



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:40 PM GMT

PDB ID : 3UMV  
Title : Eukaryotic Class II CPD photolyase structure reveals a basis for improved UV-tolerance in plants  
Authors : Arvai, A.S.; Hitomi, K.; Getzoff, E.D.; Tainer, J.A.  
Deposited on : 2011-11-14  
Resolution : 1.71 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

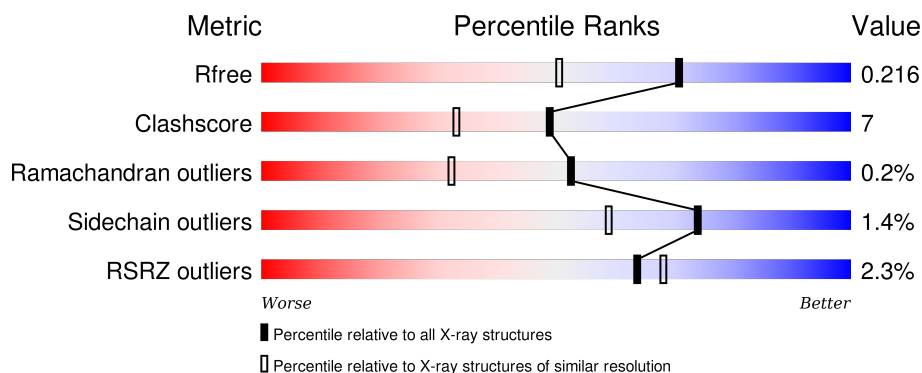
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	506	 2% 79% 14% 7%
1	B	506	 2% 80% 11% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	701	-	-	-	X
2	EDO	A	703	-	-	-	X
2	EDO	A	705	-	-	-	X
4	URE	A	901	-	-	-	X
4	URE	A	902	-	-	-	X
4	URE	A	903	-	-	-	X
4	URE	A	904	-	-	X	-
4	URE	B	902	-	-	X	X
4	URE	B	905	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8978 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	472	Total	C	N	O	S	0	7	0
			3799	2416	690	675	18			
1	B	468	Total	C	N	O	S	0	2	0
			3724	2372	670	664	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLN	ARG	SEE REMARK 999	UNP Q6F6A2
B	126	GLN	ARG	SEE REMARK 999	UNP Q6F6A2

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



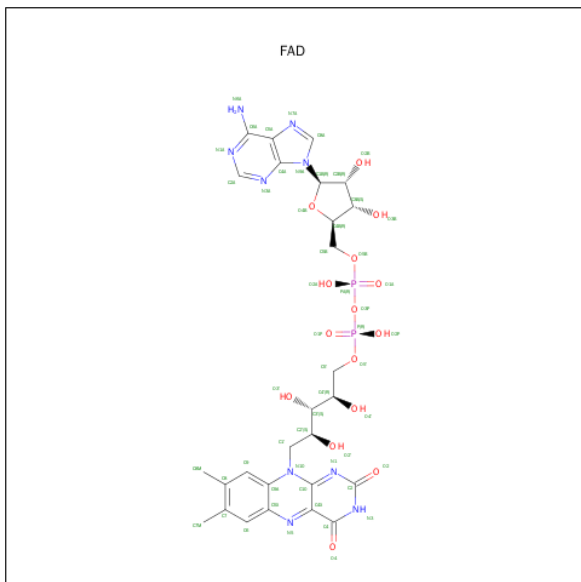
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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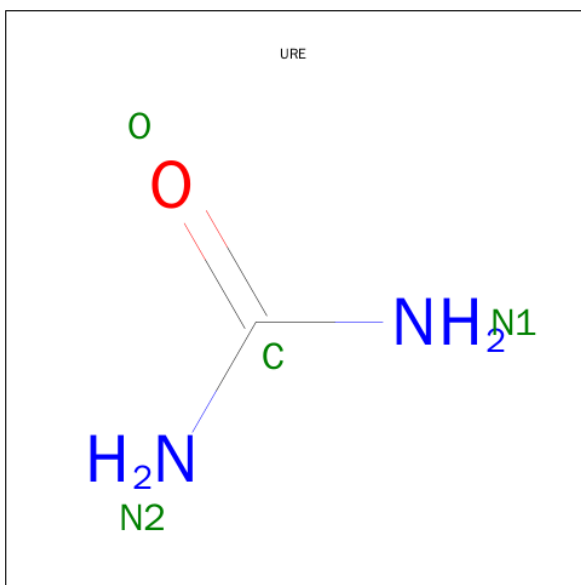
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is UREA (three-letter code: URE) (formula:  $CH_4N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			4	1	2	1		
4	A	1	Total	C	N	O	0	0
			4	1	2	1		
4	A	1	Total	C	N	O	0	0
			4	1	2	1		
4	A	1	Total	C	N	O	0	0
			4	1	2	1		
4	A	1	Total	C	N	O	0	0
			4	1	2	1		
4	B	1	Total	C	N	O	0	0
			4	1	2	1		
4	B	1	Total	C	N	O	0	0
			4	1	2	1		
4	B	1	Total	C	N	O	0	0
			4	1	2	1		

