



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:25 PM GMT

PDB ID : 2J08  
Title : THERMUS DNA PHOTOLYASE WITH 8-IOD-RIBOFLAVIN ANTENNA CHROMOPHORE  
Authors : Klar, T.; Kaiser, G.; Hennecke, U.; Carell, T.; Batschauer, A.; Essen, L.-O.  
Deposited on : 2006-08-01  
Resolution : 2.61 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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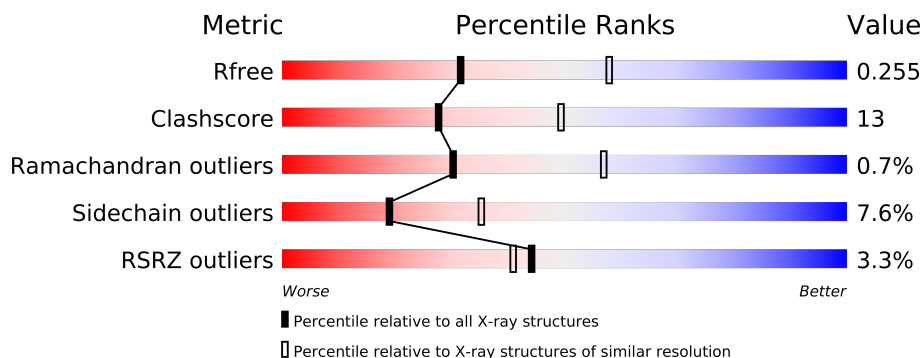
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.61 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))
$R_{free}$	66092	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (2.64-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	420	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	A	901	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3572 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

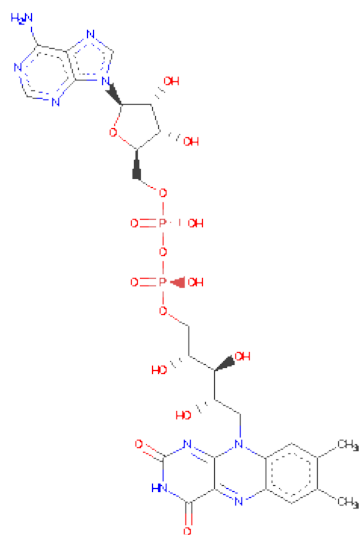
- Molecule 1 is a protein called DEOXYRIBODIPYRIMIDINEPHOTO-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3372	2175	621	572	4			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

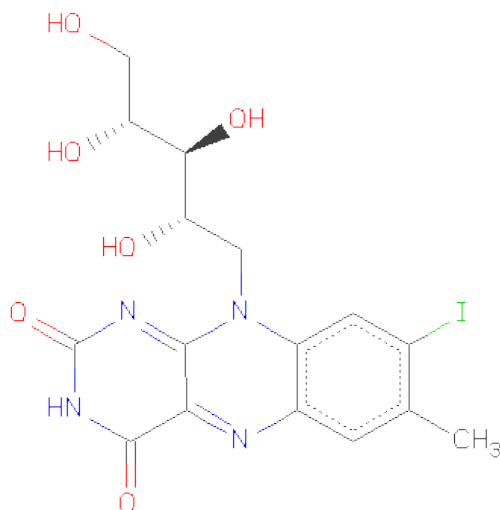
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



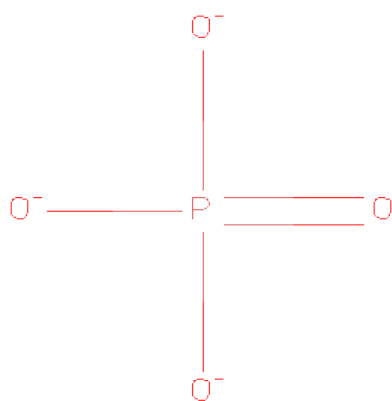
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1-DEOXY-1-(8-iodo-7-methyl-2,4-dioxo-3,4-dihydrobenzo[G]PT ERIDIN-10(2H)-YL)-D-RIBITOL (three-letter code: IRF) (formula: C<sub>16</sub>H<sub>17</sub>IN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
4	A	1	27	16	1	4	6	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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

