Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



- 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 – 2.39 31.29 – 2.39	Depositor EDS
% Data completeness (in resolution range)	83.2 (31.29-2.39) 83.3 (31.29-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.310 , 0.382 0.310 , 0.380	Depositor DCC
R_{free} test set	2399 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.58	0/3837	0.74	0/5187
1	B	0.51	0/3594	0.66	0/4858
2	C	1.04	0/315	1.09	1/484 (0.2%)
2	E	0.95	0/272	1.06	1/417 (0.2%)
3	D	1.12	2/321 (0.6%)	1.04	0/494
3	F	0.93	0/321	0.95	1/494 (0.2%)
All	All	0.64	2/8660 (0.0%)	0.76	3/11934 (0.0%)

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	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	DT	C3'-O3'	-5.07	1.37	1.44
3	D	2	DT	C3'-O3'	-5.05	1.37	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	8	DT	O4'-C1'-N1	6.20	112.34	108.00
2	C	8	DT	O4'-C1'-N1	5.64	111.95	108.00
3	F	1	DT	N3-C4-O4	5.02	122.91	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	ARG	Sidechain

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	3738	0	3676	77	0
1	B	3496	0	3405	78	0
2	C	282	0	159	6	0
2	E	244	0	135	10	0
3	D	286	0	158	5	0
3	F	286	0	158	4	0
4	A	5	0	0	1	0
5	A	53	0	33	1	0
5	B	53	0	33	2	0
6	A	91	0	0	3	0
6	B	39	0	0	4	0
6	C	8	0	0	0	0
6	D	6	0	0	1	0
6	E	4	0	0	1	0
6	F	3	0	0	1	0
All	All	8594	0	7757	175	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 11.

All (175) 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:33:ASP:OD2	1:B:280:ARG:HD2	1.86	0.75
1:A:446:GLU:N	1:A:446:GLU:OE1	2.22	0.73
3:F:12:DC:H2''	3:F:13:DG:C8	2.24	0.73
1:B:359:LEU:HD13	1:B:454:VAL:HG13	1.71	0.72
3:D:1:DT:H5''	3:D:2:DT:OP2	1.90	0.71
5:A:502:FDA:H5'2	5:A:502:FDA:H3B	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TYR:OH	1:B:356:HIS:ND1	2.26	0.69
3:D:13:DG:N3	6:D:101:HOH:O	2.27	0.68
1:A:451:LYS:NZ	2:C:9:DC:OP1	2.27	0.67
1:A:379:MET:HG3	1:A:421:TRP:HZ3	1.61	0.65
