



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 AM UTC

PDB ID : 8OYC / pdb_00008oyc
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (100 microsecond timepoint)
Authors : Lane, T.J.; Christou, N.-E.; Melo, D.V.M.; Apostolopoulou, V.; Pateras, A.; Mashhour, A.R.; Galchenkova, M.; Gunther, S.; Reinke, P.; Kremling, V.; Oberthuer, D.; Henkel, A.; Sprenger, J.; Scheer, T.E.S.; Lange, E.; Yefanov, O.N.; Middendorf, P.; Sellberg, J.A.; Schubert, R.; Fadini, A.; Cirelli, C.; Beale, E.V.; Johnson, P.; Dworkowski, F.; Ozerov, D.; Bertrand, Q.; Wranik, M.; Zitter, E.D.; Turk, D.; Bajt, S.; Chapman, H.; Bacellar, C.
Deposited on : 2023-05-03
Resolution : 2.50 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)

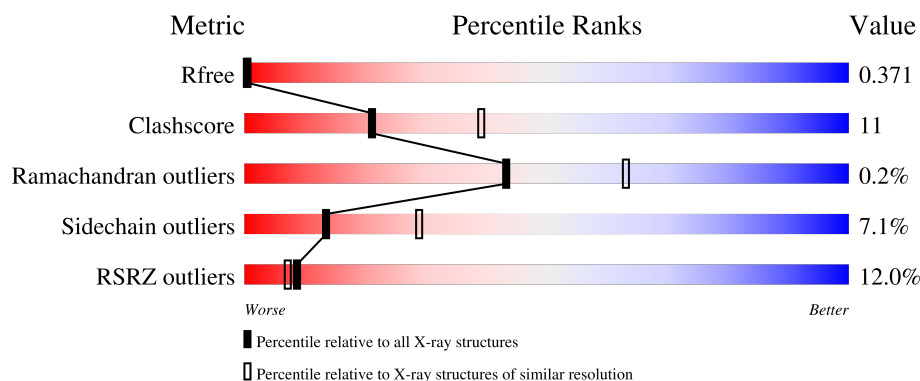
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	36%29%71%
2	E	14	43%36%50%14%
3	D	14	7%57%43%
3	F	14	43%29%64%7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8625 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	460	Total	C	N	O	S	0	3	0
			3746	2406	630	695	15			
1	B	425	Total	C	N	O	S	0	0	0
			3479	2240	585	639	15			

There are 68 discrepancies between the modelled and reference sequences:

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

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

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

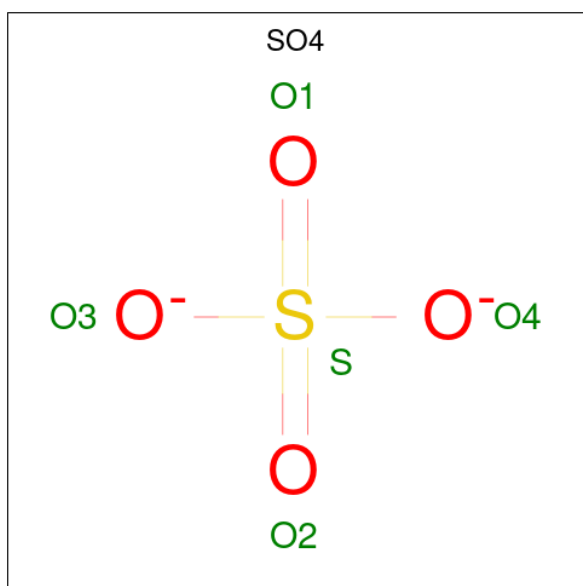
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	1	0
			302	145	53	90	14			
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.

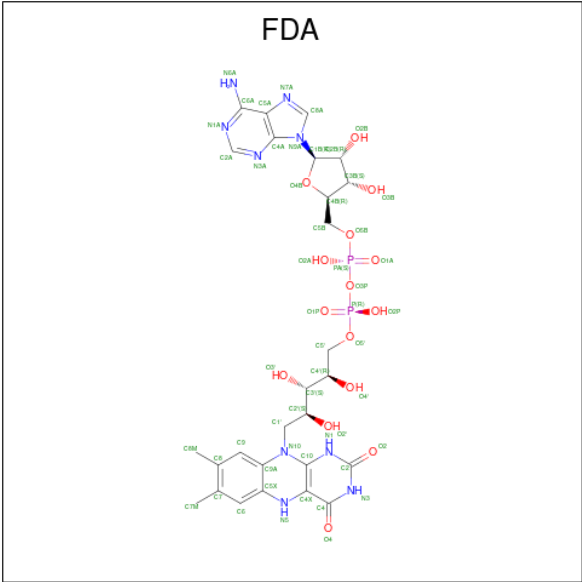
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

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



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

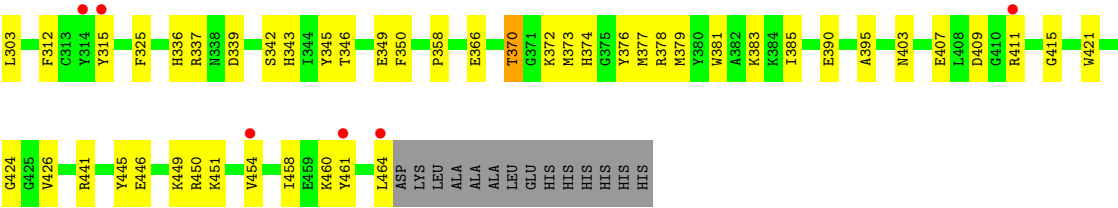
- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



