



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:39 PM UTC

PDB ID : 8OYB / pdb_00008oyb
Title : Time-resolved SFX structure of the class II photolyase complexed with a thymine dimer (30 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 : 2.25 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)

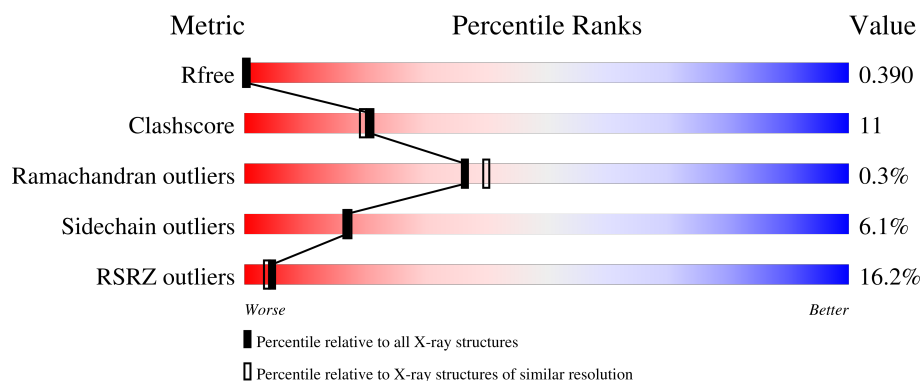
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	21% 71% 29%
2	E	14	36% 43% 36% 21%
3	D	14	7% 36% 64%
3	F	14	36% 50% 43% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8554 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	459	Total	C	N	O	S	0	1	0
			3728	2396	628	689	15			
1	B	427	Total	C	N	O	S	0	0	0
			3480	2237	587	641	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

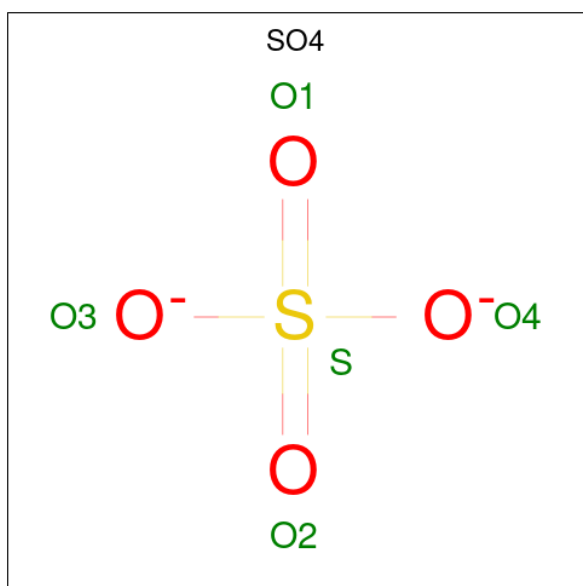
- Molecule 2 is a DNA chain called CPD-COMPRISING OLIGONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			282	135	51	83	13			
2	E	11	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

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

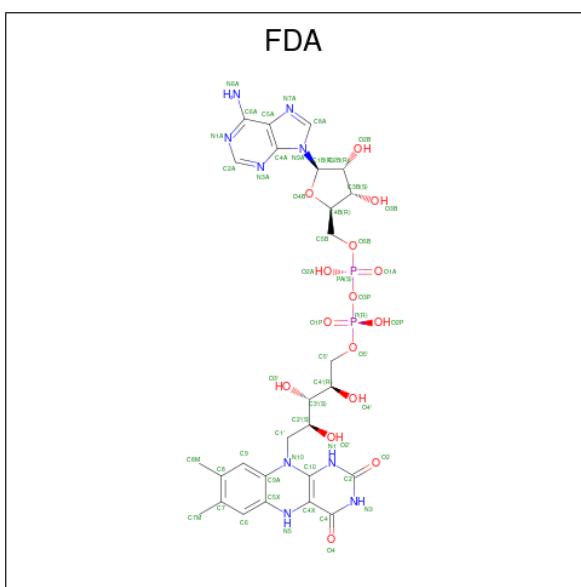
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

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



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

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



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

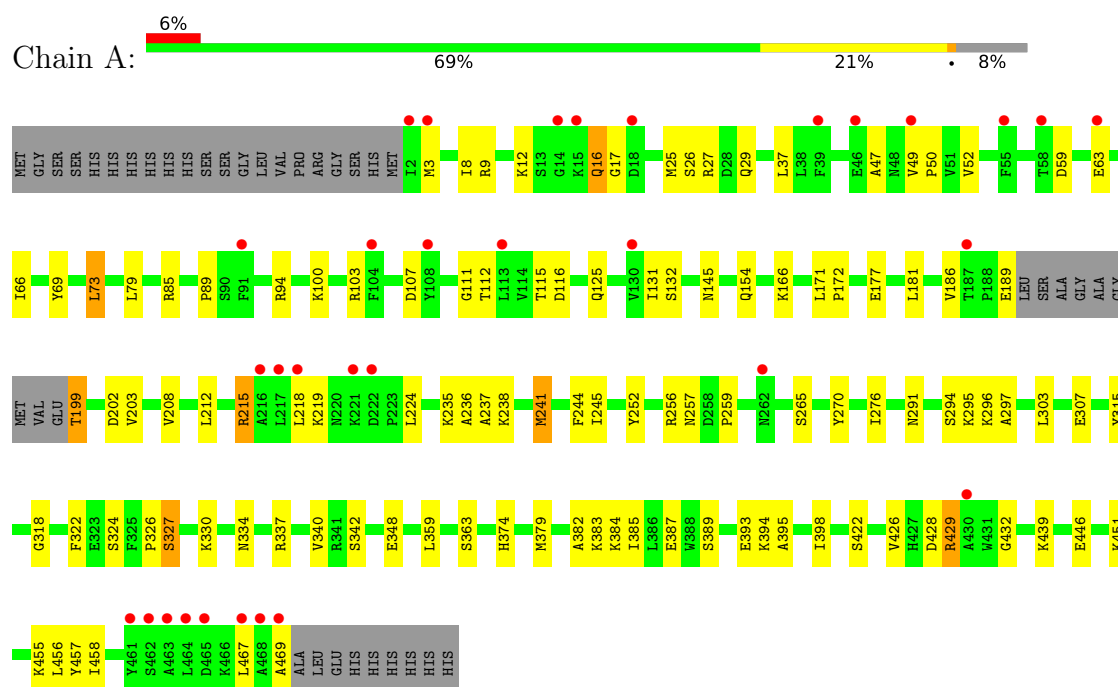
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	104	Total O 104 104	0	0
6	B	50	Total O 50 50	0	0
6	C	7	Total O 7 7	0	0
6	D	10	Total O 10 10	0	0
6	E	4	Total O 4 4	0	0
6	F	2	Total O 2 2	0	0

