



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:46 AM UTC

PDB ID : 8OY3 / pdb_00008oy3
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (3 picosecond 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 : 2.16 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)

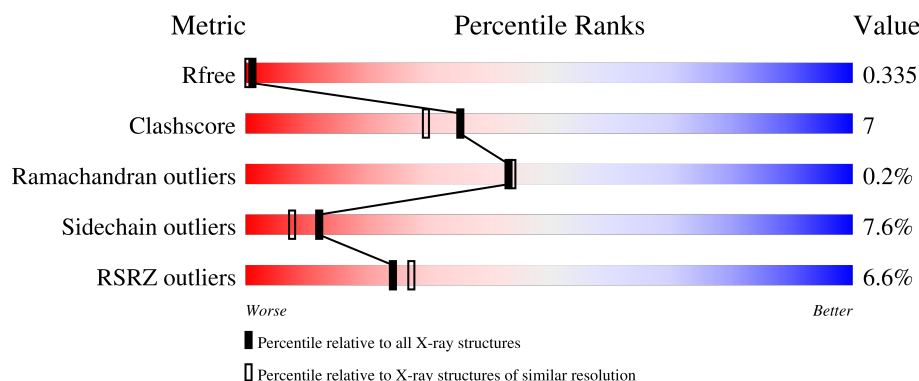
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

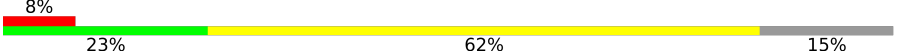
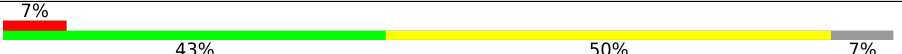
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	13	 62% 31% 8%
2	E	13	 8% 23% 62% 15%
3	D	14	 7% 64% 36%
3	F	14	 7% 43% 50% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8614 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	453	Total	C	N	O	S	0	3	0
			3701	2377	623	685	16			
1	B	427	Total	C	N	O	S	0	1	0
			3486	2240	588	643	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

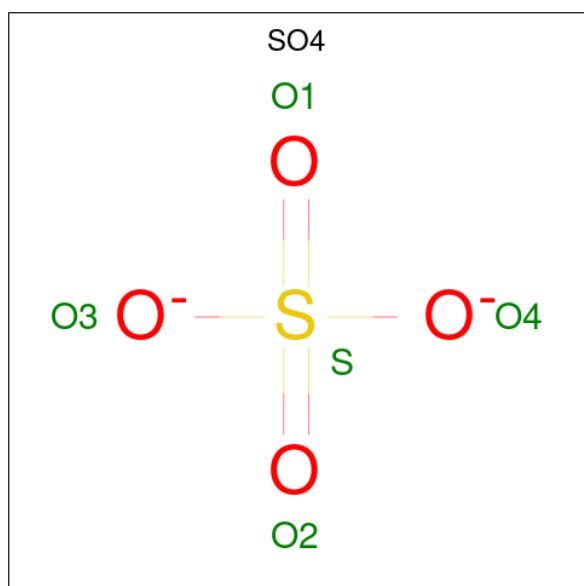
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			282	135	51	83	13			
2	E	11	Total	C	N	O	P	0	0	0
			244	115	44	73	12			

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

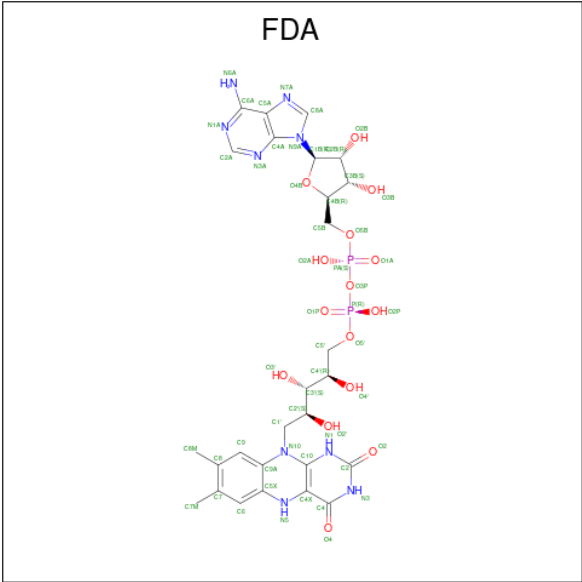
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