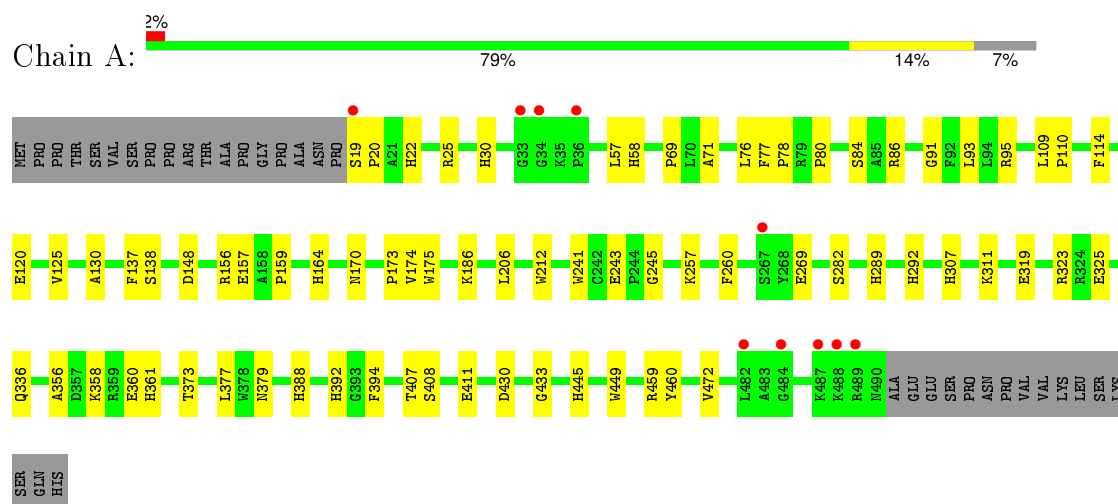
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	700	Total	O	0	0
			700	700		
5	B	589	Total	O	0	0
			589	589		

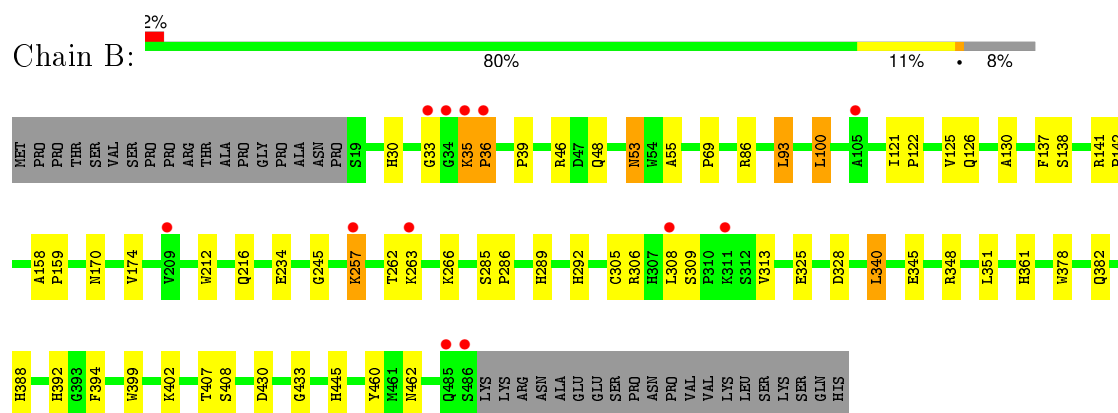
### 3 Residue-property plots [i](#)