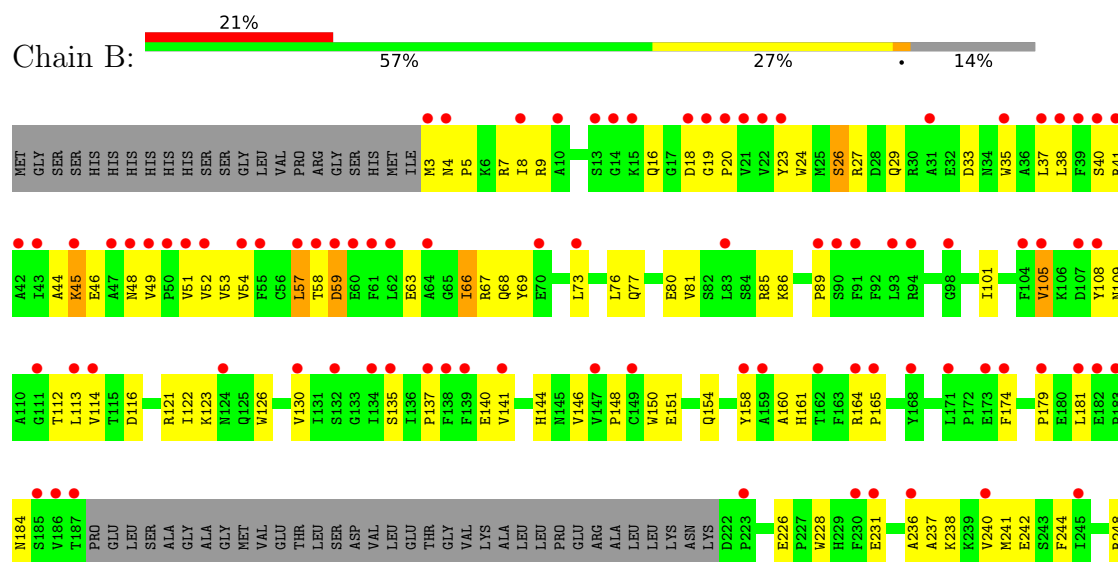
3 Residue-property plots [i](#)

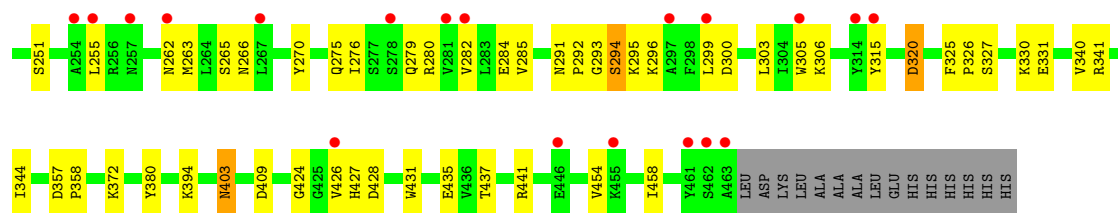
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

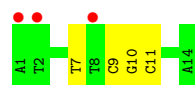


• Molecule 1: Deoxyribodipyrimidine photo-lyase

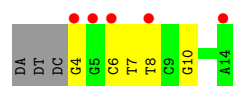
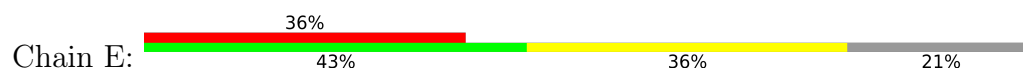




● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



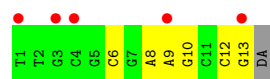
● Molecule 2: CPD-COMPRISING OLIGONUCLEOTIDE



● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



● Molecule 3: COUNTERSTRAND-OLIGONUCLEOTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.20Å 117.76Å 170.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.29 – 2.25 31.29 – 2.25	Depositor EDS
% Data completeness (in resolution range)	81.1 (31.29-2.25) 81.3 (31.29-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.317 , 0.389 0.317 , 0.390	Depositor DCC
R_{free} test set	2858 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8554	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FDA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/3827	0.66	0/5174
1	B	0.37	0/3577	0.55	0/4835
2	C	0.51	0/315	0.64	0/484
2	E	0.46	0/251	0.53	0/385
3	D	0.42	0/321	0.61	0/494
3	F	0.36	0/297	0.48	0/457
All	All	0.41	0/8588	0.60	0/11829

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	3728	0	3659	70	0
1	B	3480	0	3385	89	0
2	C	282	0	159	4	0
2	E	225	0	124	10	0
3	D	286	0	158	7	0
3	F	265	0	147	9	0
4	A	5	0	0	0	0