- 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		

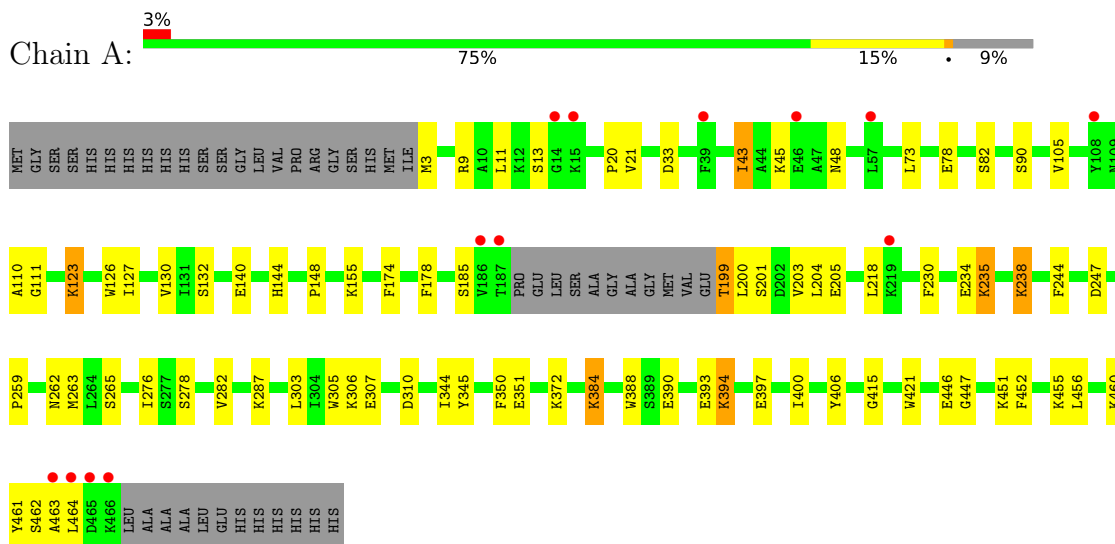
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	65	Total	O	0	0
			65	65		
6	C	14	Total	O	0	0
			14	14		
6	D	12	Total	O	0	0
			12	12		
6	E	1	Total	O	0	0
			1	1		
6	F	7	Total	O	0	0
			7	7		

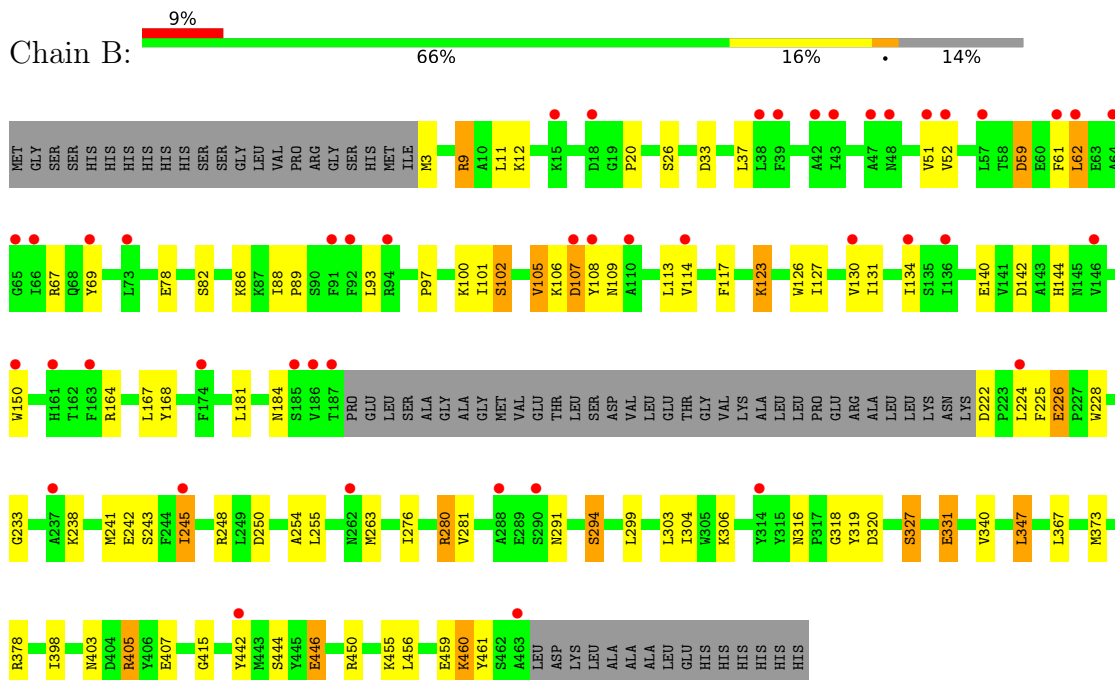
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Deoxyribodipyrimidine photo-lyase



• Molecule 1: Deoxyribodipyrimidine photo-lyase

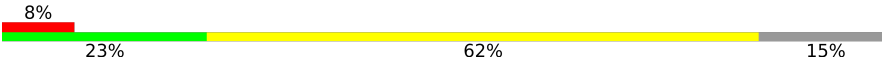


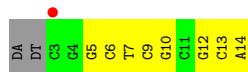
● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE

Chain C: 



● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE

Chain E: 

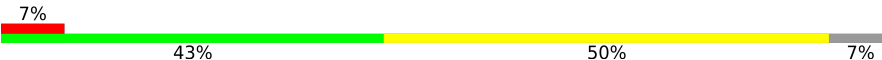


● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE

Chain D: 



● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE

Chain F: 



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 – 2.16 31.29 – 2.16	Depositor EDS
% Data completeness (in resolution range)	79.9 (31.29-2.16) 79.9 (31.29-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.273 , 0.335 0.273 , 0.335	Depositor DCC
R_{free} test set	3145 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8614	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: FDA, TTD, 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	0.49	0/3802	0.64	0/5139
1	B	0.41	0/3583	0.58	0/4843
2	C	0.46	0/270	0.54	0/412
2	E	0.38	0/227	0.46	0/345
3	D	0.45	0/321	0.60	0/494
3	F	0.42	0/297	0.54	0/457
All	All	0.45	0/8500	0.60	0/11690

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	3701	0	3625	37	0
1	B	3486	0	3389	61	0
2	C	282	0	159	7	0
2	E	244	0	135	7	0
3	D	286	0	158	4	0
3	F	265	0	147	6	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	33	1	0
5	B	53	0	33	2	0
6	A	140	0	0	4	0
6	B	65	0	0	3	0
6	C	14	0	0	0	0
6	D	12	0	0	2	0
6	E	1	0	0	0	0
6	F	7	0	0	0	0
All	All	8614	0	7679	117	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 7.