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	112	Total	O	0	0
			112	112		
6	B	60	Total	O	0	0
			60	60		
6	C	11	Total	O	0	0
			11	11		
6	D	4	Total	O	0	0
			4	4		
6	E	2	Total	O	0	0
			2	2		
6	F	3	Total	O	0	0
			3	3		



● Molecule 2: CPD-COMPRISED OLIGONUCLEOTIDE



● Molecule 2: CPD-COMPRISED 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)	30.98 – 2.50 30.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.98-2.50) 95.4 (30.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.304 , 0.371 0.304 , 0.371	Depositor DCC
R_{free} test set	2464 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8625	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: SO4, FDA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3845	0.65	0/5198
1	B	0.40	2/3575 (0.1%)	0.56	0/4831
2	C	0.38	0/337	0.62	0/518
2	E	0.37	0/272	0.56	0/417
3	D	0.41	0/321	0.52	0/494
3	F	0.33	0/297	0.48	0/457
All	All	0.41	2/8647 (0.0%)	0.60	0/11915

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	LEU	C-N	-7.01	1.24	1.34
1	B	256	ARG	C-N	5.78	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	3746	0	3669	68	0
1	B	3479	0	3390	86	0
2	C	302	0	171	11	0
2	E	244	0	135	6	0
3	D	286	0	158	6	0
3	F	265	0	147	7	0
4	A	5	0	0	0	0
5	A	53	0	33	1	0
5	B	53	0	33	2	0
6	A	112	0	0	3	0
6	B	60	0	0	3	0
6	C	11	0	0	2	0
6	D	4	0	0	0	0
6	E	2	0	0	0	0
6	F	3	0	0	1	0
All	All	8625	0	7736	175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:HB3	1:A:294:SER:HB2	1.52	0.90
1:A:3:MET:HE2	1:A:39:PHE:HB2	1.64	0.79
1:A:114:VAL:HG22	1:A:139:PHE:HB2	1.67	0.77
1:B:49:VAL:HG22	1:B:50:PRO:HD2	1.69	0.75
1:B:35:TRP:HD1	6:B:622:HOH:O	1.69	0.75
1:B:7:ARG:NH2	1:B:174:PHE:O	2.25	0.69
2:E:5:DG:H1	3:F:10:DG:H1	1.41	0.68
1:B:143:ALA:HA	6:B:622:HOH:O	1.96	0.66
1:B:12:LYS:HD3	1:B:131:ILE:HG23	1.79	0.65
1:A:441:ARG:HH12	2:C:8:DT:H5'	1.62	0.64
1:A:218:LEU:HD23	1:A:468:ALA:HB2	1.79	0.64
1:B:266:ASN:HA	1:B:372:LYS:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ARG:HH12	2:E:8:DT:H5'	1.63	0.64
2:C:2:DT:H4'	2:C:3:DC:H5'	1.79	0.64
1:B:6:LYS:HD2	1:B:174:PHE:HZ	1.63	0.63
2:C:9:DC:H2'	2:C:10:DG:C8	2.34	0.63
1:B:23:TYR:OH	1:B:116:ASP:OD1	2.17	0.62
1:B:21:VAL:HG13	1:B:112:THR:HB	1.81	0.62
1:A:21:VAL:HG21	1:A:43:ILE:HG13	1.82	0.61
1:A:86:LYS:HD2	1:A:181:LEU:HD23	1.82	0.61
1:B:52:VAL:HG12	1:B:89:PRO:HG2	1.84	0.60
1:A:441:ARG:NH1	2:C:8:DT:H5'	2.17	0.59
1:B:383:LYS:NZ	1:B:441:ARG:O	2.30	0.59
1:B:336:HIS:ND1	1:B:339:ASP:OD2	2.35	0.59
3:F:7:DG:H2''	3:F:8:DA:C8	2.38	0.58
2:C:9:DC:H2''	2:C:10:DG:H5'	1.84	0.58
1:A:459:GLU:O	1:A:462:SER:HB3	2.03	0.58
1:B:72:MET:HE3	1:B:73:LEU:HD22	1.86	0.58
1:B:35:TRP:CD1	6:B:622:HOH:O	2.50	0.57
1:B:291:ASN:HB3	1:B:294:SER:HB2	1.87	0.56
1:A:177:GLU:HG3	1:A:178:PHE:N	2.21	0.55
5:B:501:FDA:O3'	5:B:501:FDA:N1	2.38	0.55
1:B:45:LYS:NZ	1:B:182:GLU:OE2	2.39	0.55
1:A:66:ILE:HD11	1:A:212:LEU:HD23	1.88	0.55
1:B:373:MET:HE1	1:B:381:TRP:CD1	2.41	0.54
1:B:161:HIS:HA	1:B:164:ARG:HH12	1.72	0.54
1:B:282:VAL:O	1:B:286:GLU:HG2	2.08	0.54
1:B:374:HIS:CD2	1:B:376:TYR:H	2.25	0.54
1:A:348:GLU:H	1:A:348:GLU:CD	2.15	0.54