1:A:77:GLN:HG3	1:A:200:LEU:HD23	1.79	0.64
1:B:59:ASP:HA	1:B:62:LEU:HB3	1.79	0.63
1:A:411:ARG:HH11	1:A:411:ARG:HG3	1.62	0.63
1:B:336:HIS:ND1	1:B:339:ASP:OD2	2.31	0.63
1:A:348:GLU:OE1	1:A:348:GLU:N	2.31	0.62
1:A:86:LYS:HB2	1:A:88:ILE:HD12	1.82	0.61
1:B:52:VAL:HG12	1:B:89:PRO:HG2	1.82	0.61
1:B:420:ALA:HB1	1:B:426:VAL:HG21	1.83	0.61
2:C:2:DT:H4'	2:C:3:DC:H5'	1.82	0.61
1:A:212:LEU:HD23	1:A:215:ARG:HD2	1.82	0.61
1:B:67:ARG:HH21	1:B:222:ASP:HB3	1.66	0.61
1:B:366:GLU:HG3	1:B:461:TYR:CZ	2.35	0.61
1:B:7:ARG:HG2	1:B:148:PRO:HG3	1.83	0.60
1:B:450:ARG:NH2	2:E:12:DG:N7	2.49	0.60
1:B:455:LYS:O	1:B:459:GLU:HG2	2.02	0.59
1:B:144:HIS:O	1:B:306:LYS:NZ	2.36	0.59
1:B:358:PRO:HB2	1:B:458:ILE:HD13	1.84	0.58
1:A:124:ASN:O	1:A:128:GLU:HG2	2.04	0.57
1:A:155:LYS:HG2	1:A:156:HIS:H	1.69	0.57
1:B:177:GLU:OE1	1:B:280:ARG:NH2	2.38	0.57
1:B:93:LEU:HB3	1:B:100:LYS:NZ	2.20	0.57
1:A:323:GLU:HB3	6:B:612:HOH:O	2.05	0.56
1:A:352:ALA:HB3	1:A:354[B]:LYS:HE3	1.87	0.56
1:A:244:PHE:CD1	1:A:265:SER:HA	2.41	0.55
1:B:268:SER:OG	1:B:269:PRO:HD3	2.06	0.55
2:C:1:DA:H2''	2:C:2:DT:O4'	2.06	0.55
1:A:280:ARG:O	1:A:284:GLU:HG2	2.07	0.55
1:B:244:PHE:HB2	1:B:248:ARG:HH21	1.72	0.55
2:E:9:DC:H2''	2:E:10:DG:H5'	1.87	0.55
1:B:361:ASN:O	1:B:365:MET:HG2	2.06	0.54
2:E:14:DA:H2'	2:E:14:DA:OP2	2.06	0.54
2:C:9:DC:H2'	2:C:10:DG:C8	2.43	0.54
5:B:501:FDA:H5'2	5:B:501:FDA:H3B	1.88	0.54
1:B:112:THR:HG22	1:B:137:PRO:HD2	1.90	0.54
1:A:411:ARG:HH11	1:A:411:ARG:CG	2.20	0.54
1:B:28:ASP:HA	1:B:274:GLY:HA3	1.89	0.54
1:B:383:LYS:NZ	1:B:441:ARG:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:HA	1:A:337:ARG:HG3	1.90	0.53
1:A:230:PHE:CZ	1:A:372:LYS:HD3	2.43	0.53
1:A:379:MET:HG3	1:A:421:TRP:CZ3	2.42	0.53
1:A:218:LEU:CD1	1:A:224:LEU:HD13	2.38	0.53
1:A:327:SER:O	1:A:331:GLU:HG3	2.09	0.53
1:A:157:GLU:HG3	1:A:163:PHE:CD1	2.45	0.52
2:E:13:DC:H2''	2:E:14:DA:C8	2.44	0.52
1:A:12:LYS:HD2	1:A:131:ILE:HG23	1.91	0.52
