

# Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 12:29 am GMT

PDB ID	:	80Y4
Title	:	Time-resolved SFX structure of the class II photolyase complexed with a
		thymine dimer (300 ps pump-probe delay)
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		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	:	2.35  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 as $541$ be (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:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.35 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	А	498	% 68%		21%		• 9%				
1	В	498	5%	25%		•	14%				

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CCP4 Ideal geometry (proteins)

Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP) 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)

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Mol	Chain	Length		Quality of chain		
			15%			
2	С	13		62%	31%	8%
			8%			
2	Ε	13	31%	46%	8%	15%
			7%			
3	D	14		71%	29%	
3	F	14	14%	79%		7%



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8557 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1 A	452	Total	С	Ν	0	$\mathbf{S}$	0 1	1	0	
		3680	2364	620	681	15		1	0	
1	1 D	D 497	Total	С	Ν	0	S	0	1	0
I D	427	3486	2240	588	643	15	0	1	0	

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

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

There are 68 discrepancies between the modelled and reference sequences:



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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	2 C	13	Total	С	Ν	Ο	Р	0	0	0
	U		281	135	51	82	13	0	0	0
0	Б	F 11	Total	С	Ν	0	Р	0	0	0
	11	243	115	44	72	12	0	0	U	

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

Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	а	1.4	Total	С	Ν	0	Р	0	0	0
0	D	14	286	136	56	81	13	0	0	0
2	Б	12	Total	С	Ν	0	Р	0	0	0
J	Г	10	265	126	51	76	12	0	0	0

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



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

• Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
Б	Δ	1	Total	С	Ν	0	Р	0	0
0	A	L	53	27	9	15	2	0	0
F	D	1	Total	С	Ν	0	Р	0	0
0	D	L	53	27	9	15	2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	109	Total O 109 109	0	0
6	В	63	$\begin{array}{cc} \text{Total} & \text{O} \\ 63 & 63 \end{array}$	0	0
6	С	15	$\begin{array}{cc} \text{Total} & \text{O} \\ 15 & 15 \end{array}$	0	0
6	D	11	Total O 11 11	0	0
6	Е	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0	0
6	F	5	Total O 5 5	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



#### L947 E361 E365 E365 E365 E366 E386 E386







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.20Å 117.76Å 170.47Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	30.98 - 2.35	Depositor
Itesolution (A)	30.98 - 2.35	EDS
% Data completeness	89.6 (30.98-2.35)	Depositor
(in resolution range)	89.6(30.98-2.35)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.33 (at 2.34 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.301 , $0.373$	Depositor
II, II, <i>free</i>	0.301 , $0.373$	DCC
$R_{free}$ test set	2701 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.0	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $67.8$	EDS
L-test for $twinning^2$	$ < L >=0.54, < L^2>=0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: WUH, 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).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.57	0/3778	0.68	0/5107
1	В	0.49	0/3583	0.64	0/4843
2	С	0.98	0/270	0.98	0/412
2	Е	0.97	0/227	0.87	0/345
3	D	1.03	0/321	0.97	0/494
3	F	1.01	0/297	0.96	0/457
All	All	0.61	0/8476	0.71	0/11658

