



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 AM UTC

PDB ID : 8OYA / pdb_00008oya
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (10 microsecond 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 : 2.18 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)

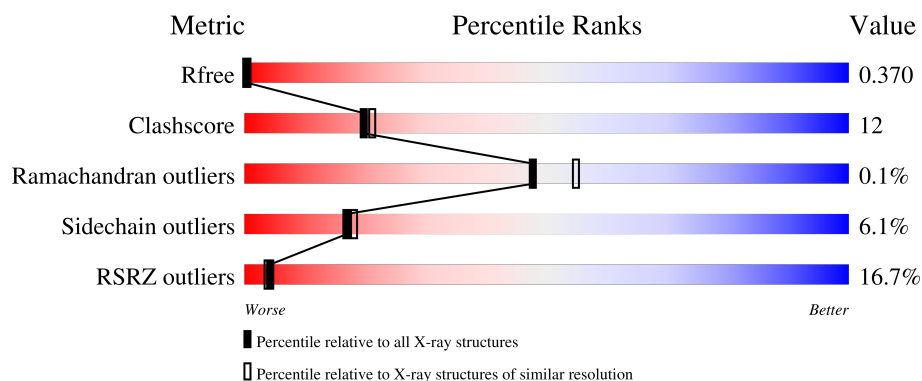
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	64% 36%
2	E	14	14% 21% 50% 7% 21%
3	D	14	7% 71% 29%
3	F	14	14% 79% 14% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8574 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	455	Total	C	N	O	S	0	0	0
			3693	2374	623	681	15			
1	B	417	Total	C	N	O	S	0	0	0
			3409	2195	573	627	14			

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

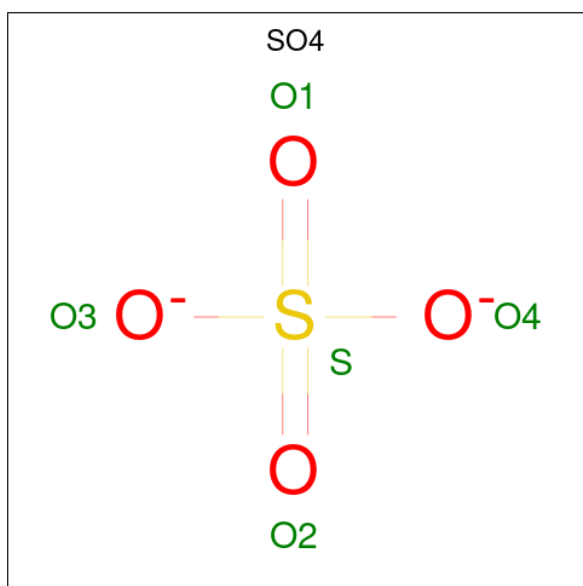
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

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	11	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

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

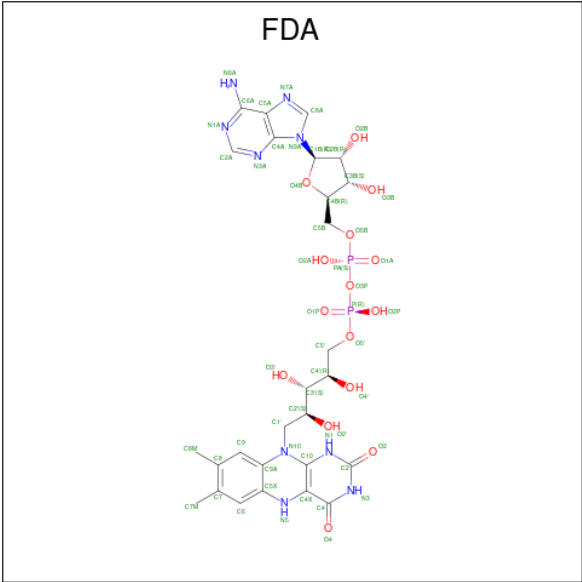
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

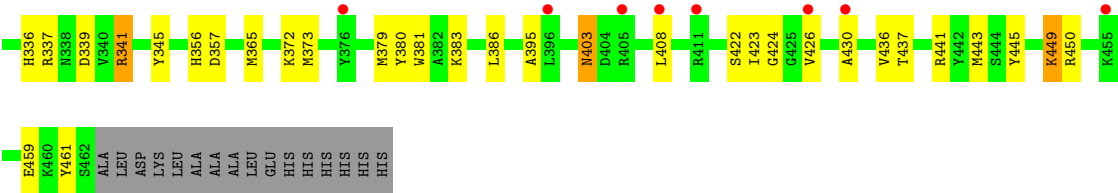
- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



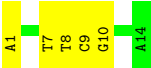
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is water.