1:A:33:ASP:HB2	6:A:668:HOH:O	2.10	0.52
1:A:55:PHE:HB3	1:A:92:PHE:CD1	2.44	0.52
1:A:376:TYR:HH	1:A:451:LYS:HZ2	1.56	0.52
1:A:412:ASP:OD1	1:A:414:ASN:HB2	2.10	0.52
1:A:367:LEU:HB2	1:A:373:MET:HE3	1.92	0.52
1:A:55:PHE:HB3	1:A:92:PHE:HD1	1.75	0.51
1:B:21:VAL:HG22	1:B:112:THR:OG1	2.09	0.51
1:A:431:TRP:CD1	1:A:441:ARG:HB2	2.45	0.51
1:B:386:LEU:HD22	1:B:437:THR:HG22	1.92	0.51
1:B:103:ARG:O	1:B:107:ASP:HB2	2.11	0.51
3:D:13:DG:H2''	3:D:14:DA:N7	2.26	0.51
1:B:86:LYS:NZ	6:B:604:HOH:O	2.44	0.51
1:B:446:GLU:OE2	2:E:11:DC:OP2	2.29	0.51
1:B:87:LYS:HB3	1:B:184:ASN:HB2	1.94	0.50
1:A:365:MET:HB3	1:A:464:LEU:HD12	1.94	0.49
1:B:12:LYS:HE2	1:B:134:ILE:O	2.12	0.49
1:A:15:LYS:O	1:A:137:PRO:HD3	2.13	0.49
1:B:312:PHE:CE2	1:B:319:TYR:HB2	2.47	0.49
1:B:37:LEU:HD11	1:B:83:LEU:HD21	1.93	0.49
1:B:415:GLY:HA2	5:B:501:FDA:C4X	2.43	0.48
1:A:16:GLN:HG2	1:A:112:THR:CG2	2.43	0.48
1:B:3:MET:HG2	1:B:35:TRP:CZ3	2.48	0.48
1:B:30:ARG:NH2	1:B:277:SER:HB2	2.29	0.48
1:B:241:MET:O	1:B:245:ILE:HG13	2.14	0.48
2:E:8:DT:OP1	6:E:101:HOH:O	2.20	0.48
1:A:22:VAL:HG23	1:A:52:VAL:HG23	1.95	0.48
1:A:89:PRO:HG2	1:A:188:PRO:HG2	1.94	0.48
1:A:218:LEU:HD12	1:A:224:LEU:HD13	1.96	0.48
1:A:67:ARG:NE	4:A:501:SO4:O3	2.45	0.47
1:A:212:LEU:O	1:A:215:ARG:HB2	2.14	0.47
1:B:392:PRO:HD2	6:B:610:HOH:O	2.13	0.47
1:A:131:ILE:HG12	1:A:138:PHE:HD2	1.80	0.47
1:A:17:GLY:CA	1:A:111:GLY:HA2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PHE:CE2	1:B:167:LEU:HD12	2.50	0.47
1:A:379:MET:HE3	1:A:379:MET:HB3	1.88	0.47
1:B:115:THR:O	1:B:140:GLU:HA	2.15	0.46
1:A:454:VAL:HG12	1:A:458:ILE:HD12	1.96	0.46
1:B:93:LEU:HB3	1:B:100:LYS:HZ3	1.81	0.46
1:B:35:TRP:CH2	1:B:179:PRO:HD2	2.51	0.46
1:A:168:TYR:CE1	1:A:304:ILE:HD11	2.52	0.45
1:A:389:SER:OG	1:A:395:ALA:HB2	2.17	0.45
1:A:404:ASP:HB3	1:A:411:ARG:HG2	1.97	0.45
2:C:4:DG:H2''	2:C:5:DG:C8	2.51	0.45
1:A:128:GLU:HG3	1:B:340:VAL:HG22	1.98	0.45
1:A:168:TYR:HE1	1:A:304:ILE:HD11	1.82	0.45