1:B:370:THR:HG23	1:B:372:LYS:H	1.73	0.54
1:A:384:LYS:HB3	1:A:388:TRP:CZ3	2.43	0.54
1:B:105:VAL:HG22	1:B:110:ALA:HB3	1.89	0.54
1:A:112:THR:HG22	1:A:137:PRO:HG2	1.91	0.53
1:A:69:TYR:CE2	1:A:207:GLY:HA3	2.43	0.53
1:B:446:GLU:HA	1:B:449:LYS:HD3	1.91	0.52
2:E:9:DC:H2'	2:E:10:DG:C8	2.45	0.52
1:B:358:PRO:HB2	1:B:458:ILE:HD13	1.92	0.52
1:B:6:LYS:HD2	1:B:174:PHE:CZ	2.44	0.52
2:C:1:DA:H2'	2:C:2:DT:C4	2.45	0.51
1:B:6:LYS:NZ	1:B:173:GLU:OE2	2.26	0.51
1:B:77:GLN:O	1:B:81:VAL:HG23	2.11	0.51
1:A:50:PRO:HD3	1:A:186:VAL:HG11	1.92	0.50
1:B:112:THR:HG23	1:B:137:PRO:HG2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:H	1:B:68:GLN:CD	2.19	0.50
1:A:177:GLU:HG3	1:A:178:PHE:H	1.76	0.50
1:B:262:ASN:OD1	1:B:262:ASN:N	2.43	0.50
1:A:93:LEU:HD11	1:A:104:PHE:HB2	1.94	0.50
1:A:426:VAL:O	1:A:427:HIS:HB2	2.11	0.50
1:B:366:GLU:O	1:B:370:THR:HG22	2.12	0.49
1:B:445:TYR:O	1:B:449:LYS:HG3	2.12	0.49
1:A:262:ASN:N	6:A:609:HOH:O	2.45	0.49
1:A:164:ARG:HB3	1:A:165:PRO:HD3	1.94	0.49
1:B:449:LYS:HG2	1:B:454:VAL:HG21	1.94	0.49
1:A:237:ALA:HB2	1:A:270:TYR:CD1	2.47	0.49
1:B:30:ARG:HG3	1:B:32:GLU:O	2.12	0.49
1:A:429:ARG:NH2	3:D:9:DA:N3	2.61	0.49
1:B:379:MET:HG2	1:B:421:TRP:CZ3	2.47	0.48
1:A:432:GLY:HA2	3:D:9:DA:H5'	1.95	0.48
2:E:12:DG:C8	2:E:12:DG:H5'	2.49	0.48
1:B:373:MET:O	1:B:378:ARG:NH1	2.46	0.48
2:E:11:DC:H2''	2:E:12:DG:H5'	1.95	0.48
1:B:385:ILE:HG22	1:B:395:ALA:HB1	1.96	0.48
1:B:64:ALA:HB3	1:B:411:ARG:HH21	1.79	0.48
2:C:9:DC:OP1	6:C:101:HOH:O	2.20	0.48
1:B:30:ARG:HD3	1:B:274:GLY:O	2.14	0.47
1:A:204:LEU:O	1:A:208:VAL:HG23	2.13	0.47
1:A:442:TYR:CE2	1:A:444:SER:HB3	2.49	0.47
1:B:407:GLU:HB3	1:B:409:ASP:OD1	2.14	0.47
1:B:61:PHE:CZ	1:B:122:ILE:HG21	2.50	0.47
3:F:12:DC:H4'	3:F:13:DG:OP1	2.14	0.47
1:B:59:ASP:HA	1:B:62:LEU:HB2	1.96	0.47
1:B:127:ILE:O	1:B:131:ILE:HG13	2.15	0.47
2:C:4:DG:H2''	2:C:5:DG:C8	2.49	0.47
1:A:259:PRO:HD2	1:A:452:PHE:CG	2.50	0.46
1:B:12:LYS:H	1:B:138:PHE:HB3	1.81	0.46
1:B:446:GLU:H	1:B:446:GLU:CD	2.23	0.46
1:A:299:LEU:O	1:A:303:LEU:HB2	2.16	0.46
1:B:346:THR:O	1:B:349:GLU:N	2.48	0.46
1:A:257:ASN:OD1	6:A:601:HOH:O	2.21	0.46
1:A:219:LYS:HE3	1:A:469:ALA:HB3	1.96	0.46
1:B:154:GLN:HA	1:B:315:TYR:OH	2.16	0.46
1:A:52:VAL:HG12	1:A:89:PRO:HG2	1.98	0.45
1:B:403:ASN:OD1	1:B:407:GLU:HG3	2.16	0.45
1:A:145:ASN:HB3	1:A:307:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:TYR:HE2	1:A:444:SER:HB3	1.80	0.45
1:B:342:SER:O	1:B:343:HIS:ND1	2.50	0.45
1:A:114:VAL:HA	1:A:139:PHE:O	2.17	0.45
1:A:394:LYS:O	1:A:398:ILE:HG13	2.16	0.45
1:A:446:GLU:OE1	1:A:446:GLU:N	2.45	0.45
1:B:376:TYR:OH	1:B:451:LYS:NZ	2.40	0.45
1:B:59:ASP:O	1:B:63:GLU:N	2.49	0.45
1:B:252:TYR:HD1	1:B:263:MET:O	2.00	0.45
1:A:394:LYS:HE2	1:A:394:LYS:HB2	1.73	0.44
1:B:345:TYR:HB2	1:B:350:PHE:CZ	2.51	0.44
1:B:460:LYS:HE3	1:B:461:TYR:CZ	2.52	0.44
1:A:285:VAL:O	1:A:295:LYS:HE3	2.17	0.44
1:B:67:ARG:HG3	1:B:68:GLN:CD	2.42	0.44
3:D:14:DA:H8	3:D:14:DA:OP2	1.99	0.44
1:A:244:PHE:CD1	1:A:265:SER:HA	2.52	0.44
1:B:415:GLY:HA2	5:B:501:FDA:N5	2.32	0.44
1:A:216:ALA:HB1	1:A:224:LEU:HD12	1.99	0.44
1:B:460:LYS:HE3	1:B:461:TYR:OH	2.17	0.44