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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	104	0	0	11	0
6	B	50	0	0	3	0
6	C	7	0	0	1	0
6	D	10	0	0	1	0
6	E	4	0	0	0	0
6	F	2	0	0	0	0
All	All	8554	0	7698	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)
2:E:4:DG:H1	3:F:12:DC:H42	1.14	0.96
1:B:41:ARG:HD2	1:B:51:VAL:HG21	1.53	0.88
1:A:219:LYS:HE3	1:A:469:ALA:HB3	1.59	0.83
2:E:6:DC:H42	3:F:9:DA:N6	1.86	0.73
1:B:51:VAL:H	1:B:184:ASN:HD21	1.38	0.71
1:A:348:GLU:OE1	1:A:348:GLU:N	2.21	0.71
2:E:6:DC:H42	3:F:9:DA:H61	1.36	0.71
1:A:428:ASP:OD1	1:A:429:ARG:N	2.26	0.67
1:A:384:LYS:NZ	1:A:387:GLU:OE2	2.22	0.67
2:E:7:DT:H1'	2:E:8:DT:O2	1.95	0.66
1:B:35:TRP:HE1	1:B:279:GLN:HE22	1.43	0.65
2:C:9:DC:H2'	2:C:10:DG:C8	2.31	0.65
1:B:73:LEU:HD13	1:B:76:LEU:HD12	1.78	0.65
1:B:435:GLU:O	1:B:437:THR:N	2.29	0.65
1:B:146:VAL:HG13	1:B:279:GLN:HG3	1.78	0.64
1:B:238:LYS:NZ	1:B:242:GLU:OE2	2.31	0.64
1:B:3:MET:SD	1:B:3:MET:N	2.71	0.64
1:B:291:ASN:HB3	1:B:294:SER:HB2	1.79	0.62
1:A:16:GLN:OE1	1:A:112:THR:OG1	2.18	0.62
1:B:26:SER:OG	1:B:27:ARG:N	2.33	0.61
1:A:125:GLN:NE2	1:B:340:VAL:HA	2.16	0.61
1:A:125:GLN:NE2	1:B:341:ARG:H	2.00	0.60
3:D:5:DG:N7	6:D:101:HOH:O	2.31	0.60
1:B:40:SER:HB2	1:B:114:VAL:HG21	1.84	0.59
1:B:409:ASP:OD1	5:B:501:FDA:N3	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:NH2	1:A:107:ASP:OD1	2.32	0.59
1:A:59:ASP:OD1	1:A:94:ARG:NH2	2.36	0.58
1:B:357:ASP:OD2	1:B:380:TYR:OH	2.21	0.58
1:A:66:ILE:H	1:A:66:ILE:HD12	1.68	0.57
1:A:382:ALA:HA	1:A:385:ILE:HD12	1.87	0.57
1:A:66:ILE:HD13	1:A:215:ARG:HG2	1.87	0.56
2:E:6:DC:N4	3:F:9:DA:H61	2.02	0.56
1:A:291:ASN:HB2	1:A:294:SER:HB2	1.89	0.55
1:B:52:VAL:HA	1:B:89:PRO:HD2	1.89	0.55
1:A:252:TYR:OH	5:A:502:FDA:O2A	2.23	0.54
1:A:318:GLY:O	1:A:324:SER:HB3	2.07	0.54
1:B:86:LYS:NZ	1:B:181:LEU:O	2.40	0.54
1:B:85:ARG:HD3	6:B:640:HOH:O	2.06	0.54
1:B:248:ARG:HD2	1:B:262:ASN:O	2.10	0.52
1:B:9:ARG:HD2	1:B:150:TRP:CD2	2.45	0.52
1:A:116:ASP:HB2	6:A:624:HOH:O	2.09	0.52
1:B:44:ALA:HB1	1:B:49:VAL:O	2.10	0.52
1:B:77:GLN:O	1:B:81:VAL:HG23	2.09	0.52
1:B:24:TRP:HA	1:B:54:VAL:HG13	1.92	0.51
1:B:266:ASN:HA	1:B:372:LYS:HE3	1.92	0.51
2:E:10:DG:H1	3:F:6:DC:H42	1.57	0.51
1:A:219:LYS:HE3	1:A:469:ALA:CB	2.36	0.51
1:A:52:VAL:HG12	1:A:89:PRO:HD2	1.92	0.51
6:A:683:HOH:O	2:C:7:DT:H2'	2.11	0.51
1:A:166:LYS:HD3	6:A:681:HOH:O	2.11	0.51
5:B:501:FDA:O3'	5:B:501:FDA:N1	2.44	0.51
1:B:262:ASN:O	1:B:263:MET:HE2	2.11	0.51
1:B:19:GLY:HA3	1:B:109:ASN:O	2.12	0.50
1:B:44:ALA:CB	1:B:51:VAL:HG22	2.41	0.50
1:A:3:MET:HE2	1:A:8:ILE:HD11	1.93	0.50
1:B:244:PHE:CD1	1:B:265:SER:HA	2.45	0.50
1:B:44:ALA:HB3	1:B:51:VAL:HG22	1.92	0.50
1:A:446:GLU:H	1:A:446:GLU:CD	2.19	0.50
3:D:7:DG:H2''	3:D:8:DA:C8	2.46	0.50
1:B:7:ARG:NH2	1:B:174:PHE:O	2.43	0.50
1:A:69:TYR:O	1:A:73:LEU:HB2	2.12	0.49
1:A:17:GLY:HA3	1:A:111:GLY:HA2	1.92	0.49
1:A:322:PHE:CE2	1:A:330:LYS:HG2	2.48	0.49
1:B:45:LYS:HG3	1:B:46:GLU:N	2.26	0.49
1:B:431:TRP:CD1	1:B:441:ARG:HB2	2.48	0.49
1:B:26:SER:OG	6:B:601:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HG3	1:B:181:LEU:HD23	1.94	0.48
1:A:25:MET:HE1	1:A:79:LEU:HD21	1.94	0.48
1:B:164:ARG:N	1:B:165:PRO:HD2	2.28	0.48
1:B:66:ILE:HG23	1:B:67:ARG:H	1.78	0.48
1:A:257:ASN:O	1:A:259:PRO:HD3	2.14	0.48
1:A:439:LYS:NZ	3:D:10:DG:OP1	2.46	0.48
3:F:8:DA:H2''	3:F:9:DA:H5'	1.94	0.48
1:A:432:GLY:HA2	3:D:9:DA:H5'	1.96	0.48
1:B:123:LYS:HA	1:B:126:TRP:HE3	1.78	0.48
2:E:6:DC:N3	3:F:9:DA:N1	2.62	0.47
1:A:241:MET:HE2	1:A:276:ILE:HD11	1.95	0.47
1:B:255:LEU:HD13	1:B:263:MET:HG3	1.96	0.47
1:A:171:LEU:N	1:A:172:PRO:HD2	2.28	0.47
1:B:59:ASP:O	1:B:63:GLU:N	2.48	0.47
1:B:241:MET:CE	1:B:284:GLU:HG3	2.45	0.47
1:B:305:TRP:HZ2	2:E:7:DT:H5'	1.79	0.47
1:A:389[A]:SER:OG	1:A:395:ALA:HB2	2.15	0.47
2:C:11:DC:H2'	6:C:101:HOH:O	2.15	0.47
1:B:160:ALA:HB3	2:E:7:DT:OP1	2.14	0.47
1:A:145:ASN:HB3	1:A:307:GLU:OE1	2.15	0.47
1:B:35:TRP:HE1	1:B:279:GLN:NE2	2.11	0.47
3:F:9:DA:C2	3:F:10:DG:N1	2.83	0.47
1:A:379:MET:O	1:A:383:LYS:HG3	2.15	0.47
1:B:121:ARG:NH2	1:B:320:ASP:OD2	2.45	0.46
1:B:69:TYR:O	1:B:73:LEU:HD23	2.15	0.46
