Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 12:16 am GMT

PDB ID	:	8OY9
Title	:	Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (1 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	:	2.24 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 (i) 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 (1)) were used in the production of this report:

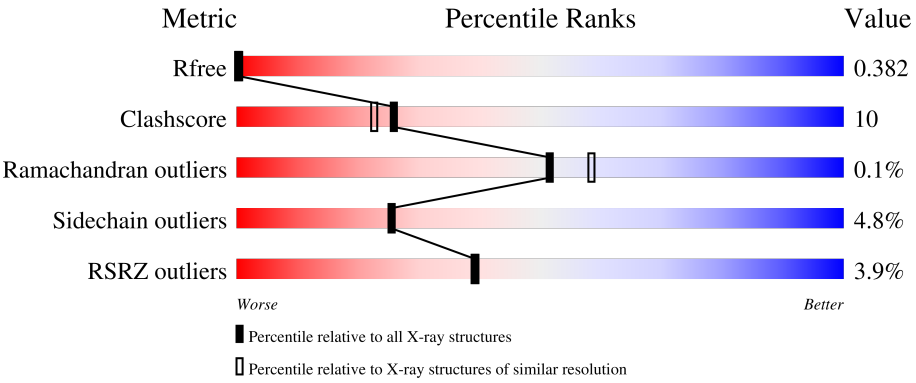
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

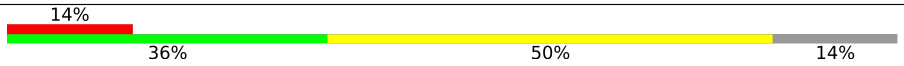
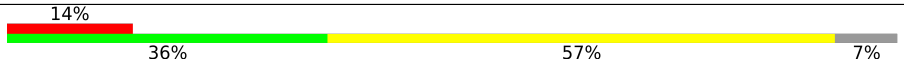
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	2% 67% 24% 8%
1	B	498	4% 60% 23% 15%

Continued on next page...

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

Continued from previous page...

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 8521 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deoxyribodipyrimidine photo-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3715	2389	626	685	15			
1	B	421	Total	C	N	O	S	0	0	0
			3440	2213	580	632	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

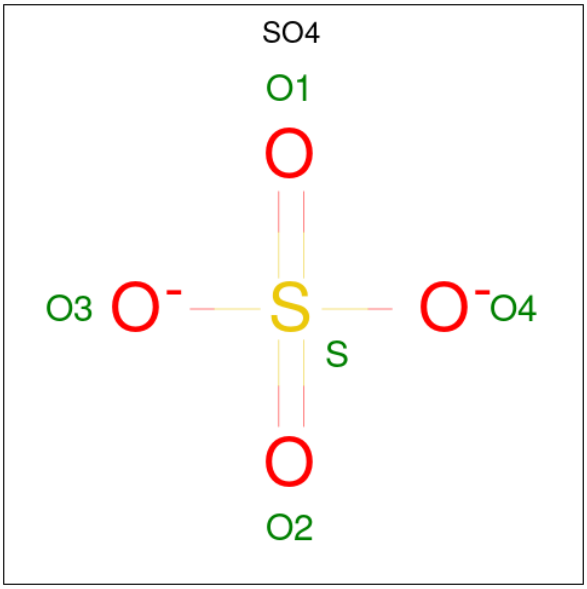
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

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

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

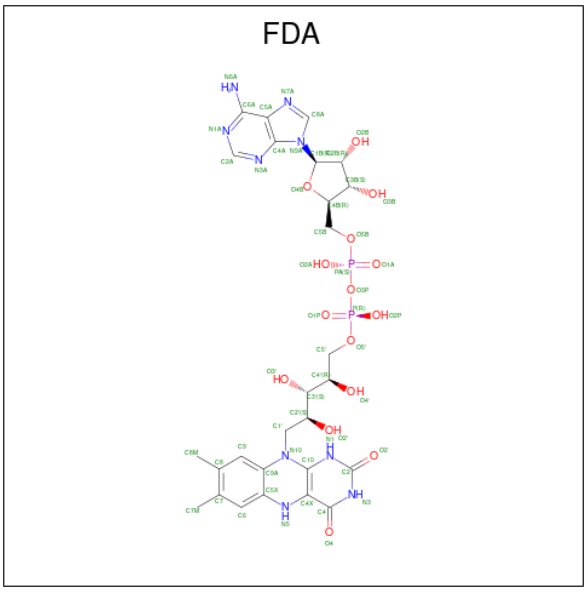
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



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.