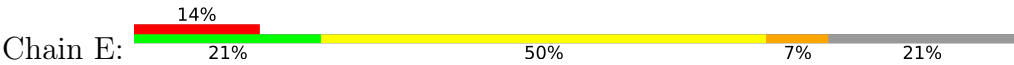
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total	O	0	0
			184	184		
6	B	85	Total	O	0	0
			85	85		
6	C	18	Total	O	0	0
			18	18		
6	D	7	Total	O	0	0
			7	7		
6	E	3	Total	O	0	0
			3	3		
6	F	6	Total	O	0	0
			6	6		



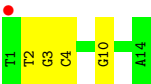
● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



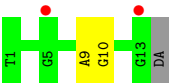
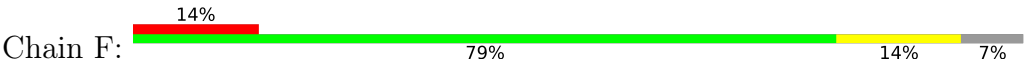
● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



● 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 – 2.18 31.29 – 2.18	Depositor EDS
% Data completeness (in resolution range)	79.0 (31.29-2.18) 79.0 (31.29-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.308 , 0.370 0.308 , 0.370	Depositor DCC
R_{free} test set	3031 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8574	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: FDA, SO4

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	0.51	0/3791	0.71	0/5124
1	B	0.41	0/3504	0.60	0/4736
2	C	0.57	0/315	0.81	0/484
2	E	0.51	0/251	0.75	1/385 (0.3%)
3	D	0.51	0/321	0.60	0/494
3	F	0.40	0/297	0.54	0/457
All	All	0.47	0/8479	0.66	1/11680 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DT	O4'-C1'-N1	5.12	116.08	108.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	341	ARG	Sidechain

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	3693	0	3626	61	0
1	B	3409	0	3314	105	0
2	C	282	0	159	11	0
2	E	225	0	124	11	0
3	D	286	0	158	3	0
3	F	265	0	147	2	0
4	A	5	0	0	0	0
5	A	53	0	33	1	0
5	B	53	0	33	1	0
6	A	184	0	0	6	0
6	B	85	0	0	8	0
6	C	18	0	0	0	0
6	D	7	0	0	0	0
6	E	3	0	0	0	0
6	F	6	0	0	0	0
All	All	8574	0	7594	181	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 12.