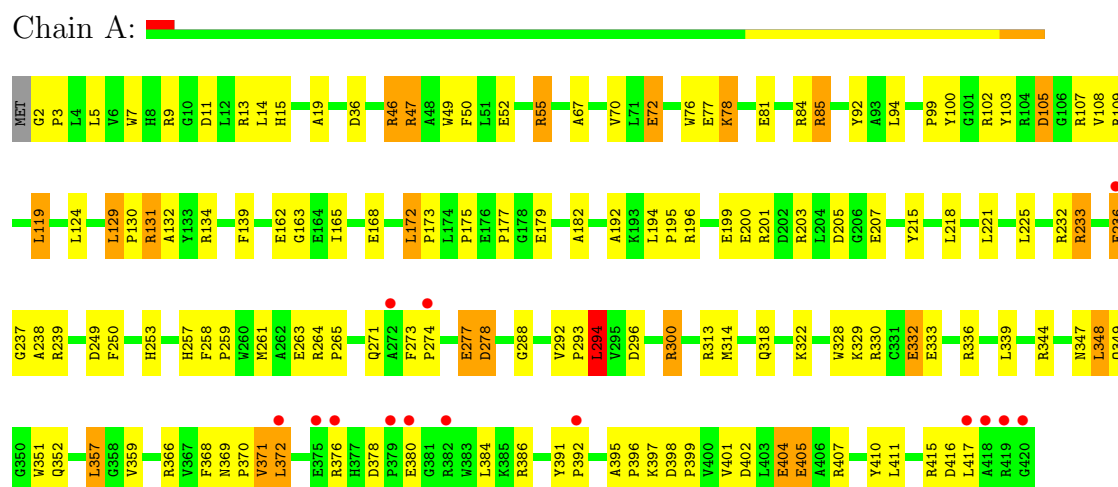
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DEOXYRIBODIPYRIMIDINEPHOTO-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.62Å 112.62Å 140.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.32 – 2.61 24.32 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.32-2.61) 91.6 (24.32-2.61)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.163 , 0.256 0.167 , 0.255	Depositor DCC
$R_{free}$ test set	771 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 15164 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IRF, FAD, CL

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	1.19	12/3487 (0.3%)	1.10	19/4759 (0.4%)