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: Deoxyribodipyrimidine photo-lyase



#### • Molecule 1: Deoxyribodipyrimidine photo-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.35Å 109.36Å 97.74Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	45.55 – 1.71 48.78 – 1.71	Depositor EDS
% Data completeness (in resolution range)	86.9 (45.55-1.71) 86.9 (48.78-1.71)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.181 , 0.217 0.180 , 0.216	Depositor DCC
$R_{free}$ test set	2000 reflections (1.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 119313 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: URE, EDO, FAD

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	0.37	0/3904	0.52	0/5295
1	B	0.31	0/3829	0.49	1/5198 (0.0%)
All	All	0.34	0/7733	0.50	1/10493 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	LEU	CA-CB-CG	5.64	128.27	115.30

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	3799	0	3732	57	0
1	B	3724	0	3655	51	0
2	A	24	0	36	6	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	20	0	20	5	0
4	B	16	0	16	2	0
5	A	700	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	589	0	0	8	0
All	All	8978	0	7521	109	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 7.

All (109) 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:B:460:TYR:H	4:B:902:URE:HN11	1.06	0.95
1:A:77:PHE:H	4:A:904:URE:HN11	1.14	0.93
1:B:289:HIS:HD2	1:B:430:ASP:OD2	1.74	0.71
1:B:257:LYS:H	1:B:257:LYS:HD2	1.56	0.69
1:A:125:VAL:HG13	1:A:130:ALA:HB3	1.75	0.68
1:A:57:LEU:HD23	1:A:206:LEU:HD12	1.74	0.68
1:A:289:HIS:HD2	1:A:430:ASP:OD2	1.77	0.68
1:B:460:TYR:N	4:B:902:URE:HN11	1.89	0.67
1:A:138:SER:OG	2:A:705:EDO:H22	1.95	0.67
1:B:407:THR:HG22	5:B:1136:HOH:O	1.95	0.67
1:B:35:LYS:H	1:B:36:PRO:HD2	1.60	0.66
1:B:33:GLY:O	1:B:36:PRO:HD2	1.97	0.65
1:A:388:HIS:HE1	2:A:701:EDO:O1	1.79	0.65
1:B:93:LEU:C	1:B:93:LEU:HD12	2.17	0.64
1:A:460:TYR:H	4:A:902:URE:HN11	1.44	0.64
1:B:382:GLN:HE21	1:B:399:TRP:HE1	1.44	0.64
1:B:245:GLY:H	1:B:292:HIS:CD2	2.17	0.63
1:A:58:HIS:HE1	1:A:164:HIS:ND1	1.97	0.63