All (181) 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:127:ILE:HG13	6:B:661:HOH:O	1.67	0.91
2:C:7:DT:H72	2:C:8:DT:H72	1.55	0.89
1:A:125:GLN:HE22	1:B:341:ARG:H	1.28	0.79
2:C:7:DT:C7	2:C:8:DT:H72	2.12	0.79
1:B:383:LYS:NZ	1:B:441:ARG:O	2.16	0.77
1:A:310:ASP:OD1	6:A:601:HOH:O	2.04	0.76
1:B:21:VAL:HG21	1:B:43:ILE:HG13	1.71	0.72
2:C:9:DC:H2'	2:C:10:DG:C8	2.26	0.71
2:C:7:DT:H72	2:C:8:DT:C7	2.20	0.71
1:B:118:SER:O	6:B:601:HOH:O	2.11	0.68
1:B:66:ILE:HG23	1:B:70:GLU:HG3	1.76	0.67
1:B:345:TYR:OH	1:B:356:HIS:ND1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ARG:HB2	1:B:35:TRP:HZ3	1.60	0.67
1:A:52:VAL:HG12	1:A:89:PRO:HG2	1.77	0.67
1:B:96:ASP:HB3	6:B:625:HOH:O	1.94	0.67
1:B:291:ASN:OD1	1:B:294:SER:N	2.23	0.66
1:A:66:ILE:HD12	1:A:215:ARG:HG3	1.79	0.65
1:A:50:PRO:HG3	1:A:186:VAL:HG22	1.79	0.65
1:B:29:GLN:HE22	1:B:72:MET:HG2	1.62	0.65
1:A:6:LYS:HE3	1:A:151:GLU:OE2	1.96	0.65
1:A:125:GLN:HE22	1:B:341:ARG:N	1.95	0.63
1:A:455:LYS:HE3	6:A:697:HOH:O	1.97	0.63
1:B:459:GLU:HB3	6:B:668:HOH:O	1.98	0.63
1:A:73:LEU:HD23	1:A:204:LEU:HB2	1.79	0.63
1:B:152:ALA:O	1:B:166:LYS:HG3	1.98	0.62
1:A:73:LEU:HD21	1:A:203:VAL:HG13	1.81	0.62
1:B:170:LEU:HD23	1:B:174:PHE:HE2	1.64	0.62
1:A:453:ASP:OD2	1:A:456:LEU:HD13	1.99	0.61
2:C:7:DT:H1'	2:C:8:DT:H5'	1.80	0.61
1:B:430:ALA:HB3	3:F:9:DA:H2''	1.83	0.61
2:E:7:DT:H72	2:E:8:DT:H71	1.83	0.60
1:B:379:MET:SD	2:E:8:DT:C6	2.94	0.60
1:B:59:ASP:N	1:B:59:ASP:OD1	2.34	0.60
1:A:379:MET:SD	2:C:8:DT:C6	2.95	0.60
1:B:241:MET:HE3	1:B:281:VAL:HA	1.84	0.60
1:B:29:GLN:HG2	1:B:76:LEU:HD21	1.83	0.59
1:A:21:VAL:HG21	1:A:43:ILE:HG13	1.84	0.58
1:A:142:ASP:OD2	1:A:148:PRO:HA	2.04	0.58
1:B:67:ARG:NE	1:B:222:ASP:OD2	2.29	0.58
1:B:177:GLU:HG3	1:B:178:PHE:H	1.69	0.58
1:B:9:ARG:HD3	1:B:140:GLU:OE2	2.03	0.58
1:B:12:LYS:NZ	1:B:134:ILE:O	2.31	0.57
1:B:373:MET:HE1	1:B:381:TRP:CD2	2.40	0.57
1:A:373:MET:HE1	1:A:381:TRP:CD1	2.39	0.57
1:B:29:GLN:NE2	1:B:72:MET:HG2	2.19	0.57
1:A:386:LEU:HD13	1:A:423:ILE:HG23	1.86	0.56
1:B:35:TRP:CD1	1:B:178:PHE:HE1	2.24	0.56
1:B:266:ASN:HA	1:B:372:LYS:HE2	1.87	0.56
1:B:450:ARG:NH2	2:E:12:DG:O6	2.39	0.56
1:A:299:LEU:O	1:A:303:LEU:HB2	2.06	0.55
1:B:336:HIS:ND1	1:B:339:ASP:OD2	2.32	0.55
3:F:9:DA:H2'	3:F:10:DG:C8	2.42	0.55
1:B:101:ILE:HD11	1:B:130:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:O	1:A:130:VAL:HG23	2.07	0.55
1:B:245:ILE:HD11	1:B:285:VAL:HG22	1.88	0.54
1:B:241:MET:HE1	1:B:284:GLU:HG3	1.89	0.54
1:B:102:SER:O	1:B:105:VAL:HG22	2.06	0.54
2:C:1:DA:H8	2:C:1:DA:H5''	1.72	0.54
1:A:256:ARG:HH22	2:C:8:DT:H3	1.54	0.54
1:B:9:ARG:HB3	1:B:140:GLU:HG3	1.90	0.54
1:A:390:GLU:OE2	1:A:394:LYS:HE3	2.08	0.53
2:C:7:DT:C4	2:C:8:DT:C5	2.97	0.53
1:B:37:LEU:HD21	1:B:181:LEU:HD22	1.90	0.53
3:D:3:DG:H1'	3:D:4:DC:H5'	1.90	0.53
1:A:125:GLN:NE2	1:B:341:ARG:H	2.03	0.53
1:B:44:ALA:HB1	1:B:49:VAL:O	2.08	0.53
1:A:259:PRO:HD2	1:A:452:PHE:CD2	2.43	0.53
1:B:60:GLU:HB3	6:B:669:HOH:O	2.08	0.53
1:A:94:ARG:HD2	1:A:94:ARG:C	2.35	0.52
1:A:72:MET:HE3	1:A:273:PHE:CD1	2.44	0.52
1:A:164:ARG:NH1	1:A:300:ASP:OD1	2.42	0.52
1:A:66:ILE:HG23	1:A:208:VAL:HG22	1.91	0.52
1:A:86:LYS:NZ	1:A:181:LEU:O	2.36	0.52
1:B:111:GLY:O	1:B:137:PRO:HD2	2.11	0.51
3:D:2:DT:H2'	3:D:3:DG:C8	2.45	0.51
2:C:9:DC:H2''	2:C:10:DG:H5'	1.92	0.51
1:B:86:LYS:O	1:B:88:ILE:HG13	2.11	0.51
1:A:59:ASP:OD1	1:A:94:ARG:NH2	2.45	0.50
1:B:7:ARG:HB2	1:B:35:TRP:CZ3	2.43	0.50
1:B:12:LYS:HG2	1:B:13:SER:H	1.76	0.50
1:A:81:VAL:O	1:A:84:SER:N	2.45	0.49
1:B:24:TRP:CH2	6:B:661:HOH:O	2.66	0.49
1:B:357:ASP:OD2	1:B:380:TYR:OH	2.24	0.49
2:E:9:DC:H2''	2:E:10:DG:H5'	1.93	0.49
1:B:124:ASN:HA	1:B:127:ILE:HD12	1.94	0.49
1:B:115:THR:O	1:B:140:GLU:HA	2.13	0.49
1:B:178:PHE:HD2	1:B:280:ARG:HH21	1.61	0.49
1:B:365:MET:HB2	1:B:461:TYR:HB3	1.95	0.49
2:E:12:DG:H1'	2:E:13:DC:H5'	1.94	0.49
1:B:386:LEU:HD13	1:B:423:ILE:HG23	1.96	0.48
2:C:1:DA:H5''	2:C:1:DA:C8	2.48	0.48
1:B:142:ASP:OD2	1:B:148:PRO:HA	2.14	0.48
1:B:154:GLN:N	1:B:154:GLN:CD	2.71	0.48
1:B:41:ARG:NH2	1:B:184:ASN:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:HE3	1:B:45:LYS:HB3	1.62	0.48