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	А	3680	0	3602	69	0
1	В	3486	0	3389	90	0
2	С	281	0	135	5	0
2	Е	243	0	111	7	0
3	D	286	0	158	3	0
3	F	265	0	147	10	0
4	А	5	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	53	0	33	6	0
5	В	53	0	33	4	0
6	А	109	0	0	2	0
6	В	63	0	0	5	0
6	С	15	0	0	0	0
6	D	11	0	0	0	0
6	Е	2	0	0	0	0
6	F	5	0	0	0	0
All	All	8557	0	7608	177	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 (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:345:TYR:HH	1:B:356:HIS:HD1	1.18	0.90
1:A:241:MET:HE3	1:A:276:ILE:HD11	1.64	0.79
1:B:241:MET:HE3	1:B:281:VAL:HA	1.65	0.79
1:B:451:LYS:NZ	2:E:10:DG:OP2	2.14	0.78
1:A:105:VAL:HG23	1:A:110:ALA:HB3	1.64	0.78
1:B:86:LYS:HG2	1:B:181:LEU:HD23	1.65	0.78
2:C:7:WUH:P1	2:C:7:WUH:C3R	2.72	0.77
1:A:220:ASN:OD1	1:A:221:LYS:N	2.18	0.76
1:B:345:TYR:OH	1:B:356:HIS:ND1	2.18	0.71
3:F:1:DT:H2'	3:F:2:DT:C6	2.26	0.70
2:E:7:WUH:C3R	2:E:7:WUH:P1	2.79	0.70
1:A:177:GLU:OE2	1:A:280:ARG:NH1	2.24	0.70
5:A:502:FDA:H5'2	5:A:502:FDA:H3B	1.73	0.69
1:A:157:GLU:OE2	1:A:166:LYS:NZ	2.24	0.67
1:B:60:GLU:OE2	1:B:411:ARG:NH2	2.27	0.66
1:B:67:ARG:NH2	1:B:368:LEU:O	2.28	0.66
1:A:3:MET:HE1	1:A:8:ILE:HD11	1.78	0.64
1:A:367:LEU:HB2	1:A:373:MET:HE2	1.78	0.64
1:A:199:THR:O	1:A:203:VAL:HG23	1.97	0.63
1:B:239:LYS:HA	1:B:242:GLU:HG2	1.81	0.62
3:F:12:DC:H2"	3:F:13:DG:C8	2.36	0.61
1:B:439:LYS:NZ	3:F:10:DG:OP1	2.22	0.60
2:E:9:DC:H42	3:F:7:DG:H1	1.48	0.60
1:B:118:SER:HB3	1:B:123:LYS:HD2	1.83	0.59
1:B:241:MET:CE	1:B:281:VAL:HA	2.31	0.59



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:12:LYS:HD3	1:B:131:ILE:HG23	1.85	0.59
1:B:222:ASP:N	1:B:222:ASP:OD1	2.35	0.59