1:B:292:PRO:O	1:B:296:LYS:HD3	2.16	0.46
1:A:451:LYS:HE2	2:C:9:DC:OP2	2.16	0.46
1:B:158:TYR:O	1:B:427:HIS:HA	2.15	0.46
1:A:393:GLU:HB2	6:A:621:HOH:O	2.15	0.46
1:A:63:GLU:OE2	6:A:601:HOH:O	2.21	0.46
1:B:161:HIS:N	2:E:7:DT:OP1	2.49	0.45
3:D:1:DT:H6	3:D:1:DT:H2'	1.59	0.45
1:A:235:LYS:HE3	1:A:235:LYS:HB2	1.66	0.45
1:A:208:VAL:O	1:A:212:LEU:HB2	2.17	0.45
1:B:325:PHE:CD1	1:B:424:GLY:HA3	2.52	0.45
1:B:326:PRO:O	1:B:330:LYS:HG3	2.16	0.45
1:B:426:VAL:C	1:B:428:ASP:H	2.25	0.45
3:D:4:DC:H2''	3:D:5:DG:C8	2.50	0.45
1:B:144:HIS:O	1:B:306:LYS:NZ	2.50	0.45
1:A:236:ALA:N	6:A:608:HOH:O	2.42	0.45
1:A:342:SER:N	6:A:607:HOH:O	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:HG2	1:B:108:TYR:HE2	1.81	0.45
1:B:23:TYR:HB3	1:B:53:VAL:HG22	1.99	0.45
1:A:12:LYS:HB2	1:A:131:ILE:HG23	1.99	0.45
1:B:8:ILE:HG12	1:B:141:VAL:HG22	1.99	0.45
1:B:41:ARG:HD2	1:B:51:VAL:CG2	2.36	0.44
1:B:68:GLN:HG2	6:B:642:HOH:O	2.18	0.44
1:A:383:LYS:NZ	1:A:422:SER:O	2.45	0.44
1:B:251:SER:HB2	1:B:255:LEU:HD12	1.98	0.44
1:A:241:MET:HE3	1:A:241:MET:HB3	1.74	0.44
3:D:13:DG:H2'	3:D:14:DA:C8	2.53	0.44
1:B:299:LEU:O	1:B:303:LEU:HB2	2.18	0.44
1:B:320:ASP:OD1	1:B:320:ASP:N	2.47	0.44
1:A:27:ARG:HB2	6:A:689:HOH:O	2.17	0.44
1:A:100:LYS:NZ	6:A:610:HOH:O	2.42	0.44
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.89	0.44
1:A:50:PRO:HG3	1:A:186:VAL:HG23	2.00	0.43
1:A:219:LYS:CE	1:A:469:ALA:HB3	2.42	0.43
1:A:394:LYS:HB2	1:A:394:LYS:HE2	1.67	0.43
1:A:47:ALA:HB3	1:A:49:VAL:HG22	2.00	0.43
1:A:154:GLN:HA	1:A:315:TYR:OH	2.19	0.43
1:B:38:LEU:HD13	1:B:179:PRO:HD2	2.01	0.43
1:B:41:ARG:HA	1:B:51:VAL:HG21	2.00	0.43
1:A:326:PRO:HD3	1:A:426:VAL:HG22	2.00	0.42
1:A:363:SER:HA	1:A:457:TYR:OH	2.19	0.42
1:A:394:LYS:O	1:A:398:ILE:HG13	2.18	0.42
1:B:35:TRP:HA	1:B:35:TRP:CE3	2.54	0.42
1:B:154:GLN:HA	1:B:315:TYR:OH	2.19	0.42
1:B:24:TRP:CD1	1:B:24:TRP:C	2.97	0.42
1:B:325:PHE:HB2	1:B:330:LYS:HG2	2.01	0.42
1:B:123:LYS:HA	1:B:126:TRP:CE3	2.54	0.42
1:B:226:GLU:HB3	1:B:228:TRP:CH2	2.54	0.42
1:B:358:PRO:HB2	1:B:458:ILE:HD13	2.00	0.42
1:B:41:ARG:NH2	1:B:184:ASN:HA	2.35	0.42
1:B:57:LEU:H	1:B:57:LEU:HG	1.58	0.42
1:B:291:ASN:OD1	1:B:293:GLY:N	2.52	0.42
1:B:105:VAL:HG21	1:B:113:LEU:HD22	2.01	0.42
1:A:326:PRO:O	1:A:327:SER:C	2.63	0.42
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.85	0.41
1:B:237:ALA:HB2	1:B:270:TYR:CD1	2.55	0.41
1:B:33:ASP:OD2	1:B:280:ARG:HB2	2.19	0.41
1:B:44:ALA:O	1:B:48:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG23	1:B:137:PRO:HG2	2.01	0.41
1:A:73:LEU:HD22	1:A:73:LEU:HA	1.81	0.41
1:A:291:ASN:HB3	1:A:294:SER:H	1.85	0.41
1:B:236:ALA:O	1:B:240:VAL:HG23	2.20	0.41
1:A:296:LYS:O	1:A:297:ALA:C	2.62	0.41
1:A:218:LEU:HD22	1:A:467:LEU:HB3	2.02	0.41
1:B:148:PRO:HG2	1:B:151:GLU:HB3	2.02	0.41
1:B:403:ASN:C	1:B:403:ASN:ND2	2.79	0.41
1:B:4:ASN:HA	1:B:5:PRO:HD3	1.87	0.41
1:B:431:TRP:NE1	1:B:441:ARG:HB2	2.35	0.41
1:A:177:GLU:HG2	6:A:664:HOH:O	2.21	0.41
1:A:334:ASN:HA	1:A:337:ARG:HG3	2.03	0.41
1:B:237:ALA:HB1	1:B:276:ILE:HB	2.03	0.41
3:F:12:DC:H2''	3:F:13:DG:O4'	2.21	0.41
1:A:29:GLN:NE2	6:A:618:HOH:O	2.53	0.41
1:A:199:THR:O	1:A:203:VAL:HG23	2.21	0.40
1:A:125:GLN:HG2	1:B:344:ILE:HD12	2.03	0.40
1:A:237:ALA:HB2	1:A:270:TYR:CD1	2.57	0.40
1:A:244:PHE:CD1	1:A:265:SER:HA	2.56	0.40
1:B:68:GLN:OE1	1:B:68:GLN:N	2.43	0.40
1:B:295:LYS:O	1:B:299:LEU:HG	2.20	0.40
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.81	0.40
1:A:115:THR:OG1	1:A:116:ASP:N	2.55	0.40
1:A:259:PRO:HA	1:A:374:HIS:CD2	2.56	0.40
1:A:359:LEU:HB2	1:A:458:ILE:HD11	2.04	0.40
1:B:29:GLN:O	1:B:275:GLN:HA	2.22	0.40
1:B:262:ASN:OD1	1:B:262:ASN:N	2.54	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	456/498 (92%)	433 (95%)	22 (5%)	1 (0%)	43	50
1	B	423/498 (85%)	400 (95%)	21 (5%)	2 (0%)	24	24
All	All	879/996 (88%)	833 (95%)	43 (5%)	3 (0%)	36	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ILE
1	A	26	SER
1	B	116	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	399/429 (93%)	378 (95%)	21 (5%)	20	22
1	B	371/429 (86%)	345 (93%)	26 (7%)	14	13
All	All	770/858 (90%)	723 (94%)	47 (6%)	17	17