1:B:176:GLU:HG2	1:B:177:GLU:O	2.13	0.48
1:A:11:LEU:HD23	1:A:138:PHE:CE2	2.50	0.47
1:B:237:ALA:HB1	1:B:276:ILE:HB	1.97	0.47
1:A:94:ARG:HD2	1:A:95:GLY:N	2.29	0.47
1:B:325:PHE:CG	1:B:424:GLY:HA3	2.50	0.47
1:A:404:ASP:HB3	1:A:411:ARG:HG3	1.96	0.47
1:B:55:PHE:HE2	1:B:57:LEU:HD23	1.80	0.47
1:B:222:ASP:N	1:B:222:ASP:OD1	2.47	0.47
1:B:403:ASN:C	1:B:403:ASN:HD22	2.22	0.47
1:A:334:ASN:HA	1:A:337:ARG:HG3	1.97	0.47
1:B:72:MET:O	1:B:75:GLY:N	2.48	0.47
1:A:446:GLU:OE1	1:A:446:GLU:N	2.43	0.46
1:B:176:GLU:O	1:B:279:GLN:NE2	2.48	0.46
1:A:3:MET:SD	1:A:39:PHE:HB2	2.55	0.46
1:B:262:ASN:HD21	1:B:266:ASN:HD21	1.62	0.46
1:B:295:LYS:O	1:B:299:LEU:HG	2.16	0.46
1:B:403:ASN:C	1:B:403:ASN:ND2	2.73	0.46
1:B:312:PHE:CE1	1:B:426:VAL:HG11	2.51	0.46
1:B:125:GLN:O	1:B:129:LYS:HG3	2.16	0.46
1:A:446:GLU:HG3	6:A:742:HOH:O	2.15	0.46
1:B:237:ALA:HB2	1:B:270:TYR:CD1	2.51	0.46
1:B:244:PHE:CD1	1:B:265:SER:HA	2.50	0.46
1:B:157:GLU:OE1	1:B:162:THR:OG1	2.30	0.46
1:B:43:ILE:HD12	1:B:112:THR:HG21	1.97	0.45
1:B:93:LEU:HB3	1:B:100:LYS:HD2	1.99	0.45
1:A:244:PHE:CD1	1:A:265:SER:HA	2.51	0.45
1:A:458:ILE:O	1:A:462:SER:HB3	2.15	0.45
1:B:51:VAL:HG12	1:B:184:ASN:HD21	1.82	0.45
1:B:8:ILE:HD12	1:B:39:PHE:CD2	2.52	0.45
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.79	0.44
1:B:121:ARG:O	1:B:125:GLN:HG3	2.17	0.44
1:B:129:LYS:HG2	6:B:657:HOH:O	2.16	0.44
1:A:215:ARG:HH11	1:A:223:PRO:HB3	1.83	0.44
1:B:86:LYS:NZ	1:B:181:LEU:O	2.51	0.43
1:A:306:LYS:O	1:A:309:SER:HB2	2.18	0.43
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.82	0.43
1:A:374:HIS:HB2	6:A:673:HOH:O	2.18	0.43
1:B:7:ARG:HG2	1:B:8:ILE:N	2.33	0.43
1:A:150:TRP:O	1:A:154:GLN:NE2	2.47	0.43
1:B:73:LEU:HD13	1:B:73:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG22	1:B:60:GLU:H	1.84	0.43
1:A:430:ALA:CB	3:D:10:DG:H5'	2.49	0.43
1:B:86:LYS:HD2	1:B:183:PRO:HG3	2.01	0.43
1:B:160:ALA:HB3	2:E:7:DT:OP1	2.18	0.43
1:B:256:ARG:NH2	2:E:8:DT:H3	2.16	0.43
1:B:222:ASP:HB2	1:B:225:PHE:HB2	2.01	0.43
1:B:314:TYR:HB3	1:B:315:TYR:CD1	2.54	0.43
2:E:4:DG:H4'	2:E:5:DG:OP1	2.18	0.42
1:B:323:GLU:HG3	1:B:323:GLU:O	2.18	0.42
2:E:7:DT:C4	2:E:8:DT:C5	3.08	0.42
1:B:97:PRO:O	1:B:101:ILE:HG12	2.20	0.42
1:A:38:LEU:HD13	1:A:179:PRO:HD2	2.01	0.42
1:A:455:LYS:HE2	1:A:455:LYS:HB3	1.62	0.42
1:B:99:GLU:HA	1:B:102:SER:OG	2.19	0.42
1:B:445:TYR:CE2	1:B:449:LYS:HD3	2.55	0.42
1:B:383:LYS:HE2	1:B:422:SER:HA	2.02	0.42
1:B:121:ARG:NH1	1:B:317:PRO:O	2.51	0.42
1:A:365:MET:HB2	1:A:461:TYR:HB3	2.02	0.41
1:A:3:MET:HE2	1:A:3:MET:HB3	1.84	0.41
1:A:12:LYS:HE2	1:A:134:ILE:O	2.20	0.41
1:A:109:ASN:CG	1:A:109:ASN:O	2.63	0.41
1:B:78:GLU:OE2	1:B:234:GLU:N	2.54	0.41
1:B:325:PHE:O	1:B:330:LYS:HE2	2.20	0.41
1:B:29:GLN:HE22	1:B:72:MET:CG	2.31	0.41
1:B:31:ALA:H	1:B:234:GLU:CD	2.28	0.41
2:E:8:DT:H4'	2:E:9:DC:OP2	2.20	0.41
1:B:24:TRP:CD1	1:B:24:TRP:C	2.98	0.41
1:B:87:LYS:O	1:B:184:ASN:HB2	2.21	0.41
1:B:408:LEU:HB2	6:B:632:HOH:O	2.19	0.41
1:A:323:GLU:HG2	1:B:337:ARG:NH2	2.36	0.41
2:E:9:DC:H2'	2:E:10:DG:C8	2.56	0.41
1:A:268:SER:HB3	5:A:502:FDA:H5'2	2.02	0.41
1:A:101:ILE:HD13	1:A:101:ILE:HA	1.81	0.41
1:A:278:SER:O	1:A:282:VAL:HG23	2.21	0.41
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.75	0.41
1:B:386:LEU:HA	1:B:395:ALA:CB	2.51	0.41
1:B:436:VAL:HG12	1:B:437:THR:HG23	2.03	0.41
1:A:257:ASN:HB2	6:A:680:HOH:O	2.20	0.41
1:A:347:LEU:HD13	1:A:398:ILE:HG23	2.02	0.40
1:B:299:LEU:O	1:B:303:LEU:HB2	2.21	0.40
1:A:446:GLU:HB3	6:A:739:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:O	1:B:38:LEU:HG	2.22	0.40
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.88	0.40
1:A:200:LEU:O	1:A:203:VAL:HG12	2.22	0.40
1:A:350:PHE:HD1	1:A:360:TRP:CH2	2.39	0.40
1:B:372:LYS:NZ	5:B:501:FDA:O2P	2.46	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	451/498 (91%)	435 (96%)	15 (3%)	1 (0%)	43	49
1	B	411/498 (82%)	388 (94%)	23 (6%)	0	100	100
All	All	862/996 (86%)	823 (96%)	38 (4%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/429 (92%)	375 (95%)	20 (5%)	21	24
1	B	364/429 (85%)	338 (93%)	26 (7%)	13	14
All	All	759/858 (88%)	713 (94%)	46 (6%)	17	18