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	A	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	GLU	CG-CD	8.66	1.65	1.51
1	A	103	TYR	CD1-CE1	-6.68	1.29	1.39
1	A	277	GLU	CG-CD	6.56	1.61	1.51
1	A	49	TRP	CB-CG	5.86	1.60	1.50
1	A	72	GLU	CD-OE1	5.78	1.32	1.25
1	A	7	TRP	CE3-CZ3	5.69	1.48	1.38
1	A	376	ARG	CB-CG	5.37	1.67	1.52
1	A	100	TYR	CD1-CE1	5.23	1.47	1.39
1	A	72	GLU	CD-OE2	5.16	1.31	1.25
1	A	376	ARG	CG-CD	5.08	1.64	1.51
1	A	76	TRP	CB-CG	5.08	1.59	1.50
1	A	207	GLU	CG-CD	5.05	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	CA-CB-CG	7.37	132.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	LEU	CB-CG-CD2	-7.08	98.97	111.00
1	A	5	LEU	CB-CG-CD1	-6.78	99.47	111.00
1	A	109	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	14	LEU	CB-CG-CD1	6.58	122.19	111.00
1	A	46	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	366	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	5	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	344	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	36	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	A	348	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	55	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	294	LEU	CB-CG-CD1	5.61	120.54	111.00
1	A	300	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	205	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	313	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	36	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	13	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	A	105	ASP	CB-CG-OD1	5.27	123.04	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ASP	Mainchain
1	A	357	LEU	Peptide
1	A	378	ASP	Peptide
1	A	47	ARG	Sidechain
1	A	77	GLU	Mainchain
1	A	85	ARG	Mainchain
1	A	99	PRO	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3372	0	3312	86	0
2	A	2	0	0	0	0
3	A	53	0	31	0	0
4	A	27	0	17	1	0
5	A	10	0	0	3	0
6	A	108	0	0	7	0
All	All	3572	0	3360	87	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (87) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:HIS:ND1	1:A:179:GLU:OE2	1.70	1.24
1:A:131:ARG:HH11	1:A:131:ARG:CG	1.64	1.10
1:A:131:ARG:HH11	1:A:131:ARG:HG3	0.87	1.01
1:A:131:ARG:HG3	1:A:131:ARG:NH1	1.55	0.99
1:A:46:ARG:NH1	5:A:1424:PO4:O1	2.01	0.92
1:A:232:ARG:HH11	1:A:232:ARG:HG2	1.41	0.84
1:A:15:HIS:CE1	1:A:179:GLU:OE2	2.39	0.75
1:A:84:ARG:NE	6:A:2033:HOH:O	2.13	0.73
1:A:232:ARG:NH1	1:A:232:ARG:HG2	2.04	0.72
1:A:332:GLU:HB2	1:A:351:TRP:CG	2.25	0.71
1:A:236:GLU:HA	6:A:2083:HOH:O	1.91	0.69
1:A:72:GLU:O	1:A:78:LYS:HD2	1.95	0.66
1:A:55:ARG:NH2	1:A:165:ILE:O	2.27	0.66
1:A:318:GLN:CG	1:A:322:LYS:HD2	2.24	0.66
1:A:258:PHE:O	1:A:261:MET:HB3	1.98	0.64
1:A:196:ARG:NH1	1:A:199:GLU:HG2	2.14	0.63
1:A:402:ASP:HB3	1:A:405:GLU:OE1	1.98	0.63
1:A:332:GLU:HB2	1:A:351:TRP:CD2	2.34	0.63
1:A:47:ARG:NH2	1:A:168:GLU:OE2	2.27	0.61
1:A:411:LEU:O	1:A:415:ARG:HG3	2.03	0.59
1:A:402:ASP:OD1	1:A:404:GLU:HG3	2.02	0.59
1:A:318:GLN:HG3	1:A:322:LYS:HD2	1.84	0.59
1:A:398:ASP:N	1:A:399:PRO:HD3	2.22	0.55
1:A:232:ARG:CG	1:A:232:ARG:NH1	2.70	0.55
1:A:192:ALA:HB2	6:A:2069:HOH:O	2.07	0.54
1:A:84:ARG:CD	6:A:2033:HOH:O	2.54	0.54
1:A:288:GLY:O	1:A:296:ASP:HB3	2.07	0.54
1:A:182:ALA:HB2	1:A:215:TYR:CD2	2.44	0.53
1:A:195:PRO:HD3	1:A:233:ARG:NH2	2.24	0.53
1:A:292:VAL:O	1:A:293:PRO:C	2.48	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:46:ARG:HH12	5:A:1424:PO4:P	2.30	0.52