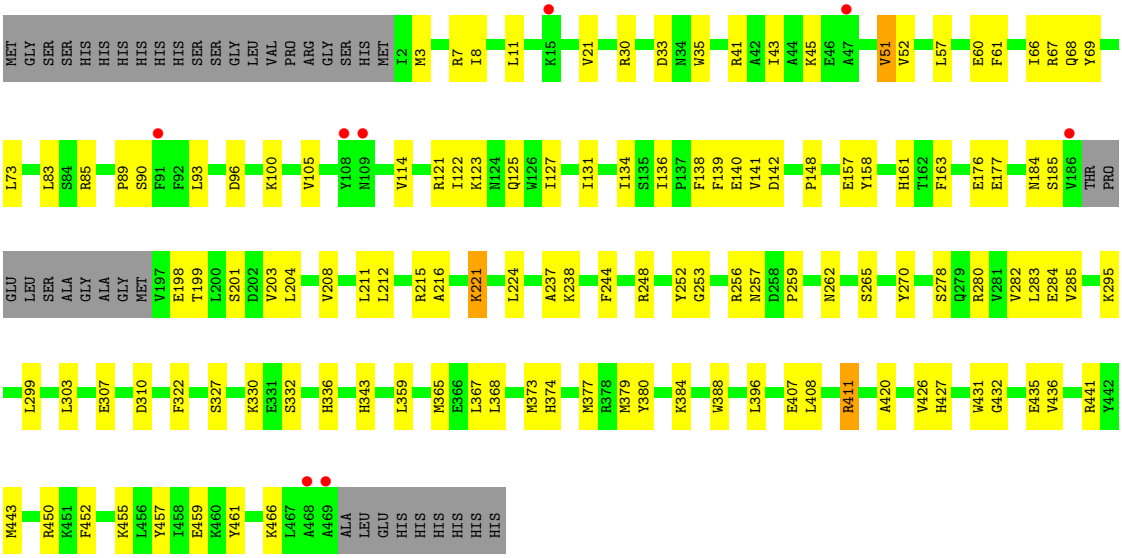
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	55	Total	O	0	0
			55	55		
6	C	12	Total	O	0	0
			12	12		
6	D	4	Total	O	0	0
			4	4		
6	F	1	Total	O	0	0
			1	1		

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.

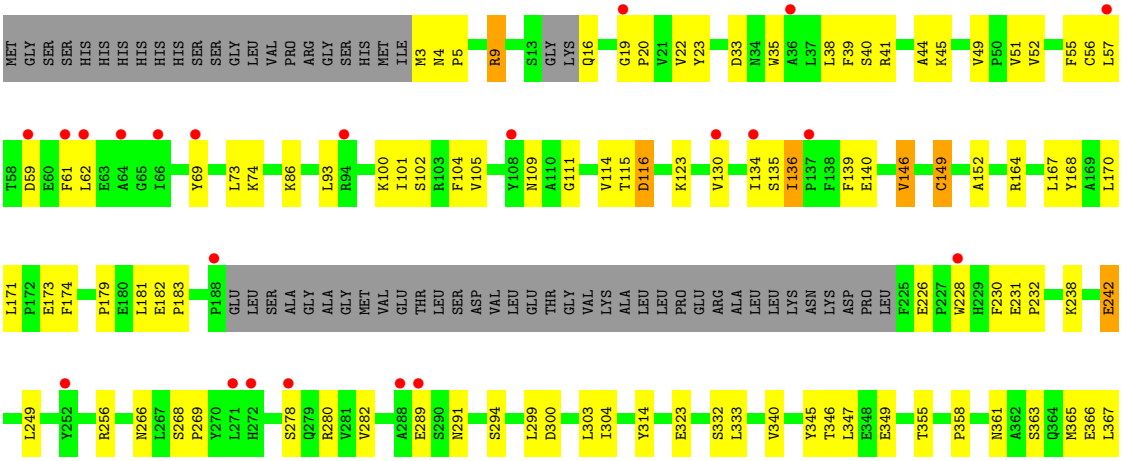
• Molecule 1: Deoxyribodipyrimidine photo-lyase

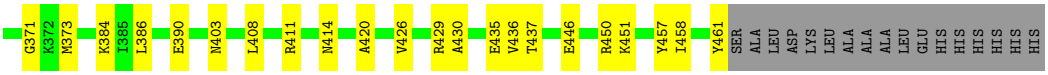
Chain A:



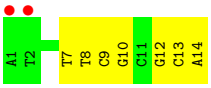
• Molecule 1: Deoxyribodipyrimidine photo-lyase

Chain B:

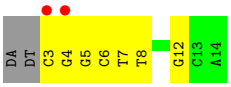




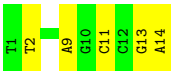
• Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



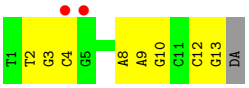
• Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



• Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



• Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



4 Data and refinement statistics (i)

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 – 2.24 31.29 – 2.24	Depositor EDS
% Data completeness (in resolution range)	80.2 (31.29-2.24) 80.3 (31.29-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.312 , 0.383 0.311 , 0.382	Depositor DCC
R_{free} test set	2782 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.57	0/3813	0.69	0/5154
1	B	0.50	1/3536 (0.0%)	0.63	0/4779
2	C	1.12	0/315	1.16	2/484 (0.4%)
2	E	0.80	0/272	1.04	1/417 (0.2%)
3	D	0.82	0/321	1.00	1/494 (0.2%)
3	F	0.85	0/297	0.92	0/457
All	All	0.60	1/8554 (0.0%)	0.73	4/11785 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	CYS	CB-SG	-6.37	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	8	DT	O4'-C1'-N1	10.72	115.50	108.00
2	C	8	DT	N3-C4-O4	5.83	123.40	119.90
2	E	8	DT	O4'-C1'-N1	5.53	111.87	108.00
3	D	2	DT	O4'-C1'-N1	5.37	111.76	108.00