1:A:161:HIS:HB3	2:C:7:DT:OP2	2.17	0.45
1:B:117:PHE:HE1	1:B:314:TYR:CE2	2.35	0.44
1:A:199:THR:O	1:A:203:VAL:HG23	2.16	0.44
1:A:365:MET:HB2	1:A:461:TYR:HB3	1.99	0.44
1:B:12:LYS:HB3	1:B:138:PHE:HB3	1.98	0.44
1:B:371:GLY:HA3	1:B:408:LEU:HG	2.00	0.44
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.89	0.44
1:B:77:GLN:O	1:B:81:VAL:HG23	2.17	0.44
1:B:257:ASN:O	1:B:259:PRO:HD3	2.18	0.44
1:A:265:SER:HB3	1:A:298:PHE:HE1	1.83	0.43
1:B:64:ALA:HB2	1:B:411:ARG:NH1	2.32	0.43
1:B:164:ARG:NH2	2:E:7:DT:OP2	2.46	0.43
1:B:176:GLU:H	1:B:279:GLN:HE21	1.66	0.43
1:B:266:ASN:HA	1:B:372:LYS:HE3	1.99	0.43
3:F:3:DG:H2''	3:F:4:DC:OP2	2.17	0.43
1:A:384:LYS:HB3	1:A:388:TRP:CZ3	2.52	0.43
1:B:299:LEU:O	1:B:303:LEU:HB2	2.17	0.43
1:A:347:LEU:HG	1:A:398:ILE:HG12	1.99	0.43
1:B:384:LYS:HD2	1:B:384:LYS:HA	1.76	0.43
1:B:379:MET:O	1:B:383:LYS:HG3	2.18	0.43
1:A:58:THR:HG22	1:A:95:GLY:O	2.19	0.43
1:B:19:GLY:HA3	1:B:109:ASN:O	2.18	0.43
1:B:244:PHE:CD1	1:B:265:SER:HA	2.54	0.43
1:B:384:LYS:NZ	1:B:387:GLU:OE1	2.32	0.43
1:B:223:PRO:HG2	1:B:224:LEU:HG	2.00	0.43
1:B:428:ASP:CG	1:B:429:ARG:H	2.23	0.43
1:B:444:SER:HB2	1:B:446:GLU:OE1	2.19	0.43
3:D:13:DG:H2''	3:D:14:DA:C8	2.53	0.43
1:A:122:ILE:HD12	1:A:122:ILE:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.91	0.42
1:B:176:GLU:H	1:B:279:GLN:NE2	2.18	0.42
1:B:303:LEU:HA	1:B:303:LEU:HD23	1.82	0.42
1:A:27:ARG:NH2	1:A:413:PRO:HG2	2.34	0.42
1:A:373:MET:HB3	1:A:378:ARG:HG2	2.02	0.42
3:D:4:DC:H2''	3:D:5:DG:C8	2.55	0.42
1:B:168:TYR:CE1	1:B:304:ILE:HD11	2.54	0.42
1:A:37:LEU:HD12	1:A:37:LEU:O	2.20	0.42
1:A:24:TRP:CZ2	1:A:97:PRO:HB3	2.54	0.42
1:A:155:LYS:HG2	1:A:156:HIS:N	2.35	0.42
1:A:217:LEU:HD23	1:A:223:PRO:HA	2.02	0.42
1:B:74:LYS:HB3	1:B:232:PRO:HG2	2.02	0.42
1:B:110:ALA:O	1:B:136:ILE:HG21	2.20	0.42
1:B:419:ILE:HG23	1:B:423:ILE:HD12	2.02	0.42
2:E:7:DT:H6	2:E:7:DT:H2'	1.72	0.42
1:B:122:ILE:HG13	1:B:126:TRP:CZ2	2.55	0.41
1:B:230:PHE:HE2	1:B:370:THR:O	2.03	0.41