1:A:415:GLY:HA2	5:A:502:FDA:N5	2.19	0.58
1:B:428:ASP:OD1	1:B:441:ARG:NH2	2.29	0.58
1:A:450:ARG:NH2	2:C:12:DG:O6	2.35	0.58
1:A:177:GLU:CD	1:A:280:ARG:HH12	2.06	0.57
1:B:393:GLU:O	1:B:397:GLU:HG3	2.04	0.57
1:B:249:LEU:O	1:B:294:SER:HB3	2.05	0.57
1:A:435:GLU:O	1:A:437:THR:N	2.31	0.56
1:A:73:LEU:HB3	1:A:204:LEU:HD12	1.86	0.56
1:A:11:LEU:HD11	1:A:140:GLU:HB2	1.88	0.55
1:B:268:SER:OG	1:B:372:LYS:HE2	2.06	0.55
1:B:86:LYS:NZ	1:B:181:LEU:HB3	2.23	0.54
1:A:237:ALA:HB2	1:A:270:TYR:CD1	2.43	0.54
1:B:123:LYS:HG2	1:B:127:ILE:HD13	1.90	0.53
1:A:75:GLY:HA3	6:A:644:HOH:O	2.08	0.53
1:B:76:LEU:HD23	1:B:79:LEU:HD23	1.90	0.53
1:A:69:TYR:OH	1:A:203:VAL:O	2.26	0.53
1:B:146:VAL:HG22	1:B:307:GLU:OE2	2.09	0.53
1:A:39:PHE:CZ	1:A:43:ILE:HD11	2.44	0.53
3:F:3:DG:H2'	3:F:3:DG:OP2	2.09	0.52
1:B:81:VAL:HA	1:B:84:SER:HB3	1.91	0.52
1:B:74:LYS:HD3	6:B:659:HOH:O	2.10	0.52
1:B:241:MET:HE2	1:B:284:GLU:HB2	1.91	0.52
1:B:282:VAL:HG21	1:B:303:LEU:HD21	1.91	0.52
1:B:12:LYS:NZ	1:B:131:ILE:O	2.41	0.51
1:B:94:ARG:H	1:B:100:LYS:NZ	2.08	0.51
1:B:112:THR:HG23	1:B:137:PRO:HG2	1.92	0.51
2:E:13:DC:H2"	2:E:14:DA:C8	2.46	0.51
1:A:384:LYS:NZ	1:A:387:GLU:OE1	2.33	0.51
1:B:312:PHE:CE1	1:B:426:VAL:HG11	2.45	0.51
3:F:7:DG:H2"	3:F:8:DA:C8	2.46	0.51
1:A:45:LYS:NZ	1:A:182:GLU:OE2	2.42	0.51
1:A:168:TYR:CE1	1:A:304:ILE:HD11	2.46	0.51
1:A:101:ILE:O	1:A:105:VAL:HG12	2.10	0.51
1:B:237:ALA:HB1	1:B:276:ILE:HB	1.92	0.51
2:C:2:DT:H2"	2:C:3:DC:OP2	2.11	0.51
1:B:144:HIS:O	1:B:306:LYS:NZ	2.40	0.50
1:B:378:ARG:HD3	1:B:407:GLU:OE2	2.11	0.50
1:A:168:TYR:HE1	1:A:304:ILE:HD11	1.77	0.50
1:A:252:TYR:OH	5:A:502:FDA:O2A	2.19	0.50