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3650	77	0
1	B	3440	0	3343	80	0
2	C	282	0	159	5	0
2	E	244	0	135	6	0
3	D	286	0	158	5	0
3	F	265	0	147	8	0
4	A	5	0	0	0	0
5	A	53	0	33	3	0
5	B	53	0	33	1	0
6	A	106	0	0	3	0
6	B	55	0	0	1	0
6	C	12	0	0	0	0
6	D	4	0	0	0	0
6	F	1	0	0	0	0
All	All	8521	0	7658	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:H	1:A:184:ASN:HD22	1.25	0.82
3:F:12:DC:H2"	3:F:13:DG:C8	2.20	0.77
1:B:450:ARG:NH2	2:E:12:DG:O6	2.18	0.76
1:B:123:LYS:NZ	6:B:601:HOH:O	2.18	0.75
1:B:358:PRO:HB2	1:B:458:ILE:HD13	1.71	0.72
1:B:40:SER:HB3	1:B:114:VAL:HG21	1.75	0.69
3:F:8:DA:H2"	3:F:9:DA:H5"	1.76	0.68
1:B:435:GLU:O	1:B:437:THR:N	2.23	0.67
1:B:3:MET:HE1	1:B:39:PHE:HB2	1.75	0.67
1:B:61:PHE:HA	1:B:411:ARG:HH12	1.59	0.66
1:A:121:ARG:NH2	1:B:390:GLU:OE2	2.29	0.66
1:A:432:GLY:HA2	3:D:9:DA:H5'	1.79	0.65
1:B:23:TYR:OH	1:B:116:ASP:OD2	2.10	0.64
1:B:3:MET:HG3	1:B:35:TRP:CE3	2.32	0.64
1:A:435:GLU:HG3	1:A:436:VAL:HG23	1.81	0.63
1:A:177:GLU:OE2	1:A:280:ARG:NH1	2.32	0.62
1:B:346:THR:HG23	1:B:349:GLU:OE2	1.99	0.62
1:A:303:LEU:O	1:A:307:GLU:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLU:HG3	1:A:163:PHE:CD1	2.34	0.61
1:B:238:LYS:NZ	1:B:242:GLU:OE2	2.33	0.61
1:B:102:SER:O	1:B:105:VAL:HG22	2.00	0.61
2:C:9:DC:H2'	2:C:10:DG:C8	2.36	0.60
1:B:429:ARG:HG2	1:B:430:ALA:H	1.67	0.60
1:A:431:TRP:CD1	1:A:441:ARG:HB2	2.37	0.60
1:B:420:ALA:HB1	1:B:426:VAL:HG21	1.84	0.58
1:A:142:ASP:OD2	1:A:148:PRO:HA	2.03	0.58
1:A:411:ARG:CZ	1:A:411:ARG:HB2	2.33	0.57
1:A:161:HIS:HB3	2:C:7:DT:OP2	2.05	0.57
1:A:367:LEU:HB2	1:A:373:MET:HE3	1.88	0.55
1:B:33:ASP:OD2	1:B:280:ARG:HD2	2.07	0.55
1:B:226:GLU:HB3	1:B:228:TRP:CZ2	2.41	0.55
1:B:366:GLU:HG2	1:B:373:MET:HA	1.88	0.54
1:A:158:TYR:CE2	3:D:11:DC:H4'	2.42	0.54
1:B:361:ASN:O	1:B:365:MET:HG2	2.07	0.54
1:B:346:THR:H	1:B:349:GLU:HG3	1.71	0.54
1:B:130:VAL:O	1:B:134:ILE:HG12	2.08	0.53
1:A:216:ALA:HB1	1:A:224:LEU:HD12	1.91	0.53
1:A:253:GLY:HA2	1:A:256:ARG:HD3	1.91	0.52
1:A:379:MET:HE3	1:A:443:MET:SD	2.48	0.52
1:B:164:ARG:HG3	1:B:304:ILE:HG13	1.91	0.52
1:B:430:ALA:HB3	3:F:9:DA:H2"	1.91	0.52
1:A:61:PHE:HD2	1:A:211:LEU:HD11	1.74	0.52
1:B:93:LEU:HD21	1:B:104:PHE:HB2	1.91	0.52
1:B:367:LEU:HB2	1:B:373:MET:HE2	1.91	0.52
1:B:22:VAL:HA	1:B:52:VAL:O	2.10	0.51
1:B:345:TYR:HB3	1:B:349:GLU:HB2	1.91	0.51
1:B:9:ARG:NH2	1:B:314:TYR:OH	2.44	0.51
1:A:237:ALA:HB2	1:A:270:TYR:CD1	2.46	0.51
1:A:68:GLN:HG3	1:A:408:LEU:HD23	1.93	0.50
1:A:21:VAL:HG21	1:A:43:ILE:HG13	1.93	0.50
1:A:121:ARG:HE	1:B:390:GLU:CG	2.24	0.50
1:A:252:TYR:OH	5:A:502:FDA:O2A	2.25	0.50
1:A:93:LEU:HD23	1:A:100:LYS:HB3	1.93	0.50
1:A:41:ARG:NH2	1:A:184:ASN:HA	2.26	0.50
1:B:59:ASP:O	1:B:62:LEU:HB3	2.12	0.50
1:B:3:MET:HG2	1:B:4:ASN:N	2.26	0.50
1:A:285:VAL:O	1:A:295:LYS:HE3	2.12	0.50
1:B:420:ALA:HB1	1:B:426:VAL:CG2	2.42	0.49
1:B:101:ILE:O	1:B:105:VAL:HG13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:NH1	6:A:603:HOH:O	2.26	0.49
1:A:57:LEU:HD13	1:A:203:VAL:HG11	1.93	0.49
1:A:280:ARG:O	1:A:284:GLU:HG2	2.13	0.49
1:B:429:ARG:HG2	1:B:430:ALA:N	2.28	0.49
1:B:74:LYS:HB3	1:B:232:PRO:HG2	1.95	0.49
3:F:2:DT:H2"	3:F:3:DG:C8	2.48	0.49
1:A:69:TYR:HB2	6:A:647:HOH:O	2.13	0.48
1:B:291:ASN:HB3	1:B:294:SER:HB2	1.94	0.48
1:A:3:MET:HG3	1:A:35:TRP:CE3	2.48	0.48
1:A:208:VAL:O	1:A:212:LEU:HG	2.12	0.48
1:B:268:SER:OG	1:B:269:PRO:HD3	2.14	0.48
1:A:127:ILE:O	1:A:131:ILE:HG13	2.14	0.48
1:B:347:LEU:HD12	1:B:347:LEU:O	2.13	0.48
1:A:8:ILE:HG13	1:A:141:VAL:HG22	1.96	0.48
1:A:30:ARG:NE	1:A:33:ASP:O	2.34	0.48
1:A:11:LEU:HD11	1:A:140:GLU:HB2	1.96	0.47
1:B:323:GLU:HG3	1:B:323:GLU:O	2.15	0.47
1:A:158:TYR:CZ	3:D:11:DC:H4'	2.50	0.47
1:A:322:PHE:CE2	1:A:330:LYS:HG2	2.50	0.47
1:A:450:ARG:NH2	2:C:12:DG:O6	2.42	0.47
1:B:38:LEU:HD13	1:B:179:PRO:HD2	1.96	0.47
1:A:52:VAL:HG12	1:A:89:PRO:HD2	1.95	0.47
1:A:455:LYS:O	1:A:459:GLU:HB2	2.15	0.47
1:A:384:LYS:HB3	1:A:388:TRP:CZ3	2.50	0.46
1:B:167:LEU:HD23	1:B:304:ILE:HD13	1.98	0.46