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	16	GLN
1	A	37	LEU
1	A	73	LEU
1	A	85	ARG
1	A	132	SER
1	A	189	GLU
1	A	199	THR
1	A	202	ASP
1	A	215	ARG
1	A	224	LEU
1	A	238	LYS
1	A	241	MET

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Mol	Chain	Res	Type
1	A	245	ILE
1	A	256	ARG
1	A	295	LYS
1	A	327	SER
1	A	340	VAL
1	A	429	ARG
1	A	455	LYS
1	A	456	LEU
1	B	16	GLN
1	B	18	ASP
1	B	26	SER
1	B	37	LEU
1	B	45	LYS
1	B	57	LEU
1	B	58	THR
1	B	59	ASP
1	B	80	GLU
1	B	101	ILE
1	B	105	VAL
1	B	122	ILE
1	B	130	VAL
1	B	135	SER
1	B	140	GLU
1	B	231	GLU
1	B	282	VAL
1	B	285	VAL
1	B	294	SER
1	B	300	ASP
1	B	320	ASP
1	B	327	SER
1	B	331	GLU
1	B	394	LYS
1	B	403	ASN
1	B	454	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	125	GLN
1	A	291	ASN
1	A	374	HIS

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Mol	Chain	Res	Type
1	B	16	GLN
1	B	257	ASN
1	B	279	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.47	0	78,89,89	0.68	2 (2%)
5	FDA	B	501	-	57,58,58	0.52	0	78,89,89	0.66	2 (2%)
4	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.54	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	-	-	5/34/50/50	0/6/6/6
5	FDA	B	501	-	-	9/34/50/50	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	FDA	C2'-C1'-N10	2.40	121.53	110.20
5	A	502	FDA	N3-C2-N1	2.40	119.50	115.74
5	A	502	FDA	O2-C2-N3	-2.31	117.75	121.86
5	B	501	FDA	N3-C2-N1	2.03	118.93	115.74