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	11	LEU
1	A	13	SER
1	A	49	VAL
1	A	70	GLU
1	A	73	LEU
1	A	90	SER
1	A	103	ARG
1	A	114	VAL
1	A	180	GLU
1	A	186	VAL
1	A	199	THR
1	A	221	LYS
1	A	250	ASP
1	A	290	SER
1	A	308	ILE
1	A	354	LYS
1	A	456	LEU
1	A	462	SER
1	A	464	LEU
1	B	12	LYS
1	B	29	GLN
1	B	54	VAL
1	B	59	ASP
1	B	62	LEU
1	B	68	GLN
1	B	72	MET
1	B	77	GLN
1	B	78	GLU
1	B	99	GLU
1	B	102	SER
1	B	127	ILE

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Mol	Chain	Res	Type
1	B	136	ILE
1	B	146	VAL
1	B	162	THR
1	B	176	GLU
1	B	222	ASP
1	B	248	ARG
1	B	250	ASP
1	B	290	SER
1	B	291	ASN
1	B	310	ASP
1	B	327	SER
1	B	403	ASN
1	B	443	MET
1	B	449	LYS

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	125	GLN
1	A	364	GLN
1	B	29	GLN
1	B	184	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 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	$\# Z > 2$
5	FDA	B	501	-	57,58,58	0.51	0	78,89,89	0.68	2 (2%)
4	SO4	A	501	-	4,4,4	0.26	0	6,6,6	0.72	0
5	FDA	A	502	-	57,58,58	0.54	0	78,89,89	0.70	1 (1%)

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	-	-	4/34/50/50	0/6/6/6
5	FDA	A	502	-	-	4/34/50/50	0/6/6/6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	FDA	N3-C2-N1	2.50	119.67	115.74
5	B	501	FDA	N3-C2-N1	2.47	119.63	115.74
5	B	501	FDA	O2-C2-N3	-2.30	117.77	121.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

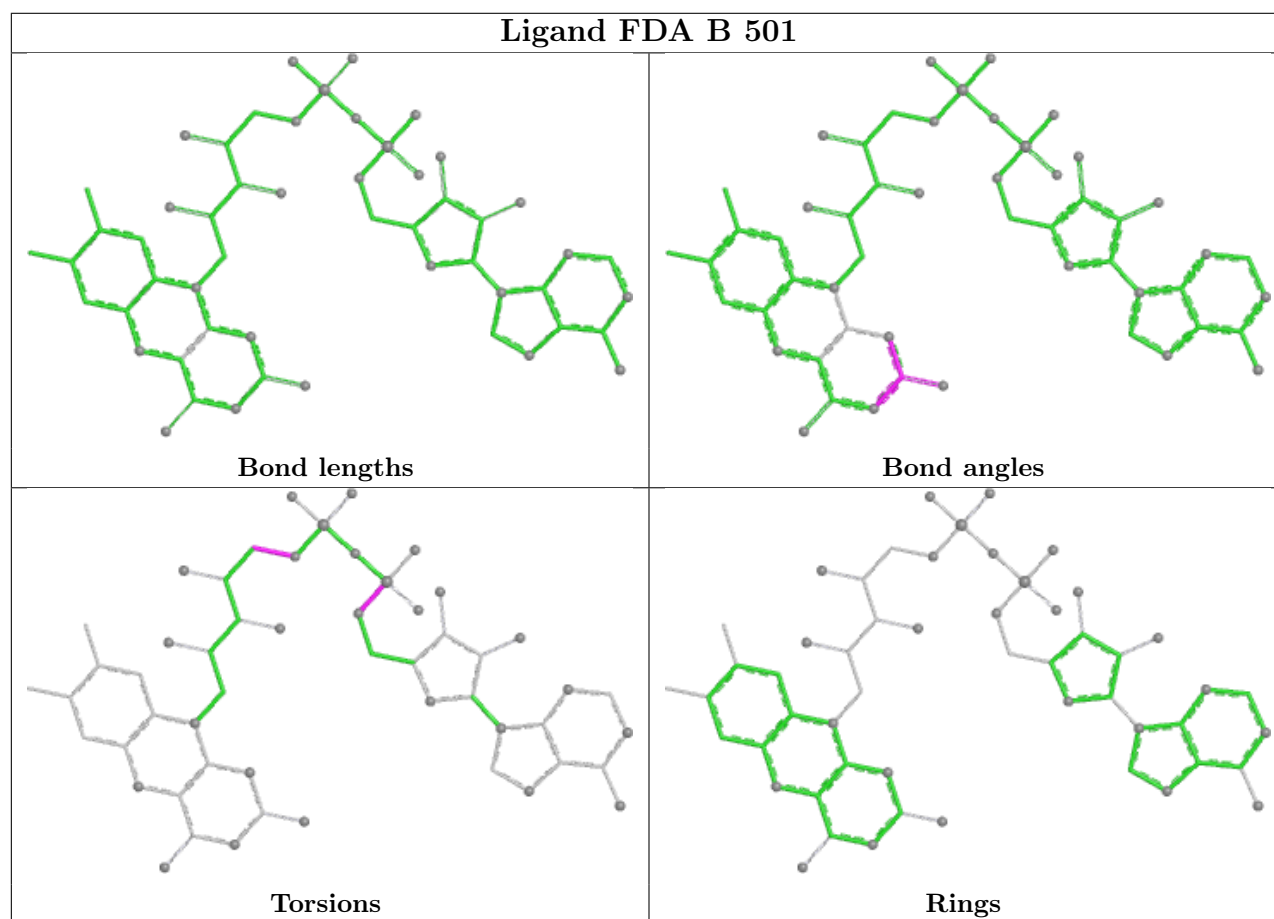
Mol	Chain	Res	Type	Atoms
5	A	502	FDA	C5B-O5B-PA-O1A
5	B	501	FDA	C5B-O5B-PA-O1A
5	B	501	FDA	C5B-O5B-PA-O3P
5	A	502	FDA	P-O3P-PA-O1A
5	A	502	FDA	C4'-C5'-O5'-P
5	B	501	FDA	C5B-O5B-PA-O2A
5	B	501	FDA	C4'-C5'-O5'-P
5	A	502	FDA	P-O3P-PA-O2A