1:B:278:SER:O	1:B:282:VAL:HG23	2.16	0.46
1:A:420:ALA:HB1	1:A:426:VAL:HG21	1.96	0.46
1:B:19:GLY:HA3	1:B:109:ASN:O	2.16	0.46
1:A:299:LEU:O	1:A:303:LEU:HB2	2.16	0.45
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.72	0.45
1:A:427:HIS:HD2	6:A:645:HOH:O	1.98	0.45
1:B:249:LEU:O	1:B:294:SER:HB3	2.16	0.45
3:F:12:DC:H2"	3:F:13:DG:N7	2.30	0.45
1:B:3:MET:O	1:B:5:PRO:HD3	2.17	0.45
1:B:115:THR:O	1:B:140:GLU:HA	2.16	0.45
1:B:152:ALA:HA	1:B:170:LEU:HD22	1.97	0.45
1:B:371:GLY:HA3	1:B:408:LEU:HD13	1.99	0.45
1:B:457:TYR:CE1	1:B:461:TYR:HE2	2.34	0.45
1:B:384:LYS:HD3	1:B:384:LYS:HA	1.65	0.45
1:B:414:ASN:HB2	5:B:501:FDA:C2	2.47	0.45
1:B:299:LEU:O	1:B:303:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG22	1:A:139:PHE:HB2	1.99	0.44
1:A:262:ASN:O	1:A:262:ASN:ND2	2.50	0.44
1:B:62:LEU:HD13	1:B:69:TYR:CG	2.52	0.44
1:B:146:VAL:O	1:B:174:PHE:HB3	2.18	0.44
5:A:502:FDA:O3'	5:A:502:FDA:N1	2.49	0.44
1:A:67:ARG:HG3	1:A:68:GLN:HG3	1.98	0.44
2:C:13:DC:H2"	2:C:14:DA:C8	2.53	0.44
1:A:134:ILE:HD12	1:A:136:ILE:O	2.18	0.44
1:A:123:LYS:O	1:A:127:ILE:HG13	2.17	0.44
1:A:221:LYS:HB3	1:A:221:LYS:HE3	1.60	0.44
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.77	0.43
1:B:44:ALA:HB1	1:B:49:VAL:O	2.18	0.43
1:A:259:PRO:HD2	1:A:452:PHE:CG	2.53	0.43
1:B:164:ARG:O	1:B:168:TYR:HD2	2.00	0.43
1:A:332:SER:O	1:A:336:HIS:HD2	2.02	0.43
1:A:377:MET:HG3	1:A:457:TYR:CE2	2.53	0.43
1:A:121:ARG:NE	1:B:390:GLU:OE2	2.52	0.43
1:A:368:LEU:HA	1:A:368:LEU:HD23	1.85	0.43
2:E:4:DG:H2'	2:E:5:DG:C8	2.54	0.43
1:A:431:TRP:NE1	1:A:441:ARG:HB2	2.34	0.43
1:B:20:PRO:HA	1:B:49:VAL:HG22	2.00	0.43
1:B:230:PHE:HE2	1:B:266:ASN:HB3	1.83	0.43
1:B:101:ILE:HD13	1:B:101:ILE:HA	1.86	0.43
2:E:12:DG:H1	3:F:4:DC:H42	1.66	0.43
1:A:7:ARG:O	1:A:141:VAL:HA	2.19	0.43
1:A:380:TYR:CE1	1:A:384:LYS:HE2	2.54	0.43
1:B:164:ARG:NH2	2:E:7:DT:OP2	2.52	0.43
2:C:9:DC:H2"	2:C:10:DG:H5'	2.00	0.43
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.80	0.43
1:A:105:VAL:HG11	1:A:134:ILE:HG22	2.01	0.42
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.82	0.42
1:B:386:LEU:HD23	1:B:437:THR:HG22	2.01	0.42
2:E:3:DC:H42	3:F:13:DG:H1	1.65	0.42
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.54	0.42
1:B:152:ALA:HA	1:B:170:LEU:CD2	2.49	0.42
1:A:244:PHE:CD1	1:A:265:SER:HA	2.54	0.42
1:A:343:HIS:O	1:A:388:TRP:HA	2.20	0.42
1:B:45:LYS:HB2	1:B:45:LYS:HE3	1.69	0.42
1:A:278:SER:O	1:A:282:VAL:HG23	2.20	0.42
5:A:502:FDA:H5'2	5:A:502:FDA:H3B	2.01	0.42
1:A:3:MET:CE	1:A:35:TRP:HB3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:HA	1:B:411:ARG:NH1	2.31	0.42
1:A:125:GLN:HE22	1:B:340:VAL:HA	1.83	0.42
1:B:41:ARG:NH2	1:B:183:PRO:O	2.41	0.42
2:E:5:DG:H2"	2:E:6:DC:C6	2.54	0.42
1:B:55:PHE:HE1	1:B:57:LEU:HB2	1.85	0.42
1:A:365:MET:CB	1:A:461:TYR:HB3	2.50	0.41
1:A:122:ILE:HD12	1:A:125:GLN:HB2	2.02	0.41
1:A:66:ILE:HD12	1:A:215:ARG:HB2	2.02	0.41
1:A:73:LEU:HD23	1:A:204:LEU:HB2	2.02	0.41
1:B:56:CYS:HA	1:B:93:LEU:O	2.20	0.41
1:B:57:LEU:HD22	1:B:73:LEU:HD21	2.01	0.41
1:B:86:LYS:NZ	1:B:181:LEU:HB3	2.35	0.41
1:B:333:LEU:HD23	1:B:333:LEU:HA	1.86	0.41
1:A:176:GLU:O	1:A:283:LEU:HD11	2.20	0.41
1:A:359:LEU:O	1:A:359:LEU:HD12	2.21	0.41
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.78	0.41
1:B:231:GLU:HA	1:B:232:PRO:HD3	1.86	0.41
1:B:429:ARG:HG3	3:F:10:DG:N2	2.35	0.41
3:D:11:DC:H6	3:D:11:DC:H2'	1.71	0.41
3:D:13:DG:H2"	3:D:14:DA:N7	2.36	0.41
1:A:57:LEU:N	1:A:93:LEU:O	2.52	0.41
1:B:45:LYS:HE2	1:B:182:GLU:CD	2.41	0.41
1:B:114:VAL:HG12	1:B:139:PHE:HB2	2.02	0.40
1:A:199:THR:HG22	1:A:201:SER:H	1.86	0.40
1:B:111:GLY:O	1:B:136:ILE:HB	2.21	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.96	0.40
1:A:367:LEU:HD13	1:A:407:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	454/498 (91%)	427 (94%)	27 (6%)	0	100 100
1	B	415/498 (83%)	397 (96%)	17 (4%)	1 (0%)	47 53
All	All	869/996 (87%)	824 (95%)	44 (5%)	1 (0%)	51 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	VAL