1:A:389[A]:SER:OG	1:A:395:ALA:HB2	2.18	0.44
2:C:9:DC:C2'	2:C:10:DG:H5'	2.48	0.44
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.80	0.43
1:A:5:PRO:C	1:A:7:ARG:H	2.25	0.43
1:B:374:HIS:HD2	1:B:377:MET:H	1.66	0.43
1:A:45:LYS:HA	6:A:673:HOH:O	2.19	0.43
1:A:199:THR:HG23	1:A:201:SER:H	1.82	0.43
1:A:458:ILE:O	1:A:462:SER:N	2.52	0.43
3:D:1:DT:H6	3:D:1:DT:H2'	1.56	0.43
1:A:41:ARG:NE	1:A:182:GLU:O	2.42	0.43
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.80	0.43
1:A:268:SER:HB3	5:A:502:FDA:H5'2	1.99	0.43
1:B:161:HIS:HA	1:B:164:ARG:NH1	2.33	0.43
1:B:178:PHE:CE2	1:B:279:GLN:HB3	2.53	0.43
1:A:332:SER:O	1:A:336:HIS:HD2	2.02	0.43
1:B:325:PHE:CD1	1:B:424:GLY:HA3	2.54	0.43
3:D:1:DT:H72	3:D:2:DT:O4'	2.18	0.43
1:B:115:THR:O	1:B:140:GLU:HA	2.18	0.43
1:B:259:PRO:HG3	1:B:374:HIS:CD2	2.54	0.42
1:B:374:HIS:CD2	1:B:376:TYR:N	2.87	0.42
1:A:5:PRO:C	1:A:7:ARG:N	2.78	0.42
1:B:23:TYR:CD1	1:B:114:VAL:HG23	2.55	0.42
1:B:41:ARG:NH2	1:B:183:PRO:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:DG:H2''	3:D:8:DA:C8	2.54	0.42
3:F:5:DG:C2	3:F:6:DC:C2	3.07	0.42
1:A:73:LEU:CB	1:A:204:LEU:HD13	2.48	0.42
1:A:323[B]:GLU:HG2	1:B:337:ARG:NH2	2.34	0.42
1:B:53:VAL:O	1:B:90:SER:HA	2.19	0.42
1:B:40:SER:HB3	1:B:51:VAL:HG21	2.01	0.42
1:B:67:ARG:HG3	1:B:68:GLN:OE1	2.20	0.42
1:B:299:LEU:O	1:B:303:LEU:HB2	2.20	0.42
2:C:11:DC:H4'	6:C:109:HOH:O	2.19	0.42
1:A:8:ILE:HG12	1:A:141:VAL:HG22	2.01	0.42
1:B:299:LEU:HA	1:B:302:ILE:HG22	2.01	0.42
1:B:312:PHE:CE1	1:B:426:VAL:HG11	2.55	0.42
1:A:100:LYS:NZ	1:A:103:ARG:HH22	2.17	0.42
1:A:121:ARG:HH21	1:B:390:GLU:CD	2.27	0.42
1:A:142:ASP:OD2	1:A:148:PRO:HA	2.19	0.42
1:A:361:ASN:O	1:A:365:MET:HG2	2.19	0.42
1:A:384:LYS:HD3	1:A:384:LYS:HA	1.78	0.42
3:F:6:DC:H5	6:F:101:HOH:O	2.03	0.42
1:A:59:ASP:OD1	1:A:94:ARG:NH2	2.43	0.41
1:B:72:MET:HE3	1:B:73:LEU:CD2	2.51	0.41
1:B:105:VAL:HG11	1:B:134:ILE:HG22	2.02	0.41
1:B:66:ILE:HD13	1:B:66:ILE:HA	1.93	0.41
1:B:161:HIS:HB3	2:E:6:DC:O3'	2.21	0.41
1:A:318:GLY:O	1:A:324:SER:HB3	2.21	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.72	0.41
1:B:44:ALA:HB1	1:B:49:VAL:O	2.20	0.41
1:A:296:LYS:NZ	2:C:7[B]:DT:O4	2.54	0.41
1:A:70:GLU:HG2	1:A:204:LEU:HD11	2.02	0.41
1:B:175:LEU:HD21	1:B:286:GLU:OE2	2.21	0.41
1:B:370:THR:CG2	1:B:372:LYS:H	2.34	0.41
3:F:1:DT:N3	3:F:2:DT:C4	2.89	0.41
3:F:6:DC:H6	3:F:6:DC:H2'	1.74	0.41
1:A:30:ARG:HD3	1:A:274:GLY:O	2.21	0.40
1:A:326:PRO:HD3	1:A:426:VAL:CG2	2.51	0.40
1:A:446:GLU:H	1:A:446:GLU:CD	2.27	0.40
1:B:23:TYR:HB3	1:B:53:VAL:HG22	2.02	0.40
1:B:337:ARG:HH11	1:B:337:ARG:HG2	1.86	0.40
1:B:105:VAL:HG21	1:B:113:LEU:HD22	2.03	0.40
1:B:291:ASN:OD1	1:B:292:PRO:HD2	2.20	0.40
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	458/498 (92%)	434 (95%)	23 (5%)	1 (0%)	43	63
1	B	417/498 (84%)	392 (94%)	24 (6%)	1 (0%)	43	63
All	All	875/996 (88%)	826 (94%)	47 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASP
1	A	453	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/429 (94%)	373 (93%)	28 (7%)	14	29
1	B	373/429 (87%)	346 (93%)	27 (7%)	13	28
All	All	774/858 (90%)	719 (93%)	55 (7%)	13	29