1:A:291:ASN:OD1	1:A:292:PRO:HD2	2.20	0.41
1:A:177:GLU:OE2	1:A:280:ARG:NH1	2.46	0.41
1:A:218:LEU:HD11	1:A:224:LEU:HD13	2.02	0.41
1:B:29:GLN:HE22	1:B:72:MET:HG3	1.86	0.41
1:B:144:HIS:HB2	6:B:628:HOH:O	2.20	0.41
1:B:97:PRO:O	1:B:101:ILE:HG12	2.20	0.41
1:A:299:LEU:O	1:A:303:LEU:HB2	2.20	0.41
1:B:74:LYS:HB2	1:B:74:LYS:HE2	1.71	0.41
2:E:4:DG:H1	3:F:12:DC:H42	1.69	0.41
1:A:8:ILE:HD13	1:A:39:PHE:CZ	2.55	0.41
1:A:121:ARG:HD3	1:A:317:PRO:O	2.21	0.41
1:A:326:PRO:HD3	1:A:426:VAL:HG22	2.02	0.41
1:B:383:LYS:HE2	1:B:422:SER:HA	2.03	0.41
1:B:384:LYS:HG3	1:B:388:TRP:CH2	2.55	0.41
1:A:127:ILE:O	1:A:131:ILE:HG13	2.20	0.41
1:A:272:HIS:ND1	1:A:412:ASP:OD2	2.37	0.41
1:A:24:TRP:N	1:A:114:VAL:O	2.49	0.40
1:B:328:TRP:HD1	6:F:101:HOH:O	2.05	0.40
1:A:9:ARG:NH2	6:A:604:HOH:O	2.51	0.40
1:B:24:TRP:C	1:B:24:TRP:CD1	2.92	0.40
1:A:19:GLY:HA3	1:A:109:ASN:O	2.22	0.40
1:A:116:ASP:HB2	6:A:629:HOH:O	2.21	0.40
1:B:386:LEU:HD12	1:B:423:ILE:HA	2.03	0.40
1:A:217:LEU:HD22	1:A:221:LYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD13	1:A:454:VAL:HG13	2.04	0.40
1:B:7:ARG:NH1	1:B:174:PHE:HD2	2.19	0.40
3:F:1:DT:H2''	3:F:2:DT:O5'	2.22	0.40
1:A:73:LEU:CB	1:A:204:LEU:HD13	2.52	0.40
2:E:5:DG:H2'	2:E:6:DC:C6	2.57	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	457/498 (92%)	436 (95%)	20 (4%)	1 (0%)	47 62
1	B	425/498 (85%)	400 (94%)	22 (5%)	3 (1%)	22 32
All	All	882/996 (89%)	836 (95%)	42 (5%)	4 (0%)	29 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	GLU
1	B	13	SER
1	A	59	ASP
1	B	222	ASP

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	400/429 (93%)	388 (97%)	12 (3%)	41	61
1	B	373/429 (87%)	347 (93%)	26 (7%)	15	24
All	All	773/858 (90%)	735 (95%)	38 (5%)	25	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	57	LEU
1	A	109	ASN
1	A	132	SER
1	A	198	GLU
1	A	215	ARG
1	A	222	ASP
1	A	224	LEU
1	A	250	ASP
1	A	290	SER
1	A	379	MET
1	A	411	ARG
1	B	6	LYS
1	B	60	GLU