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

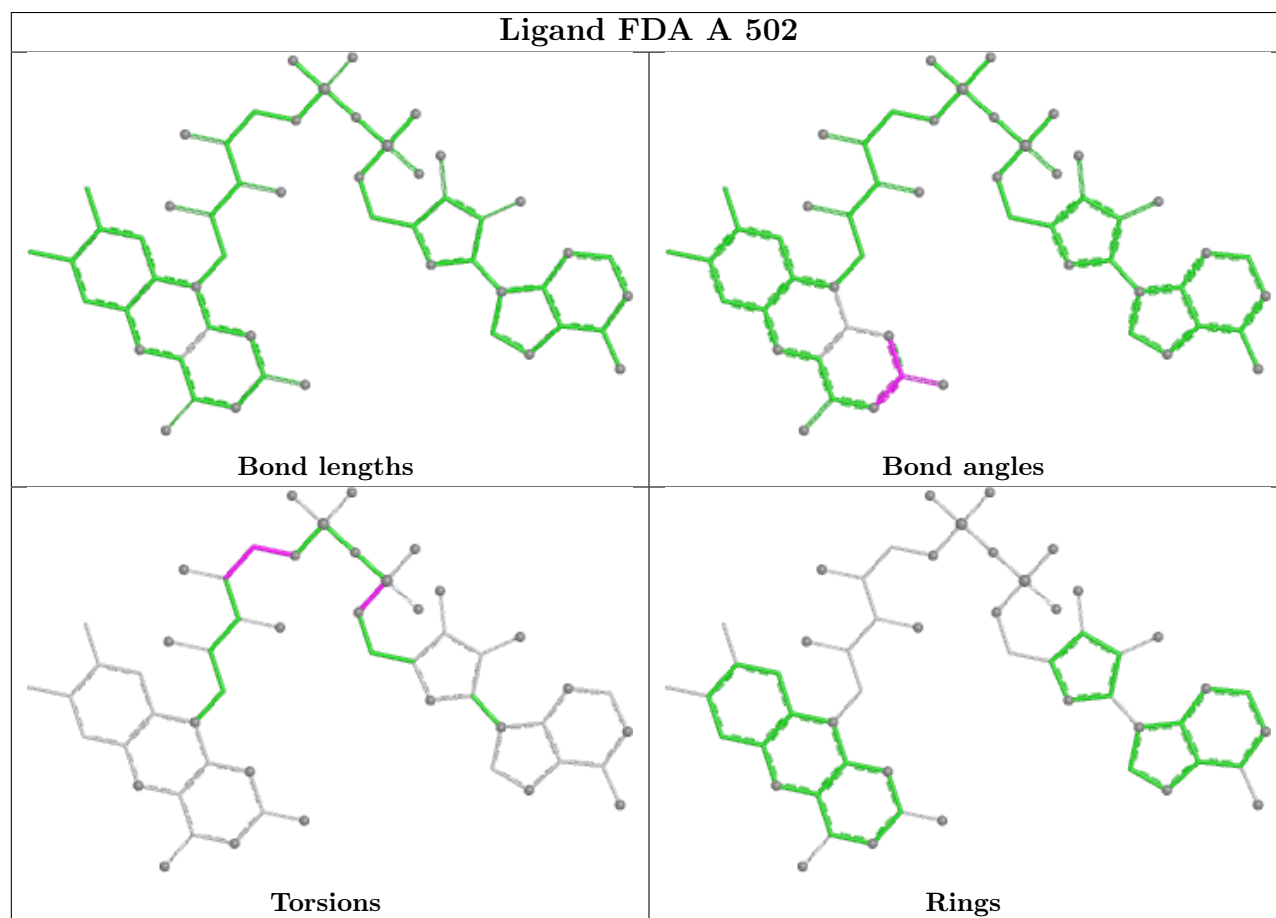
There are no ring outliers.

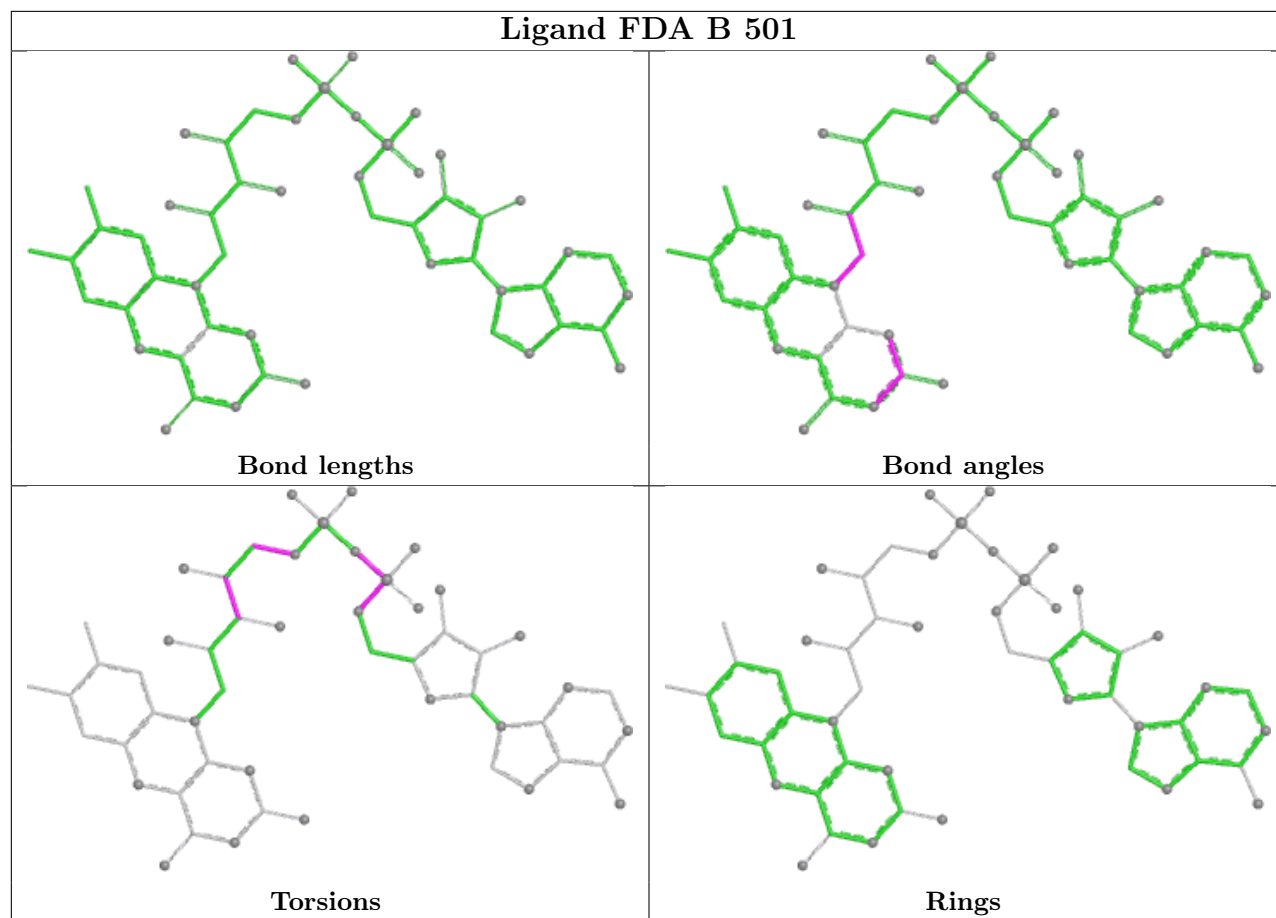
2 monomers are involved in 3 short contacts:

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	459/498 (92%)	0.67	32 (6%) 22 21	21, 41, 71, 98	1 (0%)
1	B	427/498 (85%)	1.42	106 (24%) 2 1	37, 63, 93, 108	0
2	C	14/14 (100%)	1.53	3 (21%) 2 2	45, 72, 114, 119	0
2	E	11/14 (78%)	2.09	5 (45%) 0 0	69, 77, 128, 139	0
3	D	14/14 (100%)	1.08	1 (7%) 22 20	55, 76, 88, 89	0
3	F	13/14 (92%)	1.86	5 (38%) 1 0	86, 99, 128, 132	0
All	All	938/1052 (89%)	1.06	152 (16%) 4 4	21, 51, 90, 139	1 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ALA	5.2
1	B	463	ALA	5.1
2	E	8	DT	5.1
1	A	2	ILE	4.9
1	B	257	ASN	4.3
1	B	60	GLU	4.0
1	B	49	VAL	3.9
1	B	21	VAL	3.8
1	B	57	LEU	3.7
1	A	469	ALA	3.7
2	C	1	DA	3.7
1	B	108	TYR	3.6
1	B	48	ASN	3.6
1	B	281	VAL	3.6
2	E	6	DC	3.5
1	B	40	SER	3.4
1	A	14	GLY	3.4
1	B	62	LEU	3.4
1	B	55	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	186	VAL	3.4
3	F	1	DT	3.4
1	A	18	ASP	3.3
1	A	108	TYR	3.3
1	B	93	LEU	3.2
1	B	70	GLU	3.2
1	B	89	PRO	3.2
3	D	1	DT	3.2
1	A	113	LEU	3.2
1	B	50	PRO	3.2
1	B	38	LEU	3.2
3	F	13	DG	3.2
2	C	8	DT	3.1
1	A	465	ASP	3.1
1	B	51	VAL	3.1
1	B	31	ALA	3.1
1	B	42	ALA	3.1
1	B	43	ILE	3.0
1	B	223	PRO	3.0
1	B	45	LYS	3.0
2	E	5	DG	2.9
1	B	187	THR	2.9
1	B	185	SER	2.9
1	B	446	GLU	2.9
1	B	61	PHE	2.9
1	B	58	THR	2.9
1	B	138	PHE	2.8
1	B	22	VAL	2.8
1	B	262	ASN	2.8
1	B	91	PHE	2.8
1	B	141	VAL	2.8
1	A	218	LEU	2.8
1	A	463	ALA	2.8
1	B	54	VAL	2.8
1	B	23	TYR	2.8
1	B	8	ILE	2.7
1	B	18	ASP	2.7
1	B	20	PRO	2.7
1	B	104	PHE	2.7
1	A	46	GLU	2.7
1	B	314	TYR	2.7
1	B	174	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	147	VAL	2.7
1	A	467	LEU	2.7
1	B	10	ALA	2.6
1	B	47	ALA	2.6
1	B	39	PHE	2.6
1	B	297	ALA	2.6
1	B	98	GLY	2.6
1	B	236	ALA	2.6
1	B	111	GLY	2.6
1	B	282	VAL	2.6
1	B	315	TYR	2.6
1	B	462	SER	2.6
1	B	159	ALA	2.6
1	A	104	PHE	2.6
1	B	114	VAL	2.6
1	B	73	LEU	2.5
1	B	52	VAL	2.5
1	B	15	LYS	2.5
2	E	4	DG	2.5
1	B	230	PHE	2.4
1	B	255	LEU	2.4
1	B	4	ASN	2.4
1	B	107	ASP	2.4
1	B	162	THR	2.4
2	C	2	DT	2.4
1	A	55	PHE	2.4
1	B	426	VAL	2.4
1	A	3	MET	2.4
1	B	3	MET	2.4
1	B	59	ASP	2.4
1	A	217	LEU	2.4
1	B	299	LEU	2.4
3	F	9	DA	2.3
1	A	187	THR	2.3
1	A	39	PHE	2.3
1	B	134	ILE	2.3
1	A	130	VAL	2.3
1	A	464	LEU	2.3
1	B	35	TRP	2.3
1	B	158	TYR	2.3
1	B	13	SER	2.3
1	B	139	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	37	LEU	2.3
1	B	165	PRO	2.3
1	B	183	PRO	2.3
1	A	58	THR	2.3
1	B	90	SER	2.3
1	A	15	LYS	2.3
1	A	91	PHE	2.2
1	B	267	LEU	2.2
1	B	137	PRO	2.2
1	A	468	ALA	2.2
1	B	41	ARG	2.2
1	B	231	GLU	2.2
1	A	462	SER	2.2
1	A	49	VAL	2.2
1	A	63	GLU	2.2
1	A	216	ALA	2.2
1	B	168	TYR	2.1
1	B	245	ILE	2.1
1	B	105	VAL	2.1
1	B	173	GLU	2.1
1	B	455	LYS	2.1
1	B	164	ARG	2.1
1	A	461	TYR	2.1
1	B	461	TYR	2.1
1	B	83	LEU	2.1
1	B	171	LEU	2.1
2	E	14	DA	2.1
1	B	305	TRP	2.1
1	A	221	LYS	2.1
1	B	113	LEU	2.1
1	A	262	ASN	2.1
1	B	124	ASN	2.1
1	B	179	PRO	2.1
1	B	240	VAL	2.1
1	B	14	GLY	2.1
1	B	278	SER	2.1
1	B	182	GLU	2.1
1	B	130	VAL	2.1
1	B	19	GLY	2.1
1	B	132	SER	2.0
1	B	149	CYS	2.0
1	A	222	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	135	SER	2.0
1	A	430	ALA	2.0
1	B	254	ALA	2.0
1	B	181	LEU	2.0
3	F	3	DG	2.0
1	B	94	ARG	2.0
3	F	4	DC	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