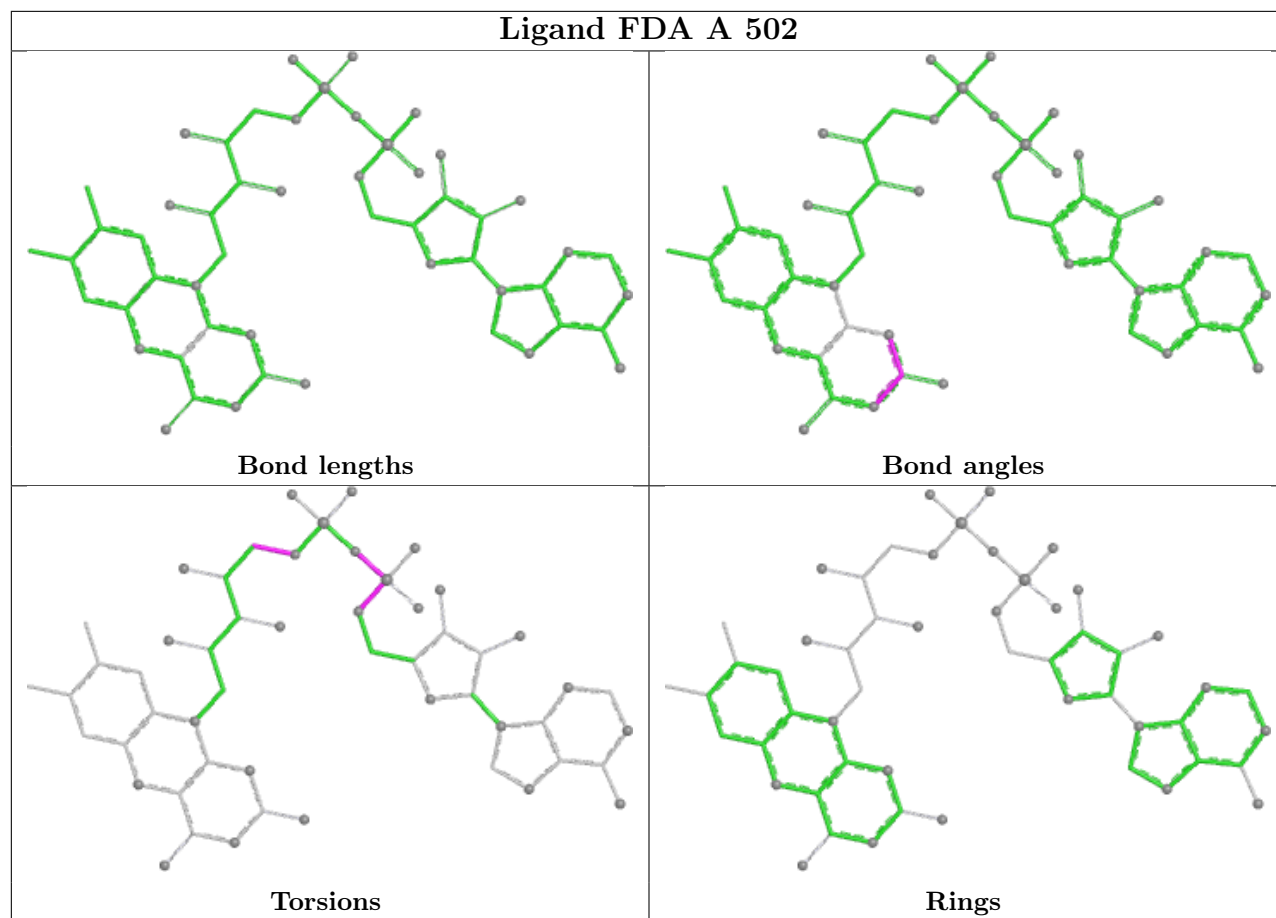
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	FDA	1	0
5	A	502	FDA	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	455/498 (91%)	0.50	18 (3%) 42 41	19, 29, 50, 79	0
1	B	417/498 (83%)	1.63	131 (31%) 1 1	30, 53, 82, 94	0
2	C	14/14 (100%)	0.53	0 100 100	30, 50, 62, 62	0
2	E	11/14 (78%)	1.17	2 (18%) 3 3	48, 62, 101, 109	0
3	D	14/14 (100%)	0.57	1 (7%) 22 21	37, 52, 59, 60	0
3	F	13/14 (92%)	1.38	2 (15%) 5 4	62, 71, 91, 104	0
All	All	924/1052 (87%)	1.03	154 (16%) 4 4	19, 39, 77, 109	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	TYR	6.0
1	B	54	VAL	5.5
1	B	108	TYR	5.4
1	B	69	TYR	5.1
1	B	141	VAL	5.1
1	B	186	VAL	5.1
1	B	136	ILE	5.0
1	B	65	GLY	5.0
1	B	50	PRO	4.9
1	B	43	ILE	4.9
1	B	104	PHE	4.9
1	B	20	PRO	4.9
1	B	52	VAL	4.8
1	B	64	ALA	4.8
1	B	35	TRP	4.7
1	B	187	THR	4.7
1	B	42	ALA	4.7
1	B	21	VAL	4.7
1	B	138	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	125	GLN	4.6
1	B	134	ILE	4.5
1	B	51	VAL	4.4
1	B	73	LEU	4.3
1	B	62	LEU	4.3
1	B	112	THR	4.2
1	B	47	ALA	4.1
1	B	57	LEU	4.1
1	B	61	PHE	4.1
1	B	45	LYS	4.0
1	B	49	VAL	4.0
1	B	130	VAL	4.0
1	B	14	GLY	3.9
1	B	24	TRP	3.8
1	B	48	ASN	3.8
1	B	11	LEU	3.8
1	B	122	ILE	3.8
1	B	53	VAL	3.8
1	B	97	PRO	3.7
1	A	15	LYS	3.6
1	B	63	GLU	3.6
1	B	111	GLY	3.6
1	B	105	VAL	3.5
1	B	135	SER	3.5
1	B	93	LEU	3.5
1	B	161	HIS	3.4
1	B	126	TRP	3.4
1	B	127	ILE	3.4
1	B	22	VAL	3.3
1	B	114	VAL	3.3
1	B	91	PHE	3.3
1	B	185	SER	3.3
1	A	463	ALA	3.3
1	B	110	ALA	3.3
1	A	465	ASP	3.3
1	B	23	TYR	3.3
1	B	159	ALA	3.3
1	B	10	ALA	3.2
1	B	55	PHE	3.2
1	B	7	ARG	3.2
1	A	467	LEU	3.2
1	B	66	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	314	TYR	3.1
1	B	92	PHE	3.1
1	B	148	PRO	3.1
1	B	150	TRP	3.1
1	B	39	PHE	3.1
1	B	137	PRO	3.1
1	B	56	CYS	3.1
1	A	39	PHE	3.0
1	B	41	ARG	3.0
1	B	71	PHE	3.0
1	B	101	ILE	3.0
1	B	184	ASN	3.0
1	B	58	THR	3.0
1	B	139	PHE	3.0
1	B	115	THR	2.9
1	B	182	GLU	2.9
1	B	160	ALA	2.9
1	B	83	LEU	2.9
1	A	222	ASP	2.9
1	B	89	PRO	2.9
1	B	174	PHE	2.9
1	B	168	TYR	2.9
1	B	129	LYS	2.8
1	B	102	SER	2.8
3	F	13	DG	2.8
1	B	103	ARG	2.8
1	A	186	VAL	2.8
1	B	8	ILE	2.8
1	B	149	CYS	2.8
1	B	305	TRP	2.8
1	B	107	ASP	2.7
1	B	315	TYR	2.7
1	A	340	VAL	2.7
1	A	462	SER	2.7
1	B	163	PHE	2.7
1	A	464	LEU	2.7
1	B	113	LEU	2.6
1	B	283	LEU	2.6
1	B	131	ILE	2.6
1	B	146	VAL	2.6
3	D	1	DT	2.6
1	B	109	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	124	ASN	2.6
1	B	37	LEU	2.6
1	B	26	SER	2.6
1	B	178	PHE	2.6
1	B	38	LEU	2.6
1	B	271	LEU	2.6
1	B	230	PHE	2.5
1	B	44	ALA	2.5
1	B	68	GLN	2.4
1	B	40	SER	2.4
1	B	76	LEU	2.4
1	B	31	ALA	2.4
1	A	136	ILE	2.4
1	B	94	ARG	2.4
1	B	411	ARG	2.4
1	B	426	VAL	2.4
1	B	162	THR	2.4
1	B	155	LYS	2.3
1	B	323	GLU	2.3
1	B	430	ALA	2.3
1	B	313	CYS	2.3
1	B	396	LEU	2.3
1	B	98	GLY	2.2
2	E	5	DG	2.2
1	B	255	LEU	2.2
1	A	126	TRP	2.2
1	B	12	LYS	2.2
1	B	408	LEU	2.2
1	B	60	GLU	2.1
1	A	21	VAL	2.1
1	B	303	LEU	2.1
1	B	88	ILE	2.1
1	B	81	VAL	2.1
1	B	175	LEU	2.1
1	A	48	ASN	2.1
1	B	70	GLU	2.1
2	E	4	DG	2.1
3	F	5	DG	2.1
1	B	455	LYS	2.1
1	B	263	MET	2.0
1	B	267	LEU	2.0
1	B	164	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	187	THR	2.0
1	A	133	GLY	2.0
1	B	376	TYR	2.0
1	B	240	VAL	2.0
1	B	72	MET	2.0
1	B	154	GLN	2.0
1	B	167	LEU	2.0
1	B	405	ARG	2.0
1	A	213	PRO	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](#)