All (117) 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:241:MET:HE3	1:B:281:VAL:HA	1.61	0.81
1:A:390:GLU:OE2	1:A:394:LYS:HD3	1.88	0.73
1:B:243:SER:OG	1:B:248:ARG:NH2	2.27	0.68
1:A:21:VAL:HG21	1:A:43:ILE:HG22	1.78	0.65
1:B:61:PHE:HB3	1:B:69:TYR:HD1	1.63	0.64
1:B:12:LYS:HB2	1:B:131:ILE:HG23	1.80	0.63
1:B:107:ASP:C	1:B:109:ASN:H	2.08	0.61
1:B:250:ASP:OD1	1:B:291:ASN:HB2	2.00	0.60
1:B:291:ASN:HB3	1:B:294:SER:HB2	1.83	0.59
1:B:367:LEU:HD11	1:B:407:GLU:HG2	1.83	0.59
1:A:11:LEU:HD11	1:A:140:GLU:HB2	1.85	0.59
3:F:12:DC:H2''	3:F:13:DG:C8	2.37	0.58
1:A:393:GLU:O	1:A:397:GLU:HG3	2.04	0.57
1:B:51:VAL:H	1:B:184:ASN:HD21	1.53	0.57
1:B:327:SER:O	1:B:331:GLU:HG3	2.04	0.57
1:A:384:LYS:HG3	1:A:388:TRP:CH2	2.40	0.57
1:B:59:ASP:HA	1:B:62:LEU:HD21	1.85	0.57
1:B:242:GLU:O	1:B:245:ILE:HG13	2.04	0.56
1:B:107:ASP:O	1:B:109:ASN:N	2.38	0.56
1:B:299:LEU:O	1:B:303:LEU:HB2	2.06	0.56
1:B:86:LYS:HG3	1:B:181:LEU:HD23	1.89	0.55
1:B:9:ARG:HB2	1:B:140:GLU:HG2	1.89	0.54
1:B:446:GLU:H	1:B:446:GLU:CD	2.15	0.54
1:B:460:LYS:HE3	1:B:461:TYR:CZ	2.43	0.53
3:F:3:DG:H2''	3:F:4:DC:OP2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LYS:HE2	1:A:461:TYR:CZ	2.44	0.53
2:E:9:DC:H2''	2:E:10:DG:H5'	1.90	0.52
1:B:127:ILE:O	1:B:131:ILE:HG13	2.09	0.52
1:B:450:ARG:NH2	2:E:12:DG:O6	2.37	0.52
1:B:222:ASP:HB3	1:B:225:PHE:HB3	1.91	0.52
1:B:241:MET:CE	1:B:281:VAL:HA	2.37	0.51
1:A:105:VAL:HG13	1:A:110:ALA:HB3	1.93	0.51
1:B:347:LEU:HD23	1:B:398:ILE:HG23	1.91	0.51
1:A:73:LEU:HD23	1:A:204:LEU:HB2	1.91	0.51
1:B:238:LYS:O	1:B:242:GLU:HG3	2.10	0.51
1:A:199:THR:O	1:A:203:VAL:HG23	2.11	0.51
1:B:123:LYS:HE3	1:B:127:ILE:HD11	1.93	0.50
2:E:10:DG:H1	3:F:6:DC:H42	1.60	0.50
3:F:1:DT:H2'	3:F:2:DT:C6	2.46	0.50
2:C:5:DG:H2''	2:C:6:DC:OP2	2.10	0.50
1:B:233:GLY:HA3	6:B:601:HOH:O	2.13	0.49
3:F:2:DT:H2''	3:F:3:DG:C8	2.46	0.49
1:A:345:TYR:HB2	1:A:350:PHE:CE2	2.48	0.49
3:D:7:DG:H2''	3:D:8:DA:C8	2.48	0.49
1:A:278:SER:O	1:A:282:VAL:HG23	2.13	0.48
1:A:303:LEU:O	1:A:307:GLU:HG3	2.12	0.48
1:A:287:LYS:NZ	6:A:607:HOH:O	2.46	0.48
1:A:235:LYS:HB2	1:A:235:LYS:HE3	1.48	0.48
1:B:117:PHE:HB3	1:B:142:ASP:HA	1.96	0.47
1:B:67:ARG:NH2	1:B:225:PHE:HB2	2.29	0.47
1:B:100:LYS:HB3	1:B:100:LYS:HE2	1.62	0.47
1:A:259:PRO:HD2	1:A:452:PHE:CG	2.50	0.47
1:A:415:GLY:HA2	5:A:502:FDA:N5	2.29	0.47
1:B:9:ARG:HG3	1:B:150:TRP:CZ2	2.49	0.47
1:A:238:LYS:HD3	1:A:276:ILE:HD12	1.95	0.47
1:B:318:GLY:C	1:B:320:ASP:H	2.23	0.47