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	9	ARG
1	A	105	VAL
1	A	108	TYR

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Mol	Chain	Res	Type
1	A	153	SER
1	A	155	LYS
1	A	171	LEU
1	A	198	GLU
1	A	199	THR
1	A	202	ASP
1	A	205	GLU
1	A	206	THR
1	A	212	LEU
1	A	221	LYS
1	A	222	ASP
1	A	235	LYS
1	A	239	LYS
1	A	256	ARG
1	A	289	GLU
1	A	294	SER
1	A	304	ILE
1	A	308	ILE
1	A	344	ILE
1	A	348	GLU
1	A	449	LYS
1	A	456	LEU
1	A	460	LYS
1	A	464	LEU
1	B	13	SER
1	B	40	SER
1	B	49	VAL
1	B	58	THR
1	B	61	PHE
1	B	66	ILE
1	B	85	ARG
1	B	94	ARG
1	B	105	VAL
1	B	129	LYS
1	B	135	SER
1	B	144	HIS
1	B	181	LEU
1	B	189	GLU
1	B	222	ASP
1	B	224	LEU
1	B	256	ARG
1	B	262	ASN

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Mol	Chain	Res	Type
1	B	263	MET
1	B	276	ILE
1	B	290	SER
1	B	294	SER
1	B	300	ASP
1	B	302	ILE
1	B	370	THR
1	B	450	ARG
1	B	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS
1	A	414	ASN
1	B	145	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	A	502	-	57,58,58	0.58	0	78,89,89	0.73	3 (3%)
4	SO4	A	501	-	4,4,4	0.30	0	6,6,6	0.81	0
5	FDA	B	501	-	57,58,58	0.54	0	78,89,89	0.74	4 (5%)

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	-	-	2/34/50/50	0/6/6/6
5	FDA	B	501	-	-	3/34/50/50	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(°)	Ideal(°)
5	A	502	FDA	N3-C2-N1	2.41	119.52	115.74
5	B	501	FDA	N3-C2-N1	2.37	119.47	115.74
5	B	501	FDA	C2'-C1'-N10	2.36	121.36	110.20
5	B	501	FDA	O2-C2-N3	-2.06	118.20	121.86
5	B	501	FDA	O4'-C4'-C3'	2.06	114.06	109.25
5	A	502	FDA	O2-C2-N3	-2.06	118.21	121.86
5	A	502	FDA	C4-C4X-N5	2.04	121.58	116.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	FDA	O4'-C4'-C5'-O5'
5	B	501	FDA	C5B-O5B-PA-O1A
5	A	502	FDA	C4'-C5'-O5'-P
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 3 short contacts:

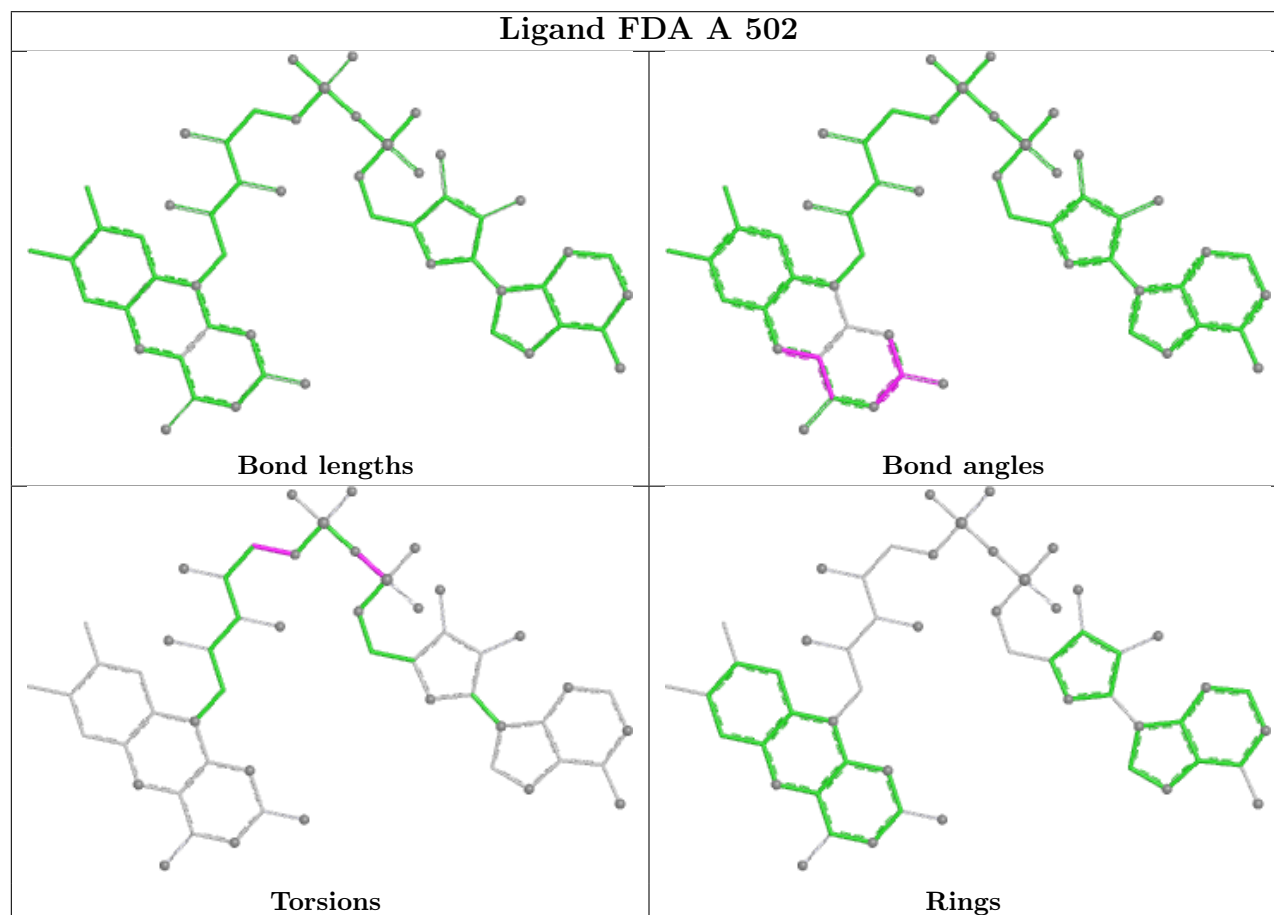
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	FDA	1	0

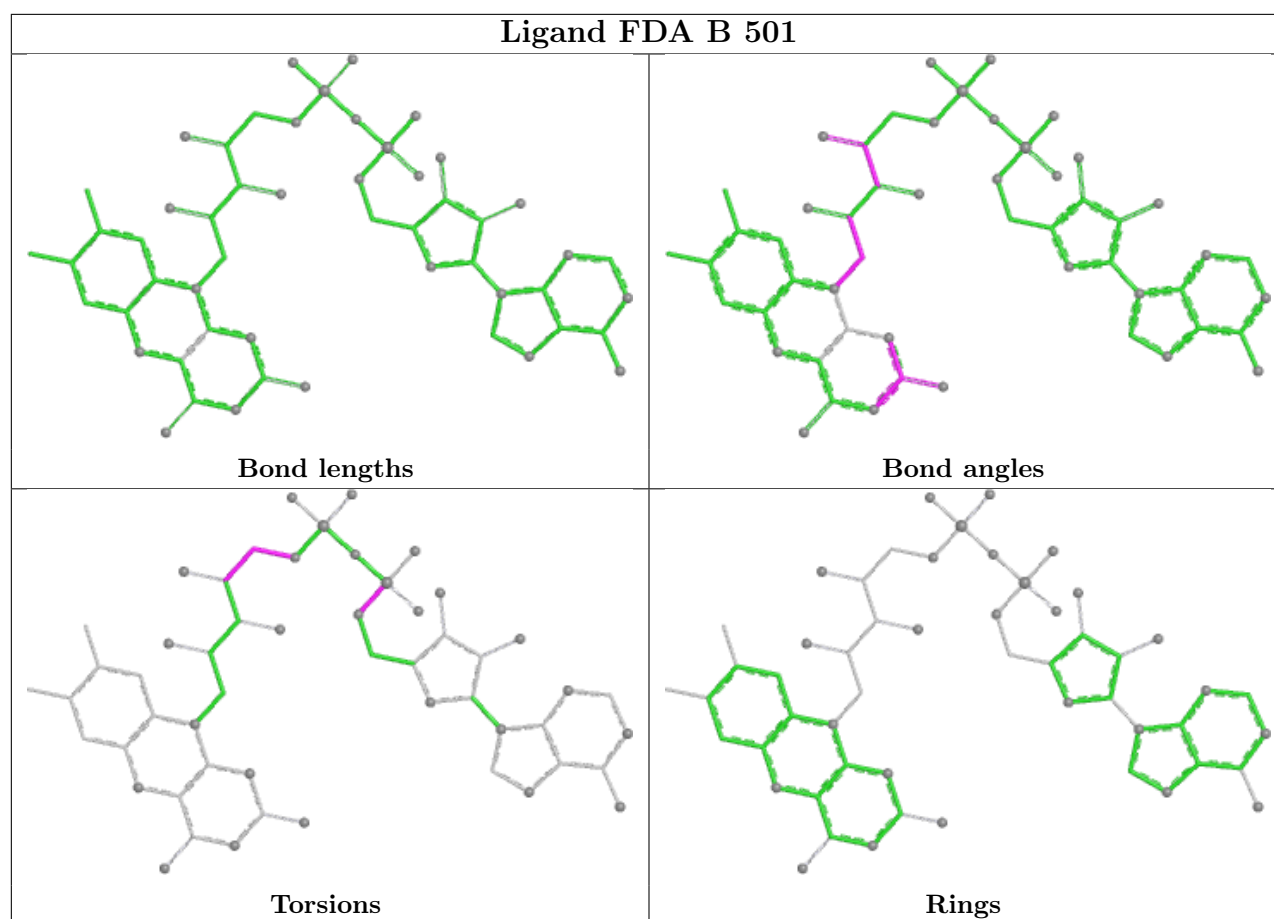
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	FDA	2	0