1:B:93:LEU:HD12	1:B:93:LEU:O	2.00	0.62
1:B:30:HIS:HE1	1:B:159:PRO:O	1.84	0.61
1:B:292:HIS:HE1	5:B:709:HOH:O	1.84	0.60
1:B:170:ASN:HD22	1:B:325:GLU:HG2	1.66	0.60
1:B:392:HIS:CD2	1:B:394:PHE:H	2.20	0.60
1:A:30:HIS:HE1	1:A:159:PRO:O	1.86	0.58
1:A:292:HIS:HE1	5:A:684:HOH:O	1.86	0.58
1:B:216:GLN:HB3	5:B:1089:HOH:O	2.03	0.57
1:B:48:GLN:NE2	1:B:93:LEU:HD13	2.19	0.57
1:B:382:GLN:NE2	1:B:399:TRP:HE1	2.03	0.57
1:A:245:GLY:H	1:A:292:HIS:CD2	2.24	0.56
1:B:46:ARG:HD2	1:B:138:SER:HB2	1.87	0.56
1:A:392:HIS:HE1	5:A:722:HOH:O	1.88	0.56
1:A:77:PHE:N	4:A:904:URE:HN11	1.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:HIS:HE1	5:B:740:HOH:O	1.89	0.54
1:A:373:THR:H	1:A:379:ASN:HD21	1.54	0.54
1:B:35:LYS:N	1:B:36:PRO:HD2	2.19	0.54
1:A:356:ALA:HB3	5:A:665:HOH:O	2.09	0.53
1:B:257:LYS:CD	1:B:257:LYS:H	2.20	0.53
1:A:91:GLY:O	1:A:95:ARG:HG3	2.09	0.53
1:A:78:PRO:HB2	2:A:708:EDO:H21	1.90	0.53
1:A:114:PHE:HB3	1:A:120:GLU:OE1	2.09	0.52
1:B:306:ARG:HA	1:B:313:VAL:HG21	1.90	0.52
1:A:170:ASN:OD1	1:A:325:GLU:HG2	2.10	0.52
1:A:392:HIS:CD2	1:A:394:PHE:H	2.28	0.52
1:B:53:ASN:C	1:B:53:ASN:HD22	2.14	0.52
1:A:19[B]:SER:OG	1:A:58:HIS:HD2	1.93	0.51
1:A:336:GLN:HG2	5:A:682:HOH:O	2.09	0.51
1:A:269:GLU:HB3	5:A:618:HOH:O	2.09	0.51
1:A:411:GLU:CD	5:A:577:HOH:O	2.50	0.51
1:B:433:GLY:HA2	3:B:801:FAD:N5	2.26	0.49
1:B:266:LYS:HG3	1:B:309:SER:HB3	1.94	0.49
1:B:445:HIS:HE1	5:B:731:HOH:O	1.96	0.49
1:A:19[A]:SER:HB3	1:A:20:PRO:HD2	1.92	0.49
1:A:25:ARG:HG2	1:A:173:PRO:HG3	1.94	0.48
1:B:36:PRO:HG3	5:B:992:HOH:O	2.13	0.48
1:A:407[B]:THR:HG22	1:A:408:SER:N	2.29	0.48
1:B:48:GLN:HE22	1:B:93:LEU:HD13	1.79	0.47
1:B:121:ILE:HB	1:B:122:PRO:HD3	1.95	0.47
1:B:285:SER:OG	1:B:286:PRO:HD3	2.14	0.47
1:B:137:PHE:CZ	1:B:174:VAL:HG11	2.50	0.46
1:B:289:HIS:CD2	1:B:430:ASP:OD2	2.62	0.46
1:A:307:HIS:HE1	5:A:1093:HOH:O	1.99	0.46
1:A:30:HIS:HD2	5:A:873:HOH:O	1.98	0.45
1:A:433:GLY:HA2	3:A:801:FAD:N5	2.32	0.45
1:B:345:GLU:OE2	1:B:348:ARG:NH2	2.49	0.45
1:A:93:LEU:C	1:A:93:LEU:HD23	2.36	0.45
1:A:148:ASP:HB3	2:A:707:EDO:H22	1.98	0.45
1:A:307:HIS:CD2	1:A:307:HIS:H	2.35	0.45