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:55:PHE:HB3	1:B:92:PHE:CD1	2.47	0.50
1:A:3:MET:CE	1:A:8:ILE:HD11	2.42	0.50
1:B:146:VAL:HG23	1:B:147:VAL:HG23	1.94	0.49
1:B:115:THR:O	1:B:140:GLU:HA	2.13	0.49
1:B:373:MET:HB3	1:B:378:ARG:HG2	1.94	0.49
2:C:1:DA:H2"	2:C:2:DT:C6	2.47	0.49
1:A:446:GLU:H	1:A:446:GLU:CD	2.16	0.49
1:B:113:LEU:O	1:B:138:PHE:HA	2.13	0.49
1:A:257:ASN:O	1:A:259:PRO:HD3	2.13	0.49
5:B:501:FDA:H5'2	5:B:501:FDA:H3B	1.94	0.49
1:A:403:ASN:ND2	1:A:404:ASP:OD1	2.46	0.48
1:B:366:GLU:HB2	1:B:461:TYR:CE2	2.48	0.48
1:A:239:LYS:O	1:A:243:SER:HB2	2.14	0.48
1:B:123:LYS:HE3	1:B:127:ILE:HD11	1.96	0.48
1:A:266:ASN:HA	1:A:372:LYS:HE3	1.94	0.48
1:B:115:THR:HG23	1:B:116:ASP:O	2.14	0.48
1:B:342:SER:HB2	6:B:652:HOH:O	2.14	0.48
1:A:268:SER:HB3	5:A:502:FDA:H5'1	1.96	0.47
1:B:3:MET:SD	1:B:179:PRO:HG2	2.54	0.47
1:B:44:ALA:HB1	1:B:49:VAL:O	2.14	0.47
1:B:67:ARG:NE	1:B:222:ASP:OD2	2.48	0.47
1:B:85:ARG:HA	1:B:85:ARG:HD2	1.67	0.47
1:B:291:ASN:HB3	1:B:294:SER:HB2	1.96	0.47
1:A:59:ASP:OD1	1:A:94:ARG:NH2	2.48	0.47
1:A:415:GLY:HA2	5:A:502:FDA:C4X	2.45	0.47
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.66	0.46
1:A:12:LYS:HB2	1:A:131:ILE:HG12	1.96	0.46
1:B:222:ASP:HB2	1:B:225:PHE:CB	2.45	0.46
1:B:68:GLN:HG2	6:B:653:HOH:O	2.16	0.46
1:A:28:ASP:OD1	1:A:144:HIS:ND1	2.42	0.46
1:B:103:ARG:HG2	1:B:107:ASP:OD2	2.16	0.46
1:B:237:ALA:HB2	1:B:270:TYR:CD1	2.51	0.46
1:A:446:GLU:HB3	6:A:664:HOH:O	2.15	0.46
1:B:176:GLU:O	1:B:283:LEU:HD11	2.16	0.46
1:B:347:LEU:O	1:B:351:GLU:HB2	2.16	0.46
1:B:76:LEU:HD22	1:B:92:PHE:CE1	2.52	0.45
1:A:452:PHE:CE1	1:A:454:VAL:HG12	2.51	0.45
1:B:389[A]:SER:OG	1:B:395:ALA:HB2	2.16	0.45
1:B:308:ILE:HA	1:B:311:ASN:HB3	1.98	0.45
1:A:184:ASN:HB3	1:A:186:VAL:O	2.17	0.45
1:A:348:GLU:H	1:A:348:GLU:CD	2.20	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:E:9:DC:N4	3:F:7:DG:H1	2.13	0.45
1:B:222:ASP:HB2	1:B:225:PHE:HB3	1.99	0.45
1:B:403:ASN:OD1	5:B:501:FDA:N5	2.49	0.45
1:A:92:PHE:CE1	1:A:200:LEU:HD11	2.52	0.45
1:A:367:LEU:HB2	1:A:373:MET:CE	2.43	0.44
1:B:7:ARG:NH2	1:B:174:PHE:O	2.45	0.44
1:A:61:PHE:HD1	1:A:211:LEU:HD11	1.82	0.44
1:A:318:GLY:HA3	1:A:323[B]:GLU:OE2	2.16	0.44
1:B:386:LEU:HD13	1:B:423:ILE:HG23	1.98	0.44
3:F:12:DC:H2"	3:F:13:DG:N7	2.31	0.44
1:A:378:ARG:HD3	1:A:407:GLU:OE2	2.17	0.44
1:B:450:ARG:NH2	2:E:12:DG:N7	2.64	0.44
1:B:267:LEU:O	1:B:271:LEU:HG	2.18	0.44
1:B:367:LEU:HD11	1:B:407:GLU:HG2	1.99	0.44
1:A:386:LEU:HD13	1:A:423:ILE:HG23	2.00	0.43
1:B:67:ARG:NH2	1:B:225:PHE:HB2	2.33	0.43
1:A:414:ASN:HB3	5:A:502:FDA:N1	2.33	0.43