1	B	61	PHE
1	B	62	LEU
1	B	67	ARG
1	B	84	SER
1	B	85	ARG
1	B	90	SER
1	B	105	VAL
1	B	107	ASP
1	B	166	LYS
1	B	171	LEU
1	B	222	ASP
1	B	224	LEU
1	B	255	LEU
1	B	256	ARG
1	B	277	SER
1	B	280	ARG
1	B	290	SER
1	B	300	ASP
1	B	342	SER
1	B	355	THR
1	B	384	LYS

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Mol	Chain	Res	Type
1	B	403	ASN
1	B	422	SER
1	B	455	LYS

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	262	ASN
1	A	266	ASN
1	B	262	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 monosaccharides 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
5	FDA	B	501	-	52,58,58	0.63	0	60,89,89	0.74	2 (3%)
5	FDA	A	502	-	52,58,58	0.63	0	60,89,89	0.85	4 (6%)
4	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.94	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
5	FDA	B	501	-	-	7/30/50/50	0/6/6/6
5	FDA	A	502	-	-	4/30/50/50	0/6/6/6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	FDA	N3-C2-N1	2.38	119.63	115.80
5	A	502	FDA	O2-C2-N3	-2.20	117.67	121.82
5	B	501	FDA	C5A-C6A-N6A	2.19	123.69	120.35
5	B	501	FDA	N3-C2-N1	2.11	119.19	115.80
5	A	502	FDA	C5A-C6A-N6A	2.08	123.51	120.35
5	A	502	FDA	O2B-C2B-C3B	-2.05	105.20	111.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

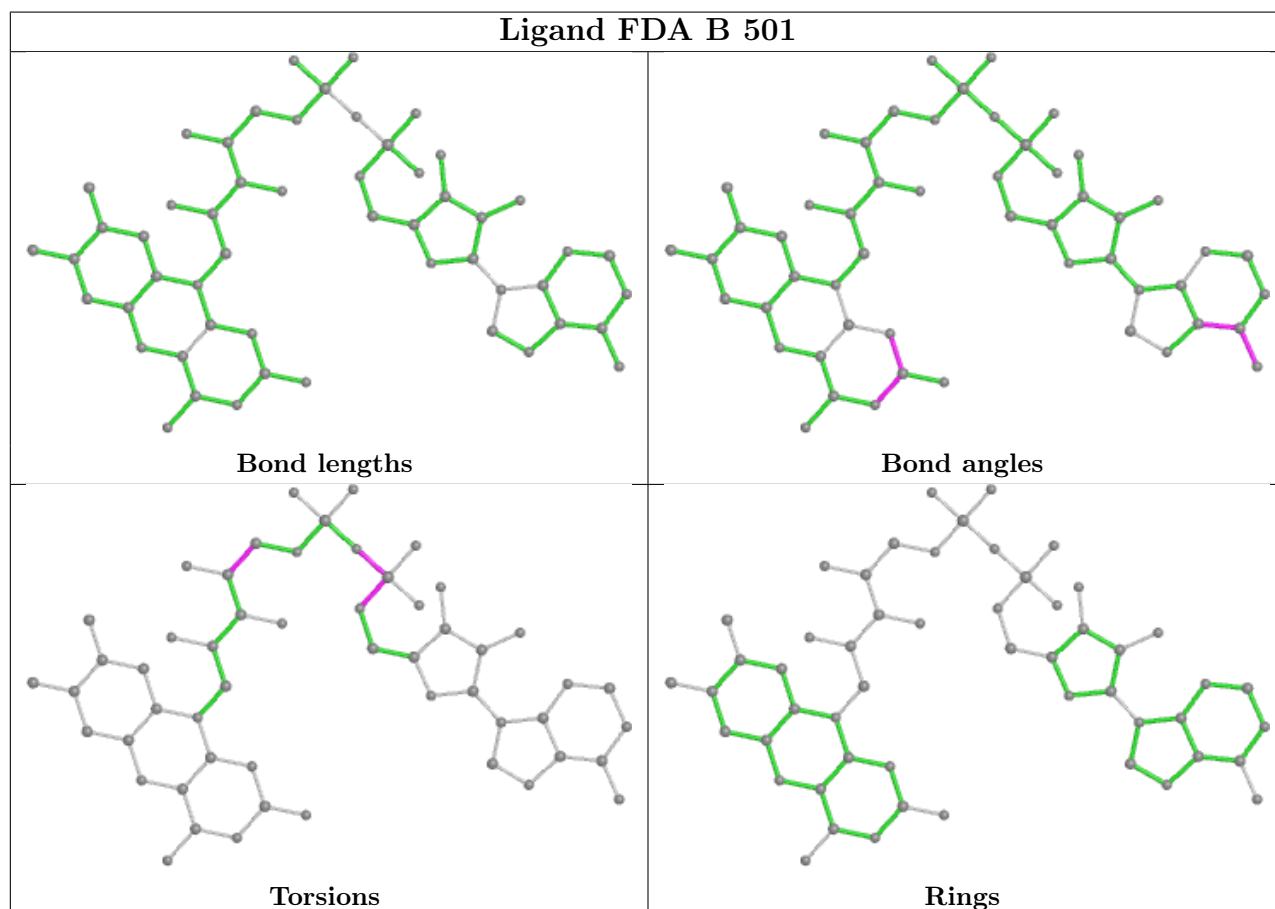
Mol	Chain	Res	Type	Atoms
5	A	502	FDA	O4'-C4'-C5'-O5'
5	B	501	FDA	C5B-O5B-PA-O1A
5	B	501	FDA	O4'-C4'-C5'-O5'
5	B	501	FDA	C5B-O5B-PA-O3P
5	A	502	FDA	P-O3P-PA-O1A
5	A	502	FDA	C3'-C4'-C5'-O5'
5	B	501	FDA	C5B-O5B-PA-O2A
5	B	501	FDA	P-O3P-PA-O1A
5	B	501	FDA	P-O3P-PA-O2A
5	B	501	FDA	C3'-C4'-C5'-O5'
5	A	502	FDA	N10-C1'-C2'-C3'

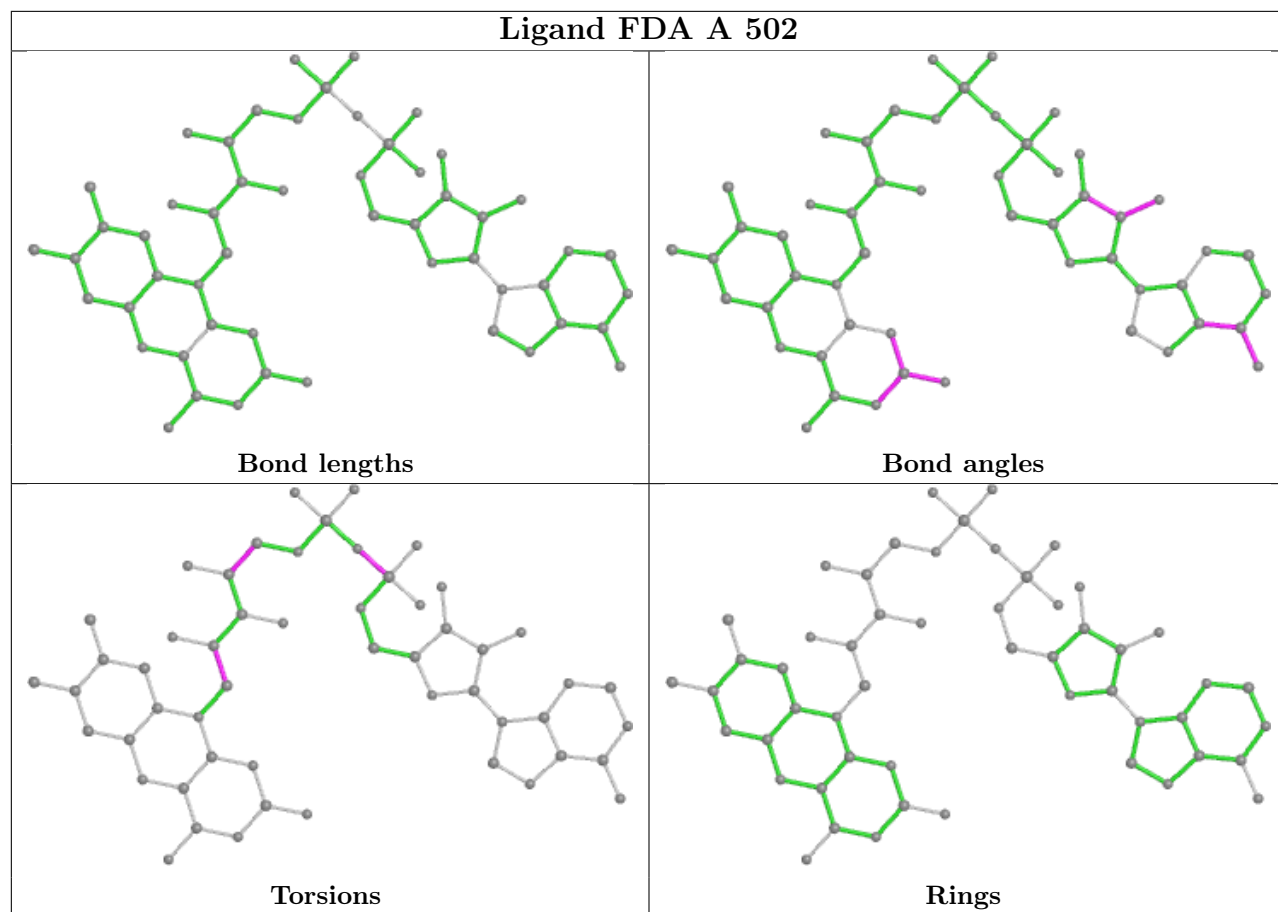
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	FDA	2	0
5	A	502	FDA	1	0
4	A	501	SO4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/498 (92%)	0.41	17 (3%) 41 41	18, 35, 69, 90	0
1	B	429/498 (86%)	0.87	52 (12%) 4 3	28, 56, 86, 116	0
2	C	14/14 (100%)	0.85	4 (28%) 0 0	27, 60, 92, 94	0