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%)	381 (96%)	16 (4%)	31 34
1	B	367/429 (86%)	346 (94%)	21 (6%)	20 19
All	All	764/858 (89%)	727 (95%)	37 (5%)	25 25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	51	VAL
1	A	60	GLU
1	A	85	ARG
1	A	90	SER
1	A	96	ASP
1	A	138	PHE
1	A	185	SER
1	A	198	GLU
1	A	221	LYS
1	A	238	LYS
1	A	257	ASN
1	A	310	ASP
1	A	327	SER
1	A	411	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	LYS
1	B	9	ARG
1	B	16	GLN
1	B	51	VAL
1	B	100	LYS
1	B	116	ASP
1	B	135	SER
1	B	136	ILE
1	B	146	VAL
1	B	149	CYS
1	B	171	LEU
1	B	173	GLU
1	B	242	GLU
1	B	256	ARG
1	B	289	GLU
1	B	300	ASP
1	B	332	SER
1	B	355	THR
1	B	363	SER
1	B	403	ASN
1	B	446	GLU
1	B	451	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	184	ASN
1	A	427	HIS
1	B	124	ASN
1	B	266	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	$\#\|Z\| > 2$
4	SO4	A	501	-	4,4,4	0.12	0	6,6,6	0.35	0
5	FDA	A	502	-	52,58,58	0.58	0	60,89,89	0.96	5 (8%)
5	FDA	B	501	-	52,58,58	0.64	0	60,89,89	0.77	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FDA	A	502	-	-	4/30/50/50	0/6/6/6
5	FDA	B	501	-	-	1/30/50/50	0/6/6/6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	FDA	O5'-P-O1P	-2.54	99.15	109.07
5	A	502	FDA	P-O3P-PA	2.48	141.34	132.83
5	A	502	FDA	N3-C2-N1	2.45	119.74	115.80
5	A	502	FDA	O2-C2-N3	-2.40	117.30	121.82
5	B	501	FDA	C5A-C6A-N6A	2.34	123.91	120.35
5	B	501	FDA	N3-C2-N1	2.22	119.36	115.80
5	A	502	FDA	C5A-C6A-N6A	2.03	123.43	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	FDA	O4B-C4B-C5B-O5B
5	A	502	FDA	C3B-C4B-C5B-O5B
5	B	501	FDA	C4'-C5'-O5'-P
5	A	502	FDA	O4'-C4'-C5'-O5'
5	A	502	FDA	C4'-C5'-O5'-P