1:B:391:SER:OG	1:B:394:LYS:HG2	2.18	0.43
1:A:11:LEU:HD12	1:A:138:PHE:CE1	2.53	0.43
1:A:130:VAL:HG12	1:A:134:ILE:HD13	2.00	0.43
1:B:415:GLY:HA2	5:B:501:FDA:N5	2.34	0.43
1:B:435:GLU:O	1:B:437:THR:N	2.47	0.43
1:B:415:GLY:HA2	5:B:501:FDA:C4X	2.48	0.43
1:B:428:ASP:CG	1:B:441:ARG:HH21	2.17	0.43
1:B:241:MET:O	1:B:245:ILE:HG13	2.18	0.43
1:A:259:PRO:HD2	1:A:452:PHE:CG	2.53	0.43
1:A:285:VAL:O	1:A:295:LYS:HE3	2.18	0.43
1:B:105:VAL:HG11	1:B:134:ILE:HG22	2.01	0.43
1:A:405:ARG:O	1:A:405:ARG:NH1	2.38	0.42
1:A:343:HIS:CE1	1:A:356:HIS:CE1	3.06	0.42
1:A:445:TYR:HB3	1:A:446:GLU:OE2	2.20	0.42
2:E:11:DC:H2"	2:E:12:DG:C8	2.54	0.42
1:A:390:GLU:CD	1:B:121:ARG:HH21	2.23	0.42
3:D:10:DG:H1'	3:D:11:DC:H5'	2.00	0.42
1:A:3:MET:HE3	1:A:3:MET:HB3	1.61	0.42
1:B:403:ASN:O	1:B:407:GLU:HB2	2.20	0.42
3:F:5:DG:H2"	3:F:6:DC:C5'	2.50	0.42
1:A:340:VAL:HA	1:B:125:GLN:HE22	1.83	0.42
1:B:55:PHE:HB3	1:B:92:PHE:CE1	2.55	0.42
1:B:93:LEU:HB3	1:B:100:LYS:HE2	2.02	0.42
1:B:347:LEU:HB2	1:B:398:ILE:HG12	2.01	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:308:ILE:HA	1:A:311:ASN:HB3	2.00	0.42
1:B:41:ARG:NH2	1:B:185:SER:H	2.18	0.42
1:B:41:ARG:NH2	6:B:607:HOH:O	2.52	0.42
2:C:1:DA:H2"	2:C:2:DT:C5	2.55	0.42
3:D:3:DG:H2"	3:D:4:DC:OP2	2.19	0.42
1:A:80:GLU:HG3	1:A:90:SER:OG	2.20	0.41
1:B:17:GLY:CA	1:B:111:GLY:HA2	2.50	0.41
1:B:45:LYS:HD2	1:B:182:GLU:OE1	2.20	0.41
1:A:33:ASP:HA	1:A:178:PHE:CD1	2.55	0.41
1:B:297:ALA:O	1:B:301:GLU:HG2	2.20	0.41
1:A:199:THR:HG23	1:A:202:ASP:H	1.85	0.41
1:B:268:SER:OG	1:B:269:PRO:HD3	2.20	0.41
1:A:19:GLY:HA3	1:A:109:ASN:O	2.21	0.41
1:B:163:PHE:CE2	1:B:167:LEU:HD12	2.55	0.41
1:B:442:TYR:CE2	1:B:444:SER:HB3	2.56	0.41
1:B:28:ASP:OD2	1:B:143:ALA:HB3	2.20	0.41
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.88	0.41
1:B:363:SER:HB2	1:B:373:MET:SD	2.61	0.41
3:F:3:DG:H2"	3:F:4:DC:OP2	2.20	0.41
1:A:157:GLU:HG3	1:A:163:PHE:CD1	2.57	0.40
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.97	0.40
1:B:67:ARG:HH21	1:B:225:PHE:HB2	1.87	0.40
1:A:24:TRP:HB2	1:A:113:LEU:HD11	2.03	0.40
1:B:253:GLY:HA3	6:B:630:HOH:O	2.20	0.40
1:A:93:LEU:N	1:A:93:LEU:HD23	2.36	0.40
1:B:89:PRO:HB2	1:B:91:PHE:HE1	1.85	0.40
1:B:114:VAL:HG22	1:B:139:PHE:HB2	2.04	0.40
1:A:158:TYR:CZ	3:D:11:DC:H4'	2.56	0.40
1:A:405:ARG:NH2	4:A:501:SO4:O4	2.47	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	Percentile	s
1	А	449/498~(90%)	430 (96%)	18 (4%)	1 (0%)	47 56	
1	В	424/498~(85%)	404 (95%)	19 (4%)	1 (0%)	47 56	
All	All	873/996~(88%)	834 (96%)	37~(4%)	2 (0%)	47 56	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	319	TYR
1	А	6	LYS