1:A:273:PHE:CD2	1:A:274:PRO:HD2	2.45	0.51
1:A:369:ASN:CG	1:A:372:LEU:HB2	2.31	0.51
1:A:263:GLU:O	1:A:263:GLU:HG2	2.11	0.51
1:A:70:VAL:O	1:A:163:GLY:HA3	2.12	0.50
1:A:84:ARG:HD2	6:A:2033:HOH:O	2.11	0.49
1:A:399:PRO:HB2	1:A:401:VAL:O	2.12	0.49
1:A:294:LEU:O	1:A:294:LEU:HD12	2.12	0.49
1:A:336:ARG:NE	5:A:1424:PO4:O3	2.44	0.49
1:A:265:PRO:HB3	1:A:357:LEU:HB3	1.95	0.49
1:A:67:ALA:HA	6:A:2060:HOH:O	2.12	0.49
1:A:175:PRO:O	1:A:177:PRO:HD3	2.12	0.48
1:A:50:PHE:HD1	1:A:218:LEU:HD22	1.78	0.48
1:A:129:LEU:HG	1:A:130:PRO:HD2	1.96	0.48
1:A:162:GLU:HG3	1:A:163:GLY:N	2.29	0.48
1:A:264:ARG:HD2	1:A:271:GLN:NE2	2.29	0.48
1:A:239:ARG:HG3	6:A:2083:HOH:O	2.13	0.47
1:A:329:LYS:O	1:A:330:ARG:C	2.52	0.47
1:A:322:LYS:HG2	1:A:410:TYR:CE1	2.49	0.47
1:A:278:ASP:OD1	1:A:278:ASP:C	2.53	0.47
1:A:402:ASP:OD1	1:A:402:ASP:C	2.52	0.47
4:A:1422:IRF:H9	4:A:1422:IRF:H1'1	1.65	0.47
1:A:371:VAL:HG22	1:A:372:LEU:N	2.29	0.46
1:A:264:ARG:HA	1:A:328:TRP:HZ2	1.81	0.45
1:A:200:GLU:O	1:A:203:ARG:HG3	2.16	0.45
1:A:369:ASN:OD1	1:A:369:ASN:C	2.54	0.45
1:A:352:GLN:HB2	1:A:359:VAL:HG23	1.98	0.45
1:A:296:ASP:O	1:A:300:ARG:HG3	2.17	0.45
1:A:258:PHE:O	1:A:261:MET:CB	2.63	0.44
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.80	0.44
1:A:332:GLU:HB2	1:A:351:TRP:CD1	2.53	0.44
1:A:318:GLN:OE1	1:A:368:PHE:CD2	2.70	0.44
1:A:236:GLU:C	1:A:238:ALA:N	2.69	0.44
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.83	0.43
1:A:52:GLU:OE2	1:A:55:ARG:NH1	2.51	0.43
1:A:293:PRO:HB3	1:A:384:LEU:HD11	1.99	0.43
1:A:172:LEU:HB2	1:A:173:PRO:HD2	2.01	0.42
1:A:131:ARG:NH1	1:A:131:ARG:CG	2.36	0.42
1:A:9:ARG:N	1:A:9:ARG:HD3	2.35	0.42
1:A:277:GLU:HG3	1:A:278:ASP:N	2.34	0.42
1:A:94:LEU:HA	1:A:119:LEU:O	2.19	0.42
1:A:253:HIS:CE1	1:A:257:HIS:CE1	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:GLU:HG2	1:A:347:ASN:ND2	2.36	0.41
1:A:2:GLY:HA2	1:A:3:PRO:HD2	1.77	0.41
1:A:395:ALA:HA	1:A:396:PRO:HD3	1.83	0.41
1:A:258:PHE:N	1:A:259:PRO:HD3	2.35	0.41
1:A:19:ALA:HB1	1:A:92:TYR:HB3	2.03	0.41
1:A:194:LEU:O	1:A:237:GLY:HA3	2.21	0.41
1:A:257:HIS:C	1:A:259:PRO:HD3	2.42	0.40
1:A:139:PHE:CE2	1:A:250:PHE:HB2	2.56	0.40
1:A:391:TYR:HA	1:A:392:PRO:HD3	1.79	0.40
1:A:81:GLU:O	1:A:85:ARG:HG3	2.21	0.40
1:A:108:VAL:O	1:A:108:VAL:HG12	2.20	0.40
1:A:124:LEU:HB2	1:A:249:ASP:OD1	2.22	0.40
1:A:15:HIS:CD2	1:A:225:LEU:HD13	2.56	0.40
1:A:318:GLN:CD	1:A:322:LYS:HD2	2.42	0.40
1:A:132:ALA:HB1	1:A:258:PHE:CZ	2.57	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	417/420 (99%)	399 (96%)	15 (4%)	3 (1%)	30 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ASP
1	A	417	LEU
1	A	278	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	329/335 (98%)	304 (92%)	25 (8%)	19	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	78	LYS
1	A	107	ARG
1	A	119	LEU
1	A	129	LEU
1	A	131	ARG
1	A	134	ARG
1	A	172	LEU
1	A	201	ARG
1	A	233	ARG
1	A	236	GLU
1	A	294	LEU
1	A	314	MET
1	A	332	GLU
1	A	333	GLU
1	A	348	LEU
1	A	349	GLN
1	A	371	VAL
1	A	372	LEU
1	A	380	GLU
1	A	386	ARG
1	A	397	LYS
1	A	404	GLU
1	A	405	GLU
1	A	407	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	97	HIS
1	A	271	GLN
1	A	310	ASN
1	A	373	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	FAD	A	1421	-	58,58,58	1.37	11 (18%)	85,89,89	2.38	23 (27%)
4	IRF	A	1422	-	29,29,29	2.13	7 (24%)	39,43,43	2.67	14 (35%)
5	PO4	A	1423	-	4,4,4	0.37	0	6,6,6	0.38	0