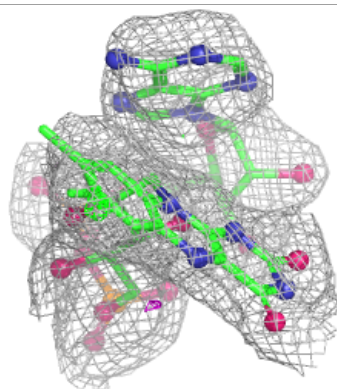
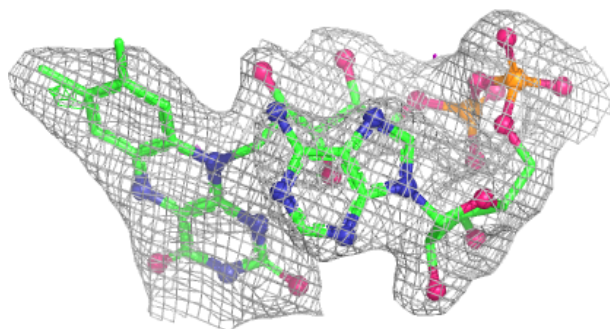
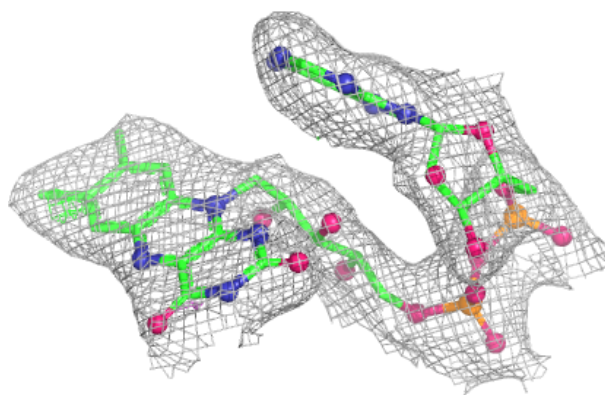
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FDA	B	501	53/53	0.92	0.09	32,39,43,45	0
5	FDA	A	502	53/53	0.95	0.08	17,22,26,27	0
4	SO4	A	501	5/5	0.98	0.05	29,30,35,35	0