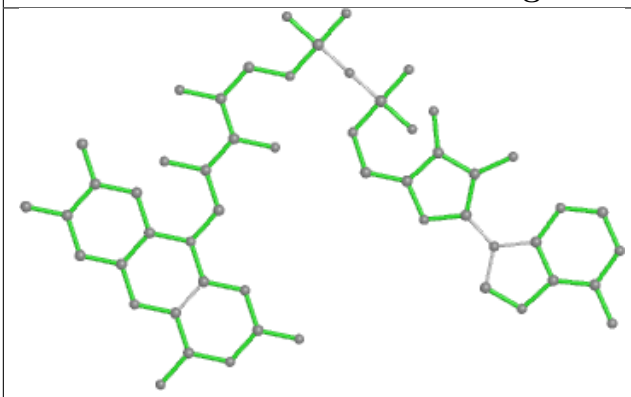
There are no ring outliers.

2 monomers are involved in 4 short contacts:

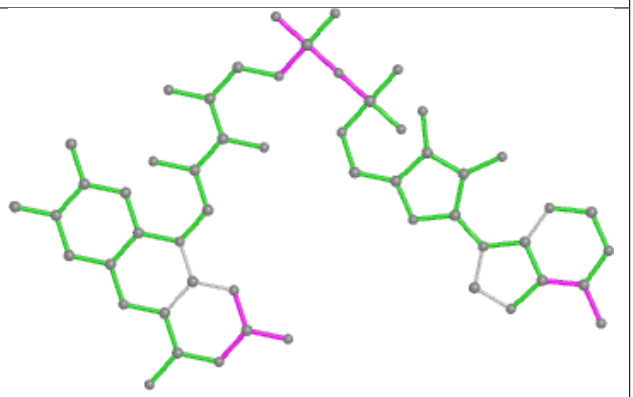
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	FDA	3	0
5	B	501	FDA	1	0

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 then 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.