1:A:123:LYS:HZ3	1:A:127:ILE:HD11	1.80	0.47
1:A:384:LYS:NZ	6:A:606:HOH:O	2.45	0.47
1:B:226:GLU:HB3	1:B:228:TRP:NE1	2.30	0.46
2:E:13:DC:H2''	2:E:14:DA:C8	2.50	0.46
1:B:52:VAL:HG12	1:B:89:PRO:HG2	1.97	0.46
1:B:318:GLY:C	1:B:320:ASP:N	2.74	0.46
1:B:442:TYR:HE2	1:B:444:SER:HB3	1.81	0.46
1:A:447:GLY:O	1:A:451:LYS:HG3	2.15	0.46
1:B:20:PRO:HG2	1:B:108:TYR:HE2	1.82	0.45
3:D:5:DG:N3	6:D:101:HOH:O	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TRP:CE2	2:C:7:TTD:H5A2	2.51	0.45
1:A:45:LYS:HA	6:A:675:HOH:O	2.16	0.45
1:B:373:MET:HG2	1:B:378:ARG:HG2	1.98	0.45
1:B:130:VAL:O	1:B:134:ILE:HG12	2.15	0.45
2:E:5:DG:H2''	2:E:6:DC:OP2	2.17	0.45
1:B:37:LEU:HG	1:B:181:LEU:HD13	1.98	0.45
1:B:167:LEU:HD23	1:B:304:ILE:HD13	1.97	0.45
1:A:462:SER:O	1:A:464:LEU:N	2.49	0.45
1:B:316:ASN:HB3	6:B:602:HOH:O	2.16	0.45
1:B:415:GLY:HA2	5:B:501:FDA:N5	2.32	0.44
2:E:7:TTD:H2R1	2:E:7:TTD:H6T	1.93	0.44
1:A:20:PRO:O	1:A:111:GLY:N	2.36	0.44
1:A:234:GLU:O	1:A:238:LYS:NZ	2.48	0.44
3:F:1:DT:H6	3:F:1:DT:O5'	2.00	0.44
3:D:14:DA:H5''	3:D:14:DA:H8	1.82	0.44
1:A:33:ASP:HA	1:A:178:PHE:CD2	2.52	0.43
1:B:11:LEU:HD11	1:B:140:GLU:HB3	2.00	0.43
1:B:107:ASP:C	1:B:109:ASN:N	2.73	0.43
1:B:9:ARG:HG3	1:B:150:TRP:CE2	2.53	0.43
1:A:446:GLU:H	1:A:446:GLU:CD	2.26	0.43
1:A:126:TRP:O	1:A:130:VAL:HG23	2.19	0.43
1:B:61:PHE:HB3	1:B:69:TYR:CD1	2.49	0.43
1:A:455:LYS:HB2	6:A:630:HOH:O	2.16	0.43
1:A:262:ASN:O	1:A:263:MET:HE2	2.18	0.43
1:B:33:ASP:OD2	1:B:280:ARG:HD2	2.18	0.43
1:B:415:GLY:HA2	5:B:501:FDA:C4X	2.49	0.42
2:C:7:TTD:H2''	2:C:7:TTD:H6	1.86	0.42
1:A:148:PRO:HD3	1:A:174:PHE:CD2	2.54	0.42
1:B:164:ARG:HD2	1:B:168:TYR:HE2	1.84	0.42
1:A:421:TRP:CE2	2:C:7:TTD:H72	2.54	0.42
1:B:20:PRO:HG2	1:B:108:TYR:CE2	2.55	0.42
1:A:244:PHE:CD1	1:A:265:SER:HA	2.54	0.42
1:B:97:PRO:HG2	1:B:126:TRP:CE2	2.54	0.42
1:B:405:ARG:O	1:B:405:ARG:HG3	2.19	0.42
1:B:86:LYS:NZ	1:B:181:LEU:HB3	2.34	0.42
1:B:254:ALA:HB3	1:B:255:LEU:HD12	2.01	0.42
1:B:306:LYS:HG2	6:B:614:HOH:O	2.19	0.42
2:C:1:DA:H4'	2:C:2:DT:OP1	2.20	0.42
2:C:7:TTD:H2R1	2:C:7:TTD:H6T	1.98	0.42
1:A:351:GLU:OE2	1:A:406:TYR:OH	2.24	0.42
1:B:164:ARG:HG3	1:B:168:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.77	0.41
1:B:102:SER:O	1:B:106:LYS:HG2	2.20	0.41
1:B:67:ARG:HH21	1:B:225:PHE:HB2	1.86	0.41
1:A:230:PHE:CZ	1:A:372:LYS:HD3	2.55	0.41
1:B:105:VAL:HG21	1:B:113:LEU:HD22	2.01	0.41
1:A:305:TRP:CZ2	2:C:7:TTD:H5A2	2.56	0.41
1:B:455:LYS:O	1:B:459:GLU:HG3	2.21	0.41