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	394/429~(92%)	374~(95%)	20~(5%)	24 27
1	В	372/429~(87%)	358~(96%)	14 (4%)	33 41
All	All	766/858~(89%)	732~(96%)	34~(4%)	27 34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	MET
1	А	13	SER
1	А	26	SER
1	А	51	VAL
1	А	57	LEU
1	А	70	GLU
1	А	73	LEU
1	А	105	VAL
1	А	132	SER
1	А	135	SER
1	А	138	PHE
1	А	200	LEU
1	А	224	LEU
1	А	243	SER



Mol	Chain	Res	Type
1	А	250	ASP
1	А	290	SER
1	А	294	SER
1	А	394	LYS
1	А	403	ASN
1	А	462	SER
1	В	32	GLU
1	В	60	GLU
1	В	90	SER
1	В	102	SER
1	В	109	ASN
1	В	116	ASP
1	В	138	PHE
1	В	149	CYS
1	В	222	ASP
1	В	276	ILE
1	В	277	SER
1	В	310	ASP
1	В	403	ASN
1	В	449	LYS

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

Mol	Chain	Res	Type
1	А	154	GLN
1	А	262	ASN
1	В	109	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)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	WUH	Е	7	2	$36,\!42,\!45$	1.60	3 (8%)	28,62,71	0.85	0
2	WUH	С	7	2	36,42,45	1.58	4 (11%)	28,62,71	1.22	3 (10%)

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).

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WUH	Е	7	2	-	13/17/83/93	0/4/4/5
2	WUH	С	7	2	-	7/17/83/93	0/4/4/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ε	7	WUH	C8-C2	5.83	1.41	1.33
2	Е	7	WUH	C5T-C4T	5.61	1.40	1.33
2	С	7	WUH	C8-C2	5.56	1.40	1.33
2	С	7	WUH	C5T-C4T	5.23	1.40	1.33
2	Е	7	WUH	C5M-C8	-3.76	1.44	1.50
2	С	7	WUH	C5M-C8	-3.75	1.44	1.50
2	C	7	WUH	C5-C8	2.42	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	7	WUH	C3-C1-N2	2.91	119.51	115.59
2	С	7	WUH	O2-C1-N2	2.59	111.72	108.65
2	С	7	WUH	C4'-O2-C1	-2.09	104.39	109.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	7	WUH	C8-C5-C6T-N1T
2	С	7	WUH	N2-C5-C6T-N1T
2	Е	7	WUH	C3R-C4R-C5R-O5R



Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	Ε	7	WUH	O4R-C4R-C5R-O5R
2	Ε	7	WUH	N2-C5-C6T-C5T
2	Ε	7	WUH	C8-C5-C6T-N1T
2	Ε	7	WUH	N2-C5-C6T-N1T
2	С	7	WUH	C2R-C1R-N1T-C6T
2	Ε	7	WUH	C2R-C1R-N1T-C6T
2	Ε	7	WUH	C2R-C1R-N1T-C2T
2	Ε	7	WUH	O4R-C1R-N1T-C2T
2	Ε	7	WUH	C3-C1-N2-C5
2	С	7	WUH	C2R-C1R-N1T-C2T
2	Ε	7	WUH	O4R-C1R-N1T-C6T
2	$\mathbf{C}$	7	WUH	O4R-C1R-N1T-C6T
2	С	7	WUH	O4R-C1R-N1T-C2T
2	C	7	WUH	C4R-C5R-O5R-PB
2	Е	7	WUH	O2-C1-N2-C5
2	Е	7	WUH	O2-C1-N2-C7
2	Ε	7	WUH	C3-C1-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	7	WUH	1	0
2	С	7	WUH	1	0