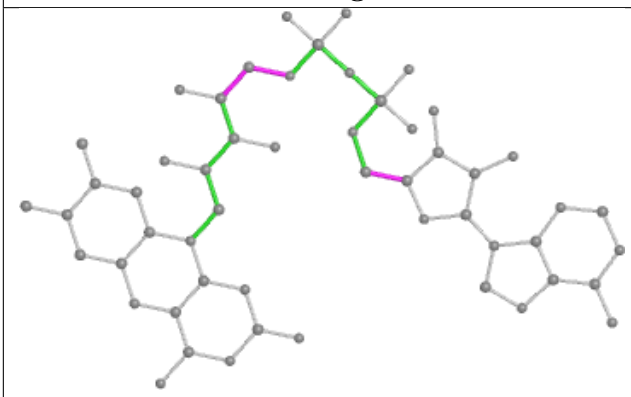
Ligand FDA A 502



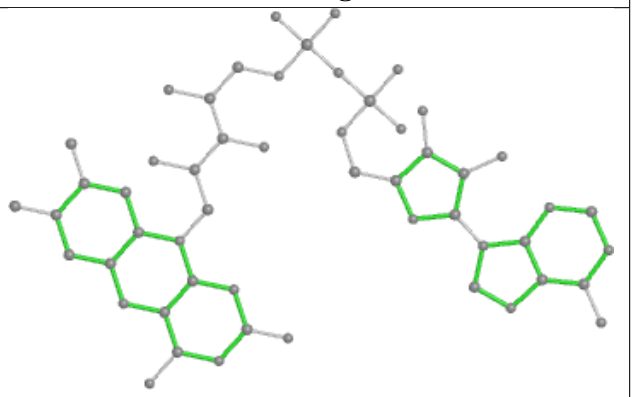
Bond lengths



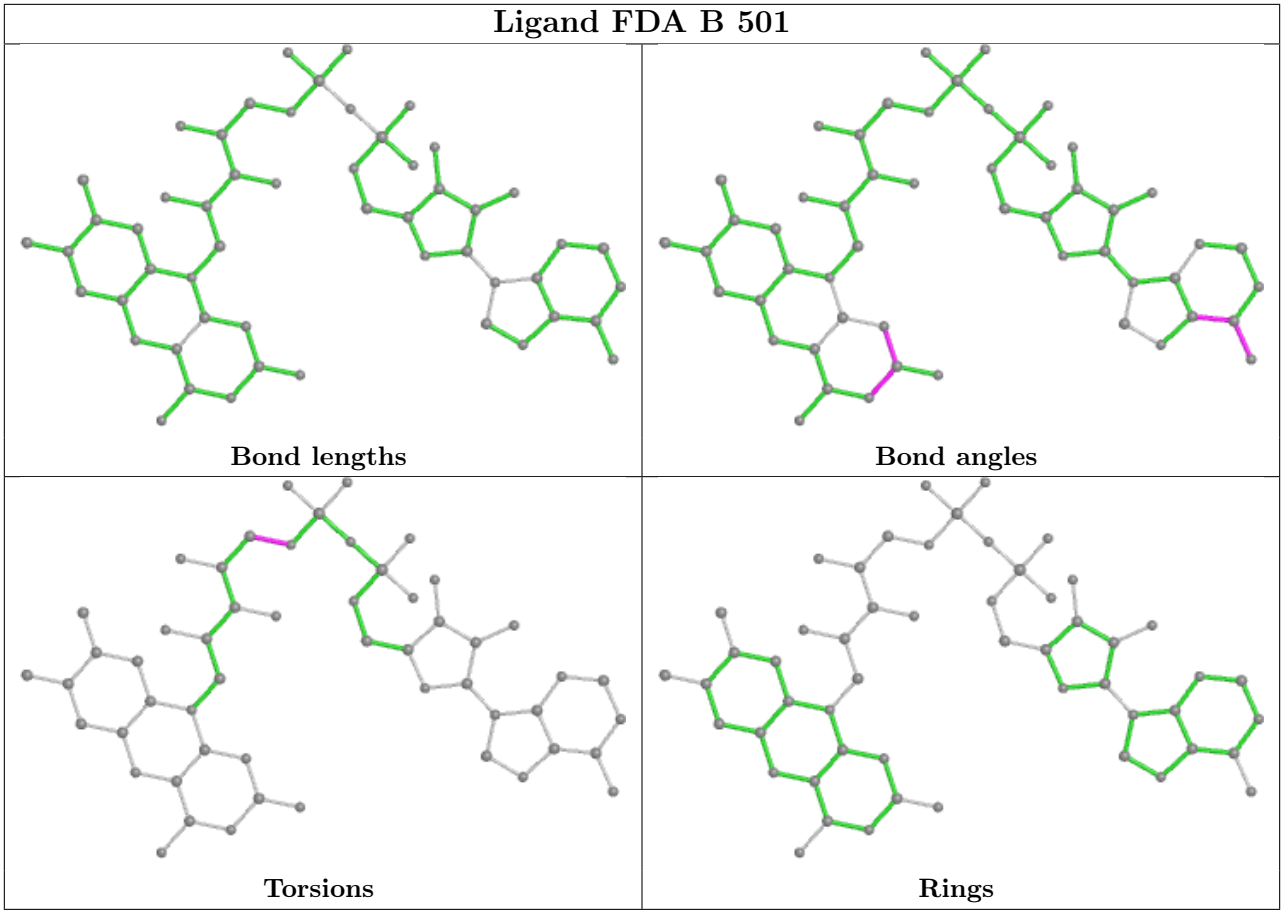
Bond angles



Torsions



Rings



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	458/498 (91%)	0.04	8 (1%) 70 71	23, 39, 73, 119	0
1	B	421/498 (84%)	0.44	22 (5%) 27 26	32, 58, 87, 103	0
2	C	14/14 (100%)	0.71	2 (14%) 2 2	42, 70, 106, 129	0
2	E	12/14 (85%)	0.54	2 (16%) 1 1	56, 79, 114, 130	0
3	D	14/14 (100%)	0.17	0 100 100	51, 72, 91, 101	0
3	F	13/14 (92%)	1.05	2 (15%) 2 1	75, 90, 110, 115	0
All	All	932/1052 (88%)	0.25	36 (3%) 39 39	23, 49, 88, 130	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ALA	4.8
1	B	252	TYR	4.8
1	B	288	ALA	4.1
1	B	61	PHE	4.1
1	A	108	TYR	4.1
1	B	108	TYR	3.9
1	B	59	ASP	3.7
2	C	2	DT	3.6
1	B	36	ALA	3.4
1	A	468	ALA	3.4
1	A	109	ASN	3.4
2	C	1	DA	2.7
1	B	69	TYR	2.7
3	F	5	DG	2.6
1	B	289	GLU	2.6
1	B	57	LEU	2.5
1	A	15	LYS	2.5
1	B	66	ILE	2.5
1	B	188	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	134	ILE	2.4
1	B	62	LEU	2.4
1	B	228	TRP	2.4
1	A	469	ALA	2.4
1	B	271	LEU	2.3
1	B	19	GLY	2.3
1	A	91	PHE	2.3
2	E	4	DG	2.3
3	F	4	DC	2.2
2	E	3	DC	2.1
1	B	130	VAL	2.1
1	A	47	ALA	2.1
1	B	94	ARG	2.1
1	B	278	SER	2.1
1	A	186	VAL	2.1
1	B	137	PRO	2.1
1	B	272	HIS	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, 95^{th} 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.