5	PO4	A	1424	-	4,4,4	0.41	0	6,6,6	0.33	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
3	FAD	A	1421	-	-	0/34/50/50	0/1/6/6
4	IRF	A	1422	-	-	0/14/14/14	0/0/3/3
5	PO4	A	1423	-	-	0/0/0/0	0/0/0/0
5	PO4	A	1424	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1422	IRF	C7-C8	6.28	1.50	1.39
4	A	1422	IRF	C4-C4A	5.28	1.49	1.41
4	A	1422	IRF	C4A-C10	3.36	1.46	1.40
3	A	1421	FAD	C8A-N9A	3.29	1.41	1.36
3	A	1421	FAD	C1'-N10	3.25	1.51	1.48
4	A	1422	IRF	C6-C5A	-3.20	1.37	1.41
3	A	1421	FAD	C1'-C2'	3.18	1.54	1.51
4	A	1422	IRF	C1'-C2'	-2.65	1.49	1.51
3	A	1421	FAD	C2A-N3A	2.54	1.37	1.32
3	A	1421	FAD	C4-N3	2.36	1.41	1.37
3	A	1421	FAD	O4B-C1B	2.31	1.44	1.41
4	A	1422	IRF	C9A-C5A	2.21	1.47	1.42
3	A	1421	FAD	C9-C9A	-2.21	1.36	1.40
3	A	1421	FAD	C5X-N5	2.18	1.38	1.35
3	A	1421	FAD	O4-C4	2.17	1.28	1.24
3	A	1421	FAD	C2A-N1A	2.16	1.38	1.33
3	A	1421	FAD	C4-C4X	2.14	1.44	1.41
4	A	1422	IRF	C9A-N10	2.09	1.41	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1421	FAD	N3A-C2A-N1A	-9.59	120.69	128.71
3	A	1421	FAD	C4X-C10-N10	9.04	125.02	120.51
4	A	1422	IRF	C2-N1-C10	6.98	122.01	114.98
4	A	1422	IRF	C4A-C10-N1	-6.86	115.88	122.73
3	A	1421	FAD	C9A-N10-C10	-6.44	115.45	121.77
4	A	1422	IRF	C4A-N5-C5A	6.16	123.61	116.69
4	A	1422	IRF	C1'-N10-C9A	-4.99	114.02	118.87
3	A	1421	FAD	C5X-C9A-N10	4.71	121.44	116.80
3	A	1421	FAD	C2-N1-C10	4.55	119.57	114.98
3	A	1421	FAD	C4X-C10-N1	-4.47	118.27	122.73
3	A	1421	FAD	C4-N3-C2	-4.04	117.10	125.39
3	A	1421	FAD	O3'-C3'-C2'	3.93	118.66	108.74
3	A	1421	FAD	N3A-C4A-N9A	3.90	132.48	125.43
3	A	1421	FAD	C2B-C1B-N9A	-3.70	103.78	113.27
4	A	1422	IRF	O2'-C2'-C3'	3.68	118.21	109.05
3	A	1421	FAD	C4-C4X-C10	3.66	122.85	116.95
4	A	1422	IRF	C9A-N10-C10	-3.33	118.50	121.77
3	A	1421	FAD	O4B-C1B-N9A	3.32	111.53	108.44
4	A	1422	IRF	O5'-C5'-C4'	-3.31	103.64	111.05
3	A	1421	FAD	C10-C4X-N5	-3.19	116.58	120.45
3	A	1421	FAD	C4X-N5-C5X	3.03	120.09	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1422	IRF	C8-C9-C9A	-2.93	117.46	120.88
3	A	1421	FAD	N7A-C8A-N9A	-2.89	106.18	114.36
4	A	1422	IRF	C5'-C4'-C3'	-2.83	105.96	112.38
4	A	1422	IRF	O4'-C4'-C3'	-2.79	102.09	109.05
4	A	1422	IRF	C4-N3-C2	-2.69	119.88	125.39
4	A	1422	IRF	C1'-N10-C10	2.67	122.96	119.17
3	A	1421	FAD	C5A-C4A-N3A	-2.56	120.12	125.70
4	A	1422	IRF	N1-C10-N10	2.56	122.69	115.97
4	A	1422	IRF	O3'-C3'-C2'	2.46	114.96	108.74
3	A	1421	FAD	C2A-N3A-C4A	2.41	120.88	114.01
3	A	1421	FAD	C1'-N10-C10	2.33	122.47	119.17
3	A	1421	FAD	C8A-N9A-C4A	2.33	108.67	106.90
3	A	1421	FAD	O3B-C3B-C4B	2.31	117.88	111.08
3	A	1421	FAD	C1'-C2'-C3'	2.11	115.86	109.82
3	A	1421	FAD	C8A-N7A-C5A	2.10	110.08	103.58
3	A	1421	FAD	C4A-C5A-N7A	-2.05	107.76	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/420 (99%)	-0.22	14 (3%) 44 41	10, 25, 43, 62	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ARG	6.6
1	A	379	PRO	5.2
1	A	272	ALA	4.6
1	A	420	GLY	4.6
1	A	417	LEU	4.3
1	A	372	LEU	3.6
1	A	418	ALA	3.3
1	A	380	GLU	3.2
1	A	392	PRO	3.1
1	A	382	ARG	3.0
1	A	376	ARG	2.8
1	A	274	PRO	2.8
1	A	375	GLU	2.5
1	A	236	GLU	2.3

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	901	1/1	0.12	2.24	57,57,57,57	0
2	CL	A	902	1/1	0.17	1.74	50,50,50,50	0
4	IRF	A	1422	27/27	0.15	-0.02	13,22,35,43	0
3	FAD	A	1421	53/53	0.13	-0.05	12,25,30,32	0
5	PO4	A	1424	5/5	0.11	-0.70	44,48,52,58	0
5	PO4	A	1423	5/5	0.09	-1.25	32,35,48,50	0

## 6.5 Other polymers

There are no such residues in this entry.