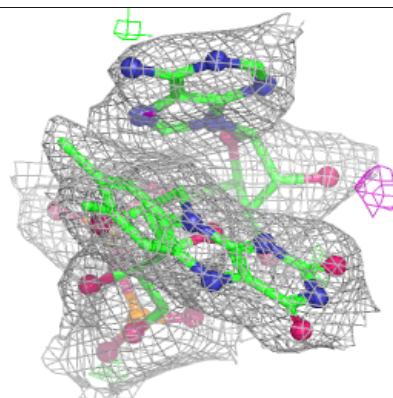
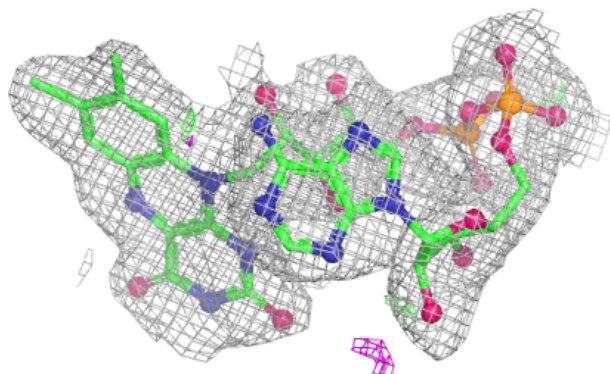
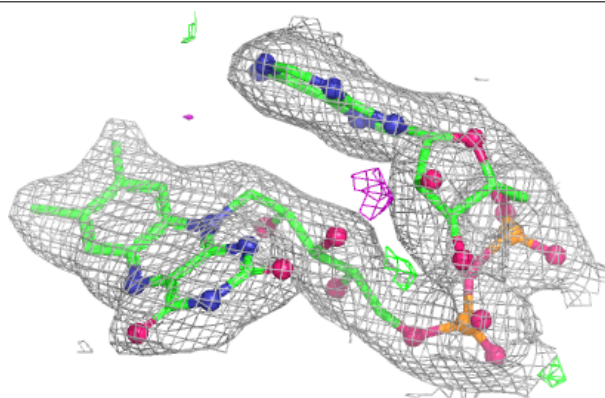
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FDA 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 FDA A 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.