2	E	12/14 (85%)	1.08	3 (25%) 0 0	47, 67, 107, 116	0
3	D	14/14 (100%)	0.91	3 (21%) 0 0	45, 65, 78, 81	0
3	F	14/14 (100%)	1.58	6 (42%) 0 0	59, 84, 110, 130	0
All	All	943/1052 (89%)	0.66	85 (9%) 9 8	18, 45, 82, 130	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	PHE	9.5
1	B	59	ASP	6.3
1	B	254	ALA	4.7
1	A	187	THR	4.6
1	B	108	TYR	4.5
1	B	60	GLU	4.0
3	F	14	DA	3.8
2	E	4	DG	3.6
1	A	197	VAL	3.5
3	D	1	DT	3.5
1	A	198	GLU	3.4
1	A	49	VAL	3.3
1	B	273	PHE	3.2
1	B	255	LEU	3.1
1	B	69	TYR	3.1
1	B	224	LEU	3.1
1	B	223	PRO	3.1
1	B	19	GLY	3.1
3	F	1	DT	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	469	ALA	3.1
1	B	178	PHE	3.0
1	A	62	LEU	3.0
1	B	94	ARG	2.9
3	F	5	DG	2.9
1	B	274	GLY	2.8
1	B	134	ILE	2.8
1	B	181	LEU	2.8
1	B	168	TYR	2.8
1	B	115	THR	2.7
1	B	22	VAL	2.7
1	B	271	LEU	2.6
2	E	5	DG	2.6
1	B	222	ASP	2.6
1	B	139	PHE	2.6
1	B	58	THR	2.6
1	B	186	VAL	2.5
1	B	23	TYR	2.5
2	C	1	DA	2.5
1	B	13	SER	2.5
2	E	3	DC	2.5
1	B	35	TRP	2.5
1	A	468	ALA	2.4
1	B	135	SER	2.4
1	B	15	LYS	2.4
3	D	5	DG	2.4
1	A	18	ASP	2.4
1	B	39	PHE	2.4
1	A	48	ASN	2.4
1	B	73	LEU	2.4
1	B	456	LEU	2.4
1	B	169	ALA	2.4
1	B	68	GLN	2.4
1	B	446	GLU	2.3
1	A	221	LYS	2.3
1	A	185	SER	2.3
1	A	3	MET	2.3
1	B	74	LYS	2.3
1	B	252	TYR	2.3
3	F	13	DG	2.3
1	B	11	LEU	2.3
1	B	18	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	8	DA	2.2
2	C	4	DG	2.2
1	B	263	MET	2.2
1	B	238	LYS	2.2
1	A	134	ILE	2.2
1	A	15	LYS	2.2
1	B	12	LYS	2.2
1	A	85	ARG	2.2
3	D	4	DC	2.2
1	B	303	LEU	2.2
1	B	167	LEU	2.1
1	B	188	PRO	2.1
1	B	289	GLU	2.1
1	B	116	ASP	2.1
1	B	302	ILE	2.1
1	B	272	HIS	2.1
1	B	305	TRP	2.1
1	A	109	ASN	2.1
3	F	3	DG	2.1
2	C	14	DA	2.1
1	B	107	ASP	2.0
1	A	463	ALA	2.0
1	B	421	TRP	2.0
2	C	2	DT	2.0

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

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

6.3 Carbohydrates [i](#)

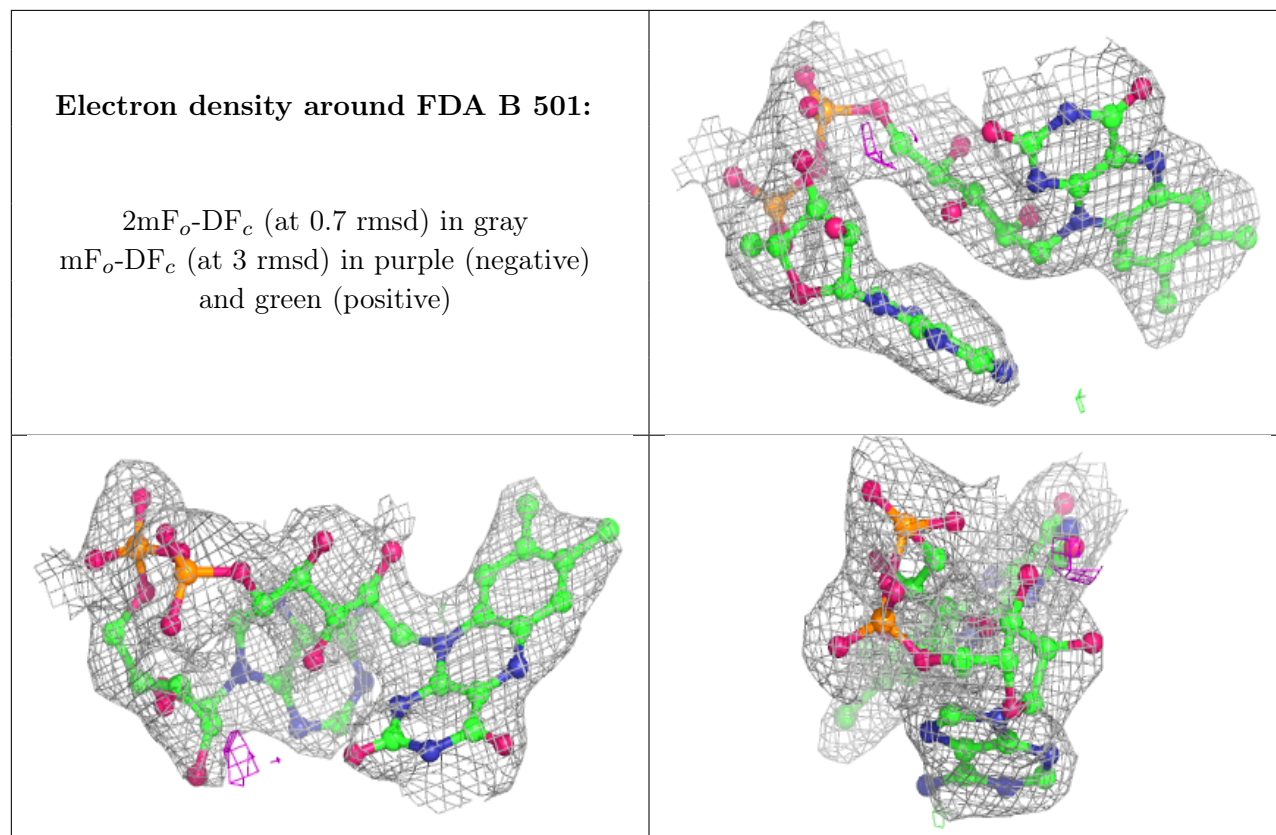
There are no monosaccharides in this entry.