2:E:7:TTD:H2''	2:E:7:TTD:H6	1.92	0.41
3:D:2:DT:H5''	6:D:105:HOH:O	2.20	0.40
1:B:88:ILE:HD12	1:B:181:LEU:HD21	2.02	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	452/498 (91%)	429 (95%)	22 (5%)	1 (0%)	43	44
1	B	424/498 (85%)	406 (96%)	17 (4%)	1 (0%)	43	44
All	All	876/996 (88%)	835 (95%)	39 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	319	TYR
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/429 (92%)	370 (93%)	27 (7%)	14	10
1	B	372/429 (87%)	341 (92%)	31 (8%)	10	6
All	All	769/858 (90%)	711 (92%)	58 (8%)	12	8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	9	ARG
1	A	13	SER
1	A	43	ILE
1	A	48	ASN
1	A	78	GLU
1	A	82	SER
1	A	90	SER
1	A	123	LYS
1	A	132	SER
1	A	144	HIS
1	A	155	LYS
1	A	185	SER
1	A	199	THR
1	A	201	SER
1	A	205	GLU
1	A	218	LEU
1	A	235	LYS
1	A	238	LYS
1	A	247	ASP
1	A	306	LYS
1	A	310	ASP
1	A	344	ILE
1	A	384	LYS
1	A	394	LYS
1	A	400	ILE
1	A	456	LEU
1	B	3	MET
1	B	9	ARG
1	B	26	SER
1	B	59	ASP
1	B	62	LEU
1	B	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	82	SER
1	B	93	LEU
1	B	101	ILE
1	B	102	SER
1	B	105	VAL
1	B	107	ASP
1	B	114	VAL
1	B	123	LYS
1	B	144	HIS
1	B	224	LEU
1	B	226	GLU
1	B	245	ILE
1	B	263	MET
1	B	276	ILE
1	B	280	ARG
1	B	294	SER
1	B	327	SER
1	B	331	GLU
1	B	340	VAL
1	B	347	LEU
1	B	403	ASN
1	B	405	ARG
1	B	446	GLU
1	B	456	LEU
1	B	460	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	B	266	ASN
1	B	272	HIS
1	B	427	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TTD	C	7	2	42,45,46	0.55	1 (2%)	61,74,77	0.71	0
2	TTD	E	7	2	42,45,46	0.40	0	61,74,77	0.67	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
2	TTD	C	7	2	-	10/22/109/110	0/5/6/6
2	TTD	E	7	2	-	11/22/109/110	0/5/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	TTD	PB-O3R	2.42	1.66	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2'-C1'-N1-C6
2	E	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	O4R-C4'-C5R-O5R
2	E	7	TTD	O4'-C1'-N1-C6
2	C	7	TTD	C2'-C1'-N1-C2
2	E	7	TTD	O4'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	7	TTD	C3'-C4'-C5R-O5R
2	E	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	O4'-C1'-N1-C6
2	C	7	TTD	C2'-C3R-O3R-PB
2	C	7	TTD	O4'-C1'-N1-C2
2	E	7	TTD	O4R-C1R-N1T-C6T
2	E	7	TTD	C2R-C1R-N1T-C2T
2	C	7	TTD	C2R-C1R-N1T-C6T
2	C	7	TTD	O4'-C4R-C5'-O5'
2	C	7	TTD	O4R-C1R-N1T-C6T
2	E	7	TTD	O4R-C1R-N1T-C2T
2	E	7	TTD	O4'-C4R-C5'-O5'
2	C	7	TTD	O4R-C1R-N1T-C2T
2	C	7	TTD	C2R-C1R-N1T-C2T