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	460/498 (92%)	0.48	21 (4%) 37 33	18, 39, 73, 103	2 (0%)
1	B	425/498 (85%)	1.20	74 (17%) 4 3	36, 63, 92, 135	0
2	C	14/14 (100%)	1.57	5 (35%) 1 1	21, 71, 114, 138	1 (7%)
2	E	12/14 (85%)	2.19	6 (50%) 0 0	66, 93, 138, 148	0
3	D	14/14 (100%)	1.02	1 (7%) 22 19	55, 79, 93, 94	0
3	F	13/14 (92%)	1.96	6 (46%) 0 0	82, 105, 135, 152	0
All	All	938/1052 (89%)	0.87	113 (12%) 9 7	18, 49, 93, 152	3 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	PHE	6.3
1	B	20	PRO	4.7
1	A	468	ALA	4.6
1	B	464	LEU	4.4
2	E	8	DT	4.4
1	B	60	GLU	4.3
1	B	48	ASN	4.1
1	A	188	PRO	3.8
1	B	186	VAL	3.8
2	C	1	DA	3.7
3	F	1	DT	3.6
2	E	5	DG	3.6
1	B	102	SER	3.5
3	F	13	DG	3.5
1	B	101	ILE	3.5
1	B	185	SER	3.4
1	B	69	TYR	3.3
2	E	3	DC	3.3
1	A	462	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	39	PHE	3.3
1	B	314	TYR	3.3
2	C	8	DT	3.2
1	B	127	ILE	3.2
1	B	262	ASN	3.1
1	A	2	ILE	3.1
1	A	198	GLU	3.1
1	B	49	VAL	3.1
1	B	134	ILE	3.1
1	B	160	ALA	3.1
1	B	108	TYR	3.0
1	B	257	ASN	3.0
1	B	89	PRO	3.0
1	B	110	ALA	3.0
1	B	82	SER	3.0
1	A	14	GLY	3.0
1	B	22	VAL	3.0
2	E	4	DG	3.0
1	A	463	ALA	2.9
1	A	465	ASP	2.9
1	B	169	ALA	2.9
1	B	252	TYR	2.9
1	B	130	VAL	2.8
3	D	1	DT	2.8
1	B	232	PRO	2.8
1	A	108	TYR	2.7
1	B	188	PRO	2.7
1	B	57	LEU	2.7
1	B	42	ALA	2.7
2	C	14	DA	2.7
1	B	40	SER	2.7
2	E	6	DC	2.7
1	A	469	ALA	2.7
1	B	454	VAL	2.6
1	B	21	VAL	2.6
1	B	105	VAL	2.6
1	B	147	VAL	2.6
1	A	136	ILE	2.5
1	B	114	VAL	2.5
1	B	286	GLU	2.5
1	B	62	LEU	2.5
1	B	159	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	31	ALA	2.4
1	B	245	ILE	2.4
1	B	83	LEU	2.4
1	B	154	GLN	2.4
1	A	189	GLU	2.4
1	B	64	ALA	2.4
1	B	411	ARG	2.4
1	B	56	CYS	2.4
1	A	3	MET	2.4
1	B	58	THR	2.3
1	A	167	LEU	2.3
1	B	43	ILE	2.3
1	B	54	VAL	2.3
1	A	109	ASN	2.3
1	B	41	ARG	2.3
2	C	7[A]	DT	2.3
1	B	135	SER	2.3
1	B	55	PHE	2.3
3	F	5	DG	2.3
1	B	90	SER	2.3
1	B	189	GLU	2.3
3	F	3	DG	2.2
1	B	461	TYR	2.2
1	B	111	GLY	2.2
1	A	466	LYS	2.2
1	B	187	THR	2.2
1	B	167	LEU	2.2
1	B	170	LEU	2.2
1	B	24	TRP	2.2
1	B	75	GLY	2.2
3	F	9	DA	2.2
1	B	146	VAL	2.1
2	E	7	DT	2.1
1	A	137	PRO	2.1
1	B	47	ALA	2.1
3	F	6	DC	2.1
1	B	181	LEU	2.1
1	B	221	LYS	2.1
2	C	2	DT	2.1
1	B	139	PHE	2.1
1	B	35	TRP	2.1
1	B	315	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	2.1
1	B	174	PHE	2.1
1	A	334	ASN	2.1
1	B	150	TRP	2.1
1	A	15	LYS	2.1
1	A	219	LYS	2.1
1	B	158	TYR	2.1
1	B	91	PHE	2.0
1	B	256	ARG	2.0
1	B	23	TYR	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](#)