## 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 Tvi	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
MOI	Type Chain Res	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
5	FDA	В	501	-	52,58,58	0.64	0	60,89,89	0.81	2 (3%)
4	SO4	А	501	-	4,4,4	0.27	0	6,6,6	0.49	0
5	FDA	А	502	-	52,58,58	0.64	0	60,89,89	0.84	3 (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	В	501	-	-	10/30/50/50	0/6/6/6
5	FDA	А	502	-	-	10/30/50/50	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	501	FDA	C5A-C6A-N6A	2.34	123.91	120.35
5	А	502	FDA	N3-C2-N1	2.33	119.55	115.80
5	А	502	FDA	O2-C2-N3	-2.16	117.75	121.82
5	А	502	FDA	O5'-P-O1P	-2.04	101.08	109.07
5	В	501	FDA	N3-C2-N1	2.04	119.08	115.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
5	А	502	FDA	C5B-O5B-PA-O1A
5	А	502	FDA	O4'-C4'-C5'-O5'
5	В	501	FDA	C5B-O5B-PA-O1A
5	В	501	FDA	P-O3P-PA-O5B
5	В	501	FDA	O3'-C3'-C4'-C5'
5	А	502	FDA	C2'-C3'-C4'-C5'
5	В	501	FDA	C2'-C3'-C4'-C5'
5	В	501	FDA	O3'-C3'-C4'-O4'
5	А	502	FDA	O3'-C3'-C4'-C5'
5	А	502	FDA	C3'-C4'-C5'-O5'
5	В	501	FDA	C2'-C3'-C4'-O4'
5	А	502	FDA	C5B-O5B-PA-O3P
5	В	501	FDA	C5B-O5B-PA-O3P



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

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	501	FDA	4	0
4	А	501	SO4	1	0
5	А	502	FDA	6	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.











## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	452/498~(90%)	-0.01	5 (1%) 80 87	18,  34,  63,  110	0
1	В	427/498~(85%)	0.48	24 (5%) 24 35	28, 53, 81, 132	0
2	С	12/13~(92%)	0.53	2(16%) 1 2	31,64,85,86	0
2	Е	10/13~(76%)	0.72	1 (10%) 7 11	43, 68, 114, 123	0
3	D	14/14~(100%)	0.30	1 (7%) 16 23	45,63,77,89	0
3	F	13/14~(92%)	0.54	0 100 100	58, 71, 86, 105	0
All	All	928/1050~(88%)	0.24	33 (3%) 42 55	18, 43, 79, 132	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	63	GLU	5.9
1	В	85	ARG	4.7
1	В	108	TYR	3.7
1	В	288	ALA	3.5
1	В	94	ARG	3.5
1	В	271	LEU	3.1
1	В	14	GLY	3.1
1	А	14	GLY	3.1
2	Е	3	DC	2.9
1	В	136	ILE	2.9
1	В	69	TYR	2.9
1	В	285	VAL	2.8
1	В	169	ALA	2.8
1	В	62	LEU	2.7
1	В	178	PHE	2.7
1	В	252	TYR	2.6
1	В	187	THR	2.6
1	В	49	VAL	2.6
1	А	15	LYS	2.6



Mol	Chain	Res	Type	RSRZ
1	В	73	LEU	2.6
1	А	221	LYS	2.6
1	В	57	LEU	2.5
3	D	1	DT	2.5
1	В	274	GLY	2.5
1	А	186	VAL	2.4
1	В	45	LYS	2.3
1	В	39	PHE	2.3
1	В	15	LYS	2.3
1	В	289	GLU	2.2
1	В	456	LEU	2.1
2	C	1	DA	2.1
1	А	219	LYS	2.1
2	C	14	DA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$B-factors(A^2)$	Q<0.9
2	WUH	Е	7	39/41	0.90	0.18	$35,\!43,\!52,\!59$	0
2	WUH	С	7	39/41	0.95	0.15	20,28,33,42	0

### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
5	FDA	В	501	53/53	0.95	0.17	$27,\!38,\!44,\!47$	0
5	FDA	А	502	53/53	0.96	0.14	13,22,26,29	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
4	SO4	А	501	5/5	0.97	0.11	31,33,36,37	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.







## 6.5 Other polymers (i)

There are no such residues in this entry.