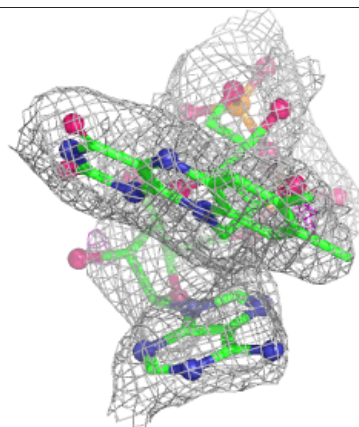
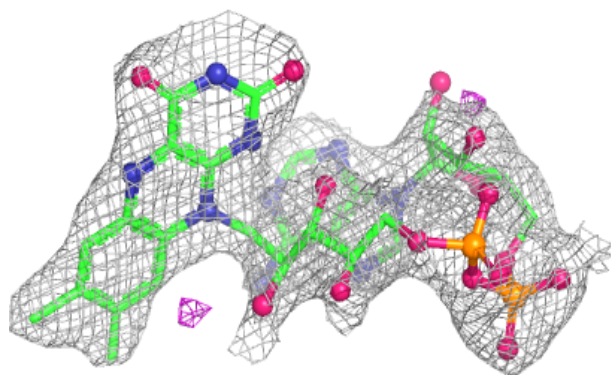
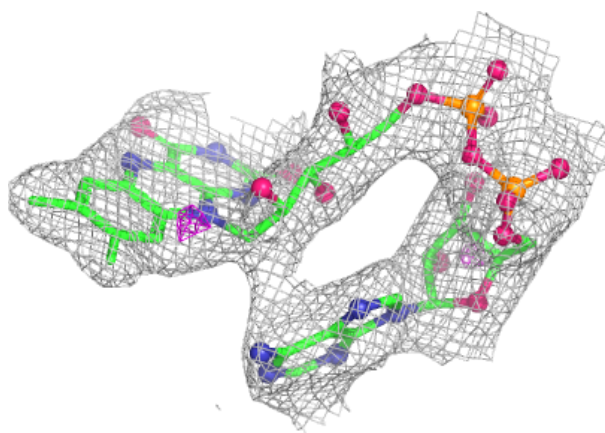
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FDA	B	501	53/53	0.92	0.10	38,46,52,58	0
4	SO4	A	501	5/5	0.94	0.08	30,38,43,45	0
5	FDA	A	502	53/53	0.95	0.08	21,28,34,35	0

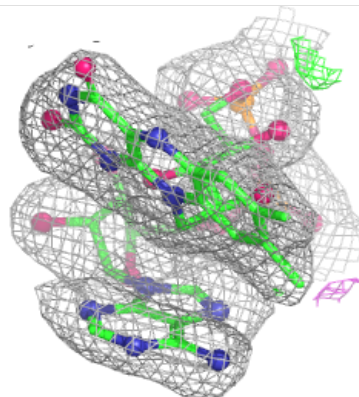
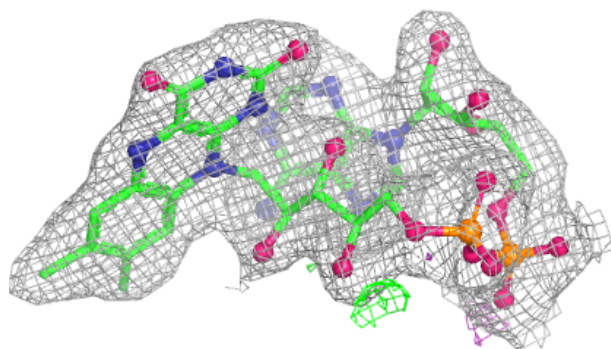
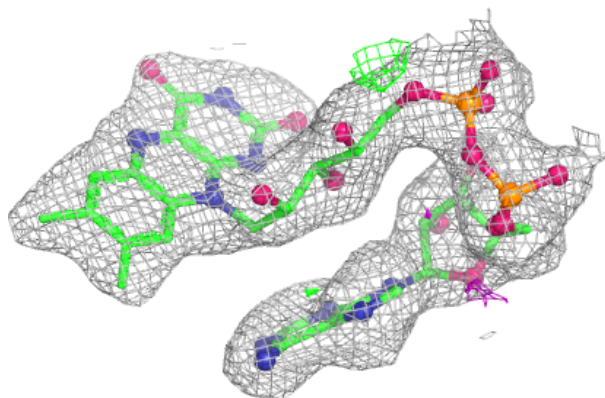
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA B 501:

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

**Electron density around FDA A 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.