1:A:241:TRP:CZ3	2:A:701:EDO:H12	2.51	0.45
1:B:125:VAL:HG13	1:B:130:ALA:HB3	1.98	0.45
1:B:53:ASN:HD21	1:B:55:ALA:HB3	1.82	0.45
1:A:319:GLU:OE1	1:A:323[B]:ARG:HD3	2.17	0.45
1:A:377:LEU:HD13	1:A:472:VAL:HG13	1.99	0.45
1:A:19[A]:SER:HB2	1:A:58:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PRO:HB2	1:A:212:TRP:CE3	2.52	0.44
1:B:388:HIS:HE1	5:B:737:HOH:O	1.98	0.44
1:B:35:LYS:O	1:B:36:PRO:C	2.56	0.44
2:A:701:EDO:O1	4:A:901:URE:N2	2.51	0.44
1:B:86:ARG:HD2	1:B:234:GLU:HB3	1.99	0.43
1:A:445:HIS:HD2	5:A:749:HOH:O	2.02	0.43
1:A:109:LEU:HA	1:A:110:PRO:HD3	1.89	0.43
1:A:19[A]:SER:HB3	1:A:20:PRO:CD	2.49	0.43
1:A:71:ALA:HB2	1:A:212:TRP:CZ3	2.53	0.43
1:B:340:LEU:HD21	1:B:351:LEU:HD12	2.01	0.43
1:A:86:ARG:HG2	5:A:1100:HOH:O	2.18	0.43
1:A:76:LEU:HD12	4:A:904:URE:N1	2.35	0.42
1:A:449:TRP:CD1	1:A:459:ARG:HB2	2.55	0.42
1:B:257:LYS:N	1:B:257:LYS:HD2	2.29	0.42
1:B:126:GLN:HG2	1:B:158:ALA:HB2	2.00	0.42
1:A:360:GLU:HG3	1:A:361:HIS:CD2	2.55	0.42
1:A:257:LYS:HE2	1:A:257:LYS:HB3	1.68	0.42
1:A:80:PRO:HG2	5:A:562:HOH:O	2.19	0.42
1:A:260:PHE:CD1	1:A:282:SER:HA	2.55	0.42
1:B:93:LEU:C	1:B:93:LEU:CD1	2.87	0.42
1:A:388:HIS:HD2	5:A:1168:HOH:O	2.03	0.41
1:A:22:HIS:HB3	1:A:25:ARG:HG3	2.02	0.41
1:B:305:CYS:HB2	1:B:308:LEU:HD23	2.02	0.41
1:B:378:TRP:CD1	1:B:402:LYS:HB2	2.56	0.41
1:B:361:HIS:HB3	5:B:833:HOH:O	2.19	0.41
1:B:460:TYR:CE1	1:B:462:ASN:HB3	2.56	0.41
1:A:57:LEU:CD2	1:A:206:LEU:HD12	2.46	0.41
1:B:39:PRO:HB3	1:B:69:PRO:HG2	2.02	0.41
1:B:69:PRO:HB2	1:B:212:TRP:CE3	2.56	0.41
1:A:186:LYS:C	1:A:186:LYS:HD3	2.42	0.41
1:A:84:SER:O	1:A:86:ARG:HD3	2.20	0.40
1:A:137:PHE:CZ	1:A:174:VAL:HG11	2.55	0.40
1:B:262:THR:O	1:B:263:LYS:HD2	2.22	0.40
1:A:360:GLU:HG3	1:A:361:HIS:HD2	1.86	0.40
1:A:156:ARG:HG2	1:A:157:GLU:HG2	2.03	0.40
1:B:141:ARG:HG3	1:B:142:PRO:HD3	2.03	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	476/506 (94%)	467 (98%)	9 (2%)	0	100	100
1	B	468/506 (92%)	456 (97%)	10 (2%)	2 (0%)	39	20
All	All	944/1012 (93%)	923 (98%)	19 (2%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	PRO
1	B	35	LYS