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	TTD	5	0
2	E	7	TTD	2	0

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	A	502	-	57,58,58	0.52	0	78,89,89	0.72	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FDA	B	501	-	57,58,58	0.55	0	78,89,89	0.68	2 (2%)
4	SO4	A	501	-	4,4,4	0.18	0	6,6,6	0.64	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	A	502	-	-	3/34/50/50	0/6/6/6
5	FDA	B	501	-	-	5/34/50/50	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	B	501	FDA	N3-C2-N1	2.52	119.70	115.74
5	A	502	FDA	N3-C2-N1	2.39	119.50	115.74
5	A	502	FDA	O2-C2-N3	-2.35	117.68	121.86
5	B	501	FDA	O2-C2-N3	-2.28	117.80	121.86
5	A	502	FDA	C5X-N5-C4X	-2.05	116.35	121.08
5	A	502	FDA	C2'-C1'-N10	2.03	119.79	110.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

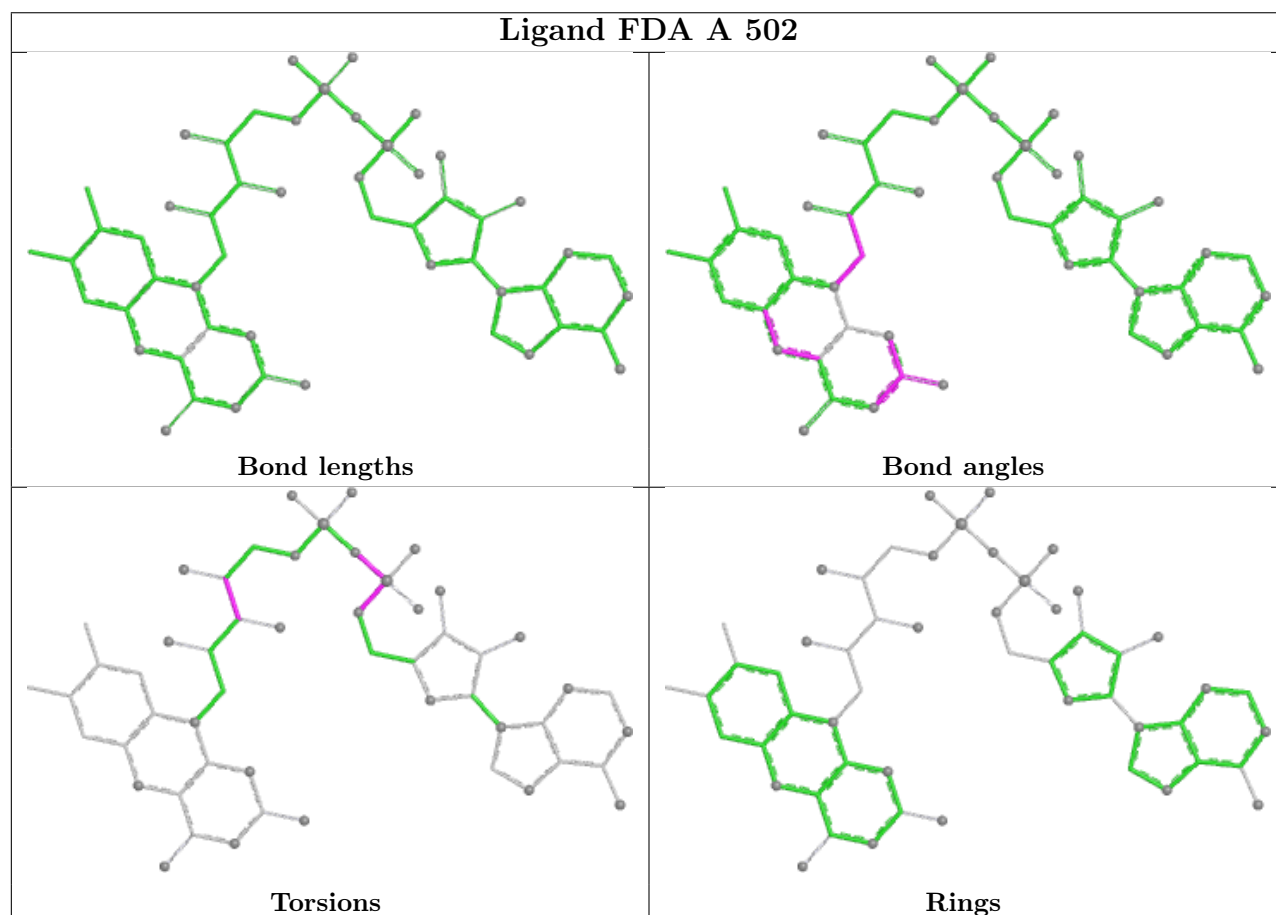
Mol	Chain	Res	Type	Atoms
5	A	502	FDA	C5B-O5B-PA-O1A
5	B	501	FDA	C5B-O5B-PA-O1A
5	B	501	FDA	C5B-O5B-PA-O3P
5	B	501	FDA	N10-C1'-C2'-C3'
5	B	501	FDA	O4'-C4'-C5'-O5'
5	B	501	FDA	C5B-O5B-PA-O2A
5	A	502	FDA	O3'-C3'-C4'-C5'
5	A	502	FDA	P-O3P-PA-O2A