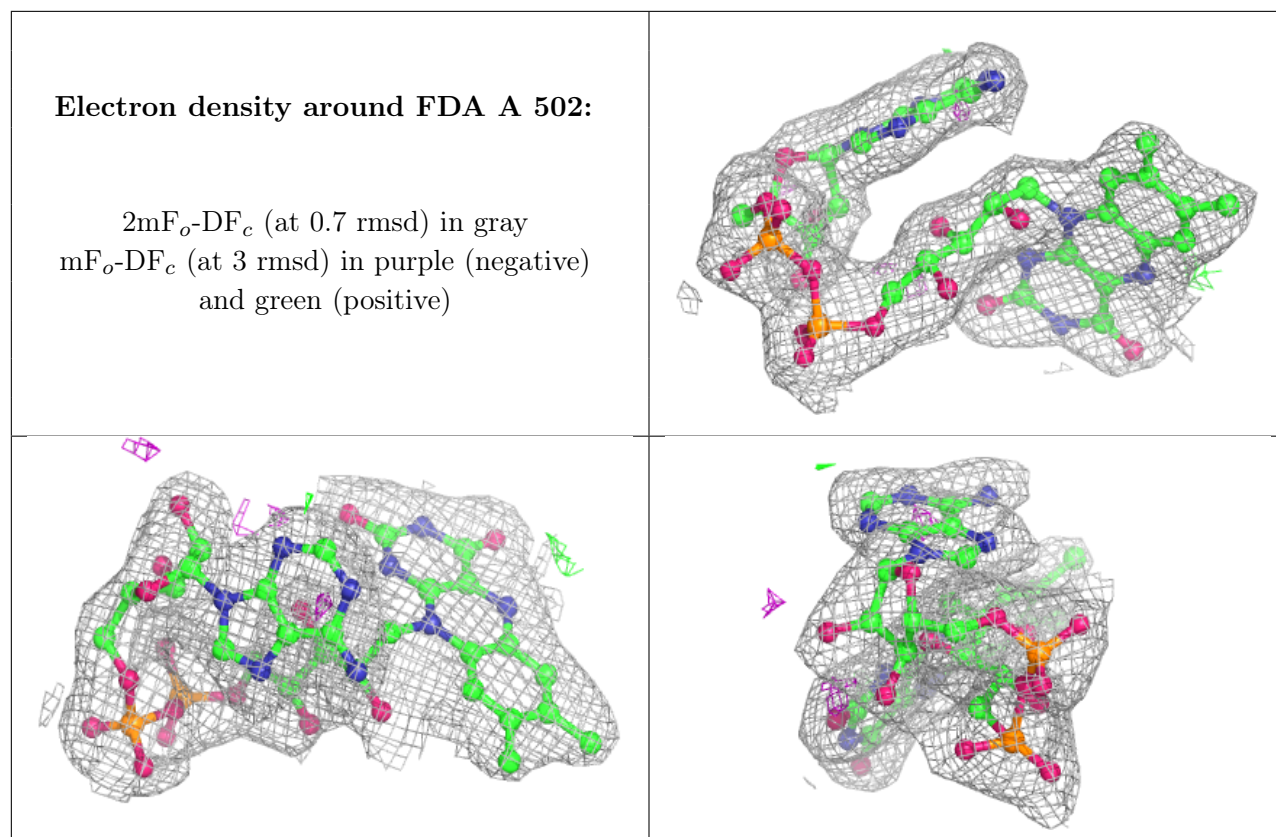
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
5	FDA	B	501	53/53	0.95	0.16	29,41,51,53	0
5	FDA	A	502	53/53	0.96	0.14	15,22,26,27	0
4	SO4	A	501	5/5	0.98	0.11	26,27,31,33	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.