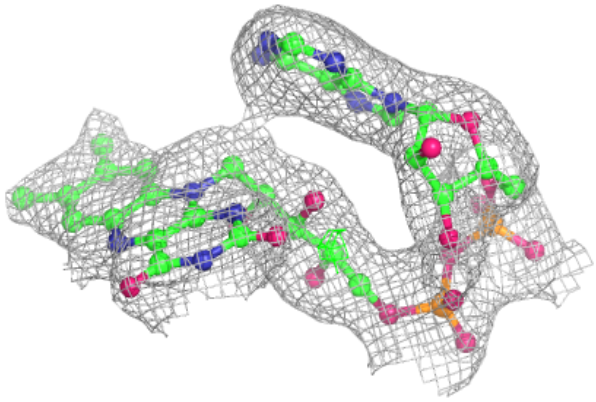
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FDA	B	501	53/53	0.94	0.17	35,45,51,56	0
5	FDA	A	502	53/53	0.96	0.14	17,26,31,35	0
4	SO4	A	501	5/5	0.98	0.11	27,34,39,40	0

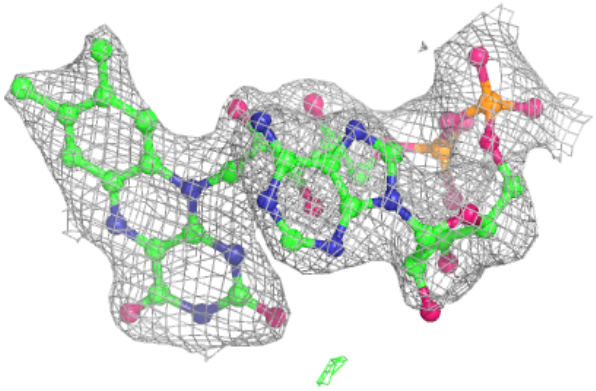
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

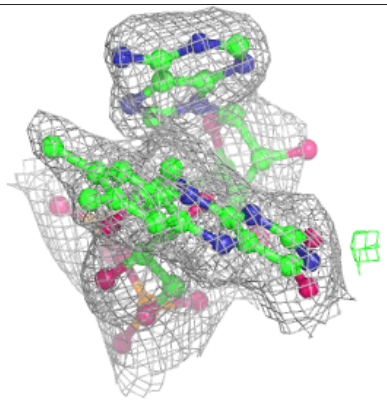
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

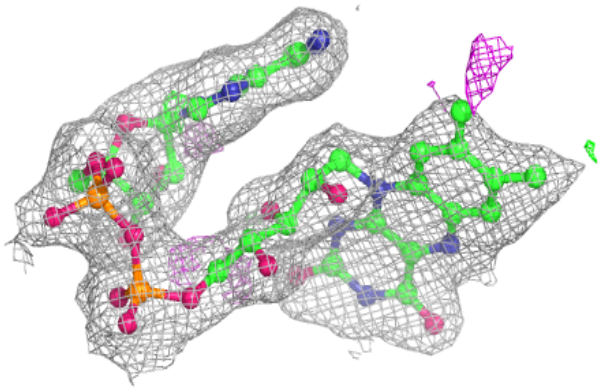


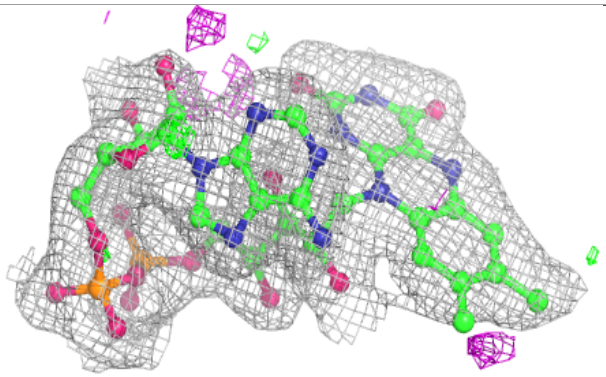


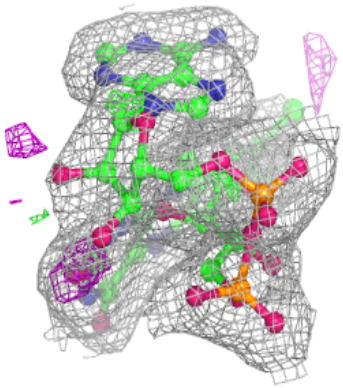


Electron density around FDA A 502:

$2mF_o$-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.