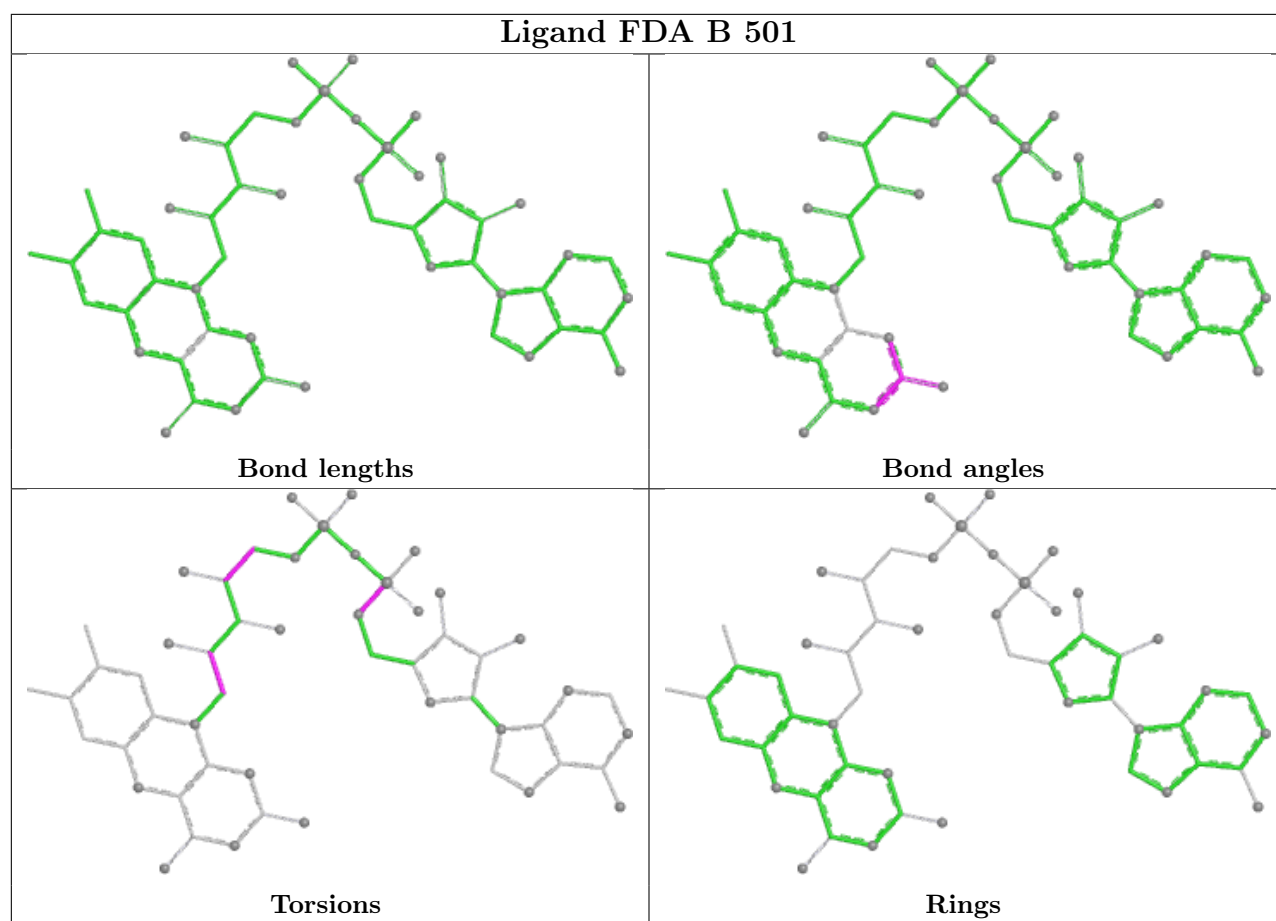
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	FDA	1	0
5	B	501	FDA	2	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	453/498 (90%)	0.27	13 (2%) 53 57	19, 39, 70, 109	3 (0%)
1	B	427/498 (85%)	0.86	45 (10%) 11 13	18, 58, 91, 141	1 (0%)
2	C	12/13 (92%)	0.37	0 100 100	37, 70, 88, 93	0
2	E	10/13 (76%)	0.69	1 (10%) 12 14	52, 76, 110, 131	0
3	D	14/14 (100%)	0.44	1 (7%) 22 25	50, 67, 90, 95	0
3	F	13/14 (92%)	0.93	1 (7%) 19 22	71, 79, 109, 109	0
All	All	929/1050 (88%)	0.56	61 (6%) 24 27	18, 49, 88, 141	4 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	PHE	5.6
1	B	64	ALA	4.6
1	B	108	TYR	4.2
1	B	136	ILE	3.7
1	B	73	LEU	3.6
1	A	465	ASP	3.5
1	B	186	VAL	3.4
1	B	130	VAL	3.2
1	B	62	LEU	3.2
1	A	466	LYS	3.2
1	B	69	TYR	3.1
1	B	18	ASP	3.1
3	D	1	DT	3.0
1	B	134	ILE	3.0
1	A	186	VAL	2.8
1	B	107	ASP	2.7
1	B	65	GLY	2.7
1	A	108	TYR	2.7
1	B	146	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	47	ALA	2.6
1	B	48	ASN	2.6
1	B	39	PHE	2.6
1	B	150	TRP	2.6
1	A	39	PHE	2.6
1	A	187	THR	2.5
1	B	185	SER	2.5
1	B	187	THR	2.5
1	B	15	LYS	2.4
1	B	38	LEU	2.4
1	B	262	ASN	2.4
1	B	245	ILE	2.4
1	B	92	PHE	2.3
1	B	42	ALA	2.3
1	A	46	GLU	2.3
1	B	290	SER	2.3
1	B	114	VAL	2.3
1	B	94	ARG	2.3
1	A	14	GLY	2.3
1	A	464	LEU	2.3
1	B	66	ILE	2.2
1	B	237	ALA	2.2
1	A	219	LYS	2.2
1	B	43	ILE	2.2
1	B	463	ALA	2.2
1	B	224	LEU	2.2
1	B	161	HIS	2.2
1	B	174	PHE	2.2
1	A	463	ALA	2.2
1	B	57	LEU	2.2
1	B	442	TYR	2.2
1	A	15	LYS	2.2
1	B	110	ALA	2.1
3	F	1	DT	2.1
1	B	314	TYR	2.1
1	B	52	VAL	2.1
1	A	57	LEU	2.1
1	B	51	VAL	2.1
1	B	163	PHE	2.1
1	B	91	PHE	2.0
1	B	288	ALA	2.0
2	E	3	DC	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TTD	E	7	40/41	0.93	0.09	39,47,67,74	0
2	TTD	C	7	40/41	0.94	0.08	25,34,49,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