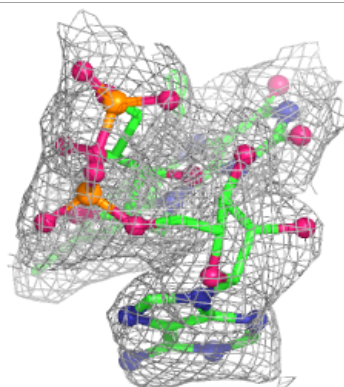
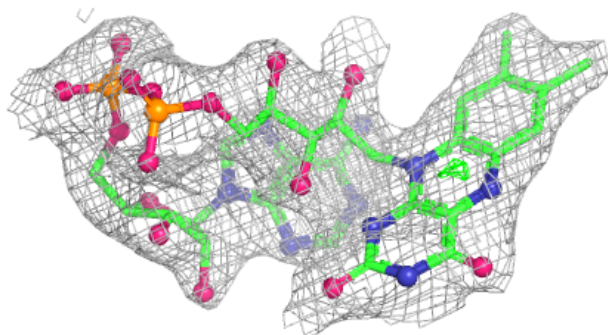
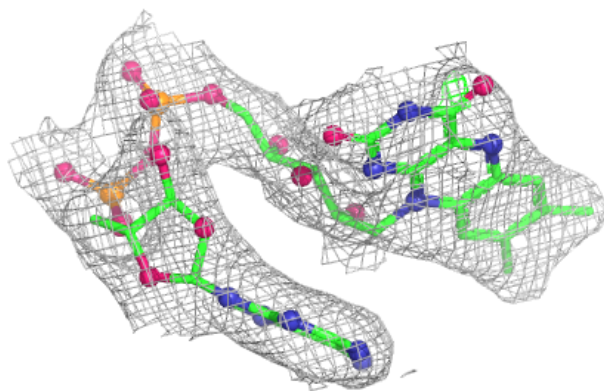
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FDA	B	501	53/53	0.92	0.10	35,46,51,52	0
4	SO4	A	501	5/5	0.93	0.10	25,31,39,40	0
5	FDA	A	502	53/53	0.96	0.08	17,23,26,27	0

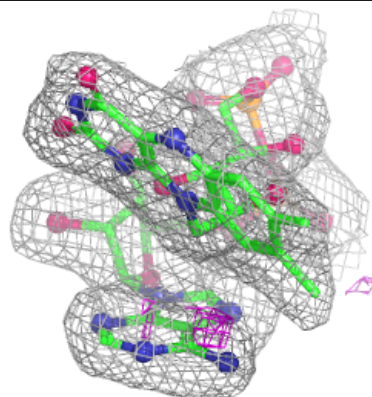
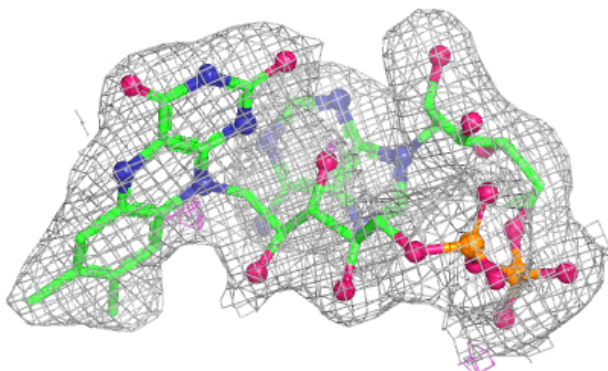
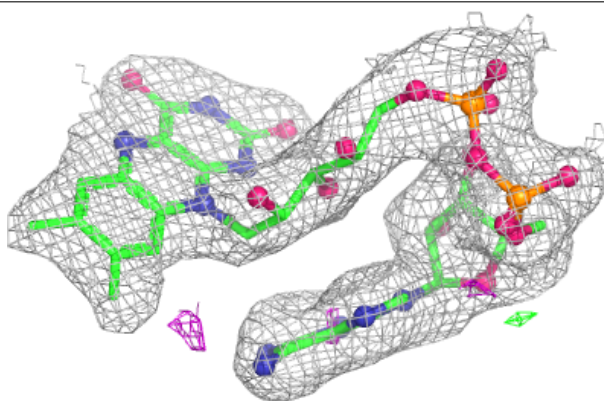
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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