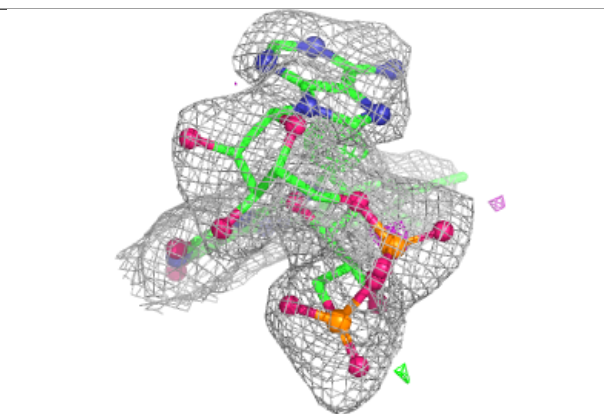
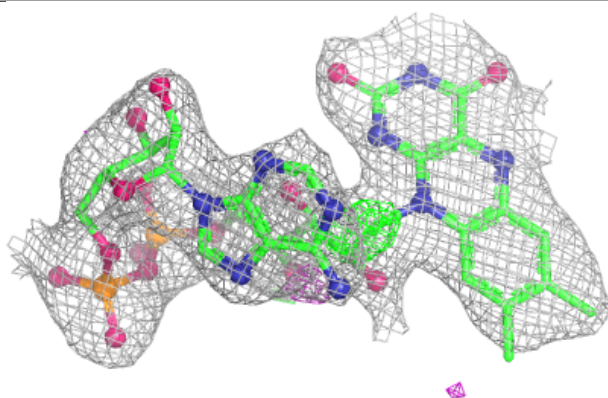
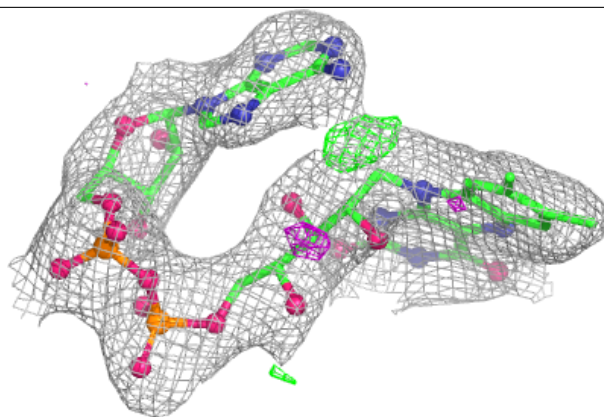
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	36,44,53,57	0
5	FDA	A	502	53/53	0.94	0.07	23,31,38,42	0
4	SO4	A	501	5/5	0.98	0.06	36,37,46,46	0

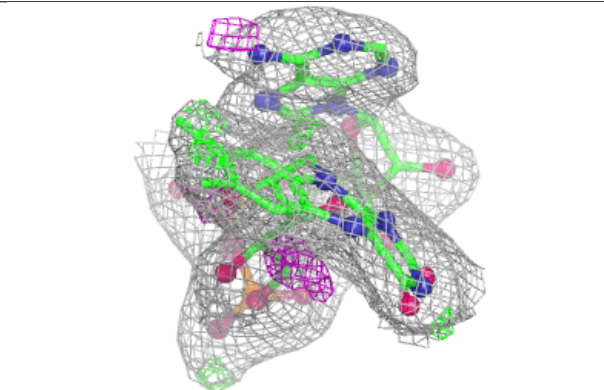
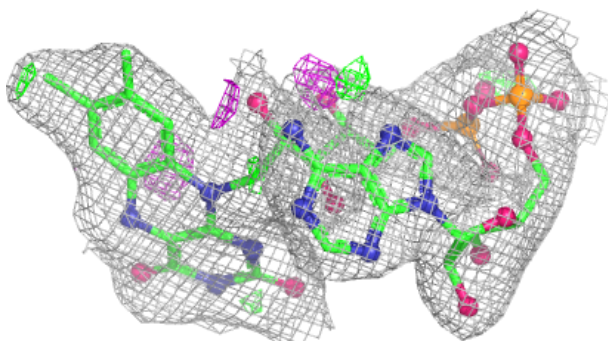
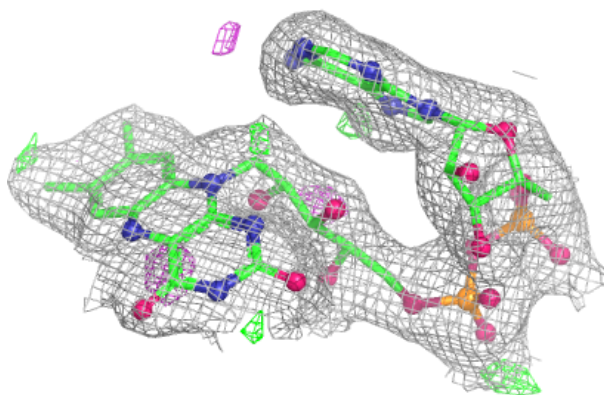
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.