### 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	389/415 (94%)	385 (99%)	4 (1%)	82	72
1	B	382/415 (92%)	375 (98%)	7 (2%)	66	49
All	All	771/830 (93%)	760 (99%)	11 (1%)	74	59

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	TRP
1	A	243	GLU
1	A	311	LYS
1	A	358	LYS

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Mol	Chain	Res	Type
1	B	53	ASN
1	B	93	LEU
1	B	100	LEU
1	B	257	LYS
1	B	328	ASP
1	B	340	LEU
1	B	408	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	58	HIS
1	A	289	HIS
1	A	292	HIS
1	A	307	HIS
1	A	361	HIS
1	A	379	ASN
1	A	388	HIS
1	A	392	HIS
1	A	445	HIS
1	A	485	GLN
1	B	30	HIS
1	B	48	GLN
1	B	53	ASN
1	B	126	GLN
1	B	170	ASN
1	B	289	HIS
1	B	292	HIS
1	B	370	ASN
1	B	382	GLN
1	B	388	HIS
1	B	392	HIS
1	B	445	HIS
1	B	485	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

17 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	$\# Z  > 2$
2	EDO	A	701	-	3,3,3	1.05	0	2,2,2	0.69	0
2	EDO	A	703	-	3,3,3	1.02	0	2,2,2	1.25	0
2	EDO	A	705	-	3,3,3	1.03	0	2,2,2	0.97	0
2	EDO	A	706	-	3,3,3	1.08	0	2,2,2	1.01	0
2	EDO	A	707	-	3,3,3	1.06	0	2,2,2	1.04	0
2	EDO	A	708	-	3,3,3	1.02	0	2,2,2	1.11	0
3	FAD	A	801	-	48,58,58	1.29	6 (12%)	54,89,89	2.18	11 (20%)
4	URE	A	901	-	3,3,3	0.85	0	3,3,3	0.56	0
4	URE	A	902	-	3,3,3	0.77	0	3,3,3	0.50	0
4	URE	A	903	-	3,3,3	0.94	0	3,3,3	0.69	0
4	URE	A	904	-	3,3,3	0.89	0	3,3,3	0.42	0
4	URE	A	905	-	3,3,3	1.01	0	3,3,3	0.78	0
3	FAD	B	801	-	48,58,58	1.27	6 (12%)	54,89,89	2.27	6 (11%)
4	URE	B	901	-	3,3,3	0.92	0	3,3,3	0.67	0
4	URE	B	902	-	3,3,3	0.72	0	3,3,3	0.55	0
4	URE	B	904	-	3,3,3	0.98	0	3,3,3	0.88	0
4	URE	B	905	-	3,3,3	0.98	0	3,3,3	0.62	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
2	EDO	A	701	-	-	0/1/1/1	0/0/0/0
2	EDO	A	703	-	-	0/1/1/1	0/0/0/0
2	EDO	A	705	-	-	0/1/1/1	0/0/0/0
2	EDO	A	706	-	-	0/1/1/1	0/0/0/0
2	EDO	A	707	-	-	0/1/1/1	0/0/0/0
2	EDO	A	708	-	-	0/1/1/1	0/0/0/0
3	FAD	A	801	-	-	0/30/50/50	0/6/6/6
4	URE	A	901	-	-	0/0/0/0	0/0/0/0
4	URE	A	902	-	-	0/0/0/0	0/0/0/0
4	URE	A	903	-	-	0/0/0/0	0/0/0/0
4	URE	A	904	-	-	0/0/0/0	0/0/0/0
4	URE	A	905	-	-	0/0/0/0	0/0/0/0
3	FAD	B	801	-	-	0/30/50/50	0/6/6/6
4	URE	B	901	-	-	0/0/0/0	0/0/0/0
4	URE	B	902	-	-	0/0/0/0	0/0/0/0
4	URE	B	904	-	-	0/0/0/0	0/0/0/0
4	URE	B	905	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FAD	C5X-N5	2.04	1.38	1.35
3	A	801	FAD	C2A-N1A	2.17	1.38	1.33
3	B	801	FAD	C2A-N1A	2.32	1.38	1.33
3	B	801	FAD	C5X-N5	2.61	1.39	1.35
3	B	801	FAD	C4-N3	2.92	1.38	1.33
3	A	801	FAD	C4X-N5	2.97	1.38	1.33
3	A	801	FAD	C4-N3	3.06	1.38	1.33
3	B	801	FAD	C2A-N3A	3.30	1.38	1.32
3	A	801	FAD	C2A-N3A	3.38	1.38	1.32
3	B	801	FAD	C4X-N5	3.44	1.38	1.33
3	B	801	FAD	C1'-N10	3.50	1.52	1.48
3	A	801	FAD	C1'-N10	4.06	1.52	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	FAD	N3A-C2A-N1A	-12.54	119.29	128.89
3	A	801	FAD	N3A-C2A-N1A	-11.37	120.19	128.89
3	A	801	FAD	C4X-C4-N3	-3.76	118.45	123.59
3	B	801	FAD	C4X-C4-N3	-3.23	119.18	123.59
3	A	801	FAD	C4A-C5A-N7A	-2.69	107.01	109.48
3	B	801	FAD	C2B-C1B-N9A	-2.42	110.59	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	C2B-C1B-N9A	-2.16	110.99	114.29
3	A	801	FAD	O3P-P-O5'	-2.09	97.39	102.94
3	A	801	FAD	C4-C4X-N5	2.13	121.30	118.72
3	A	801	FAD	C4X-C10-N10	2.36	121.91	120.52
3	A	801	FAD	C5X-C9A-N10	2.52	119.53	117.62
3	A	801	FAD	C1'-N10-C9A	2.72	121.92	118.86
3	B	801	FAD	C1'-N10-C9A	2.99	122.22	118.86
3	B	801	FAD	C5X-C9A-N10	3.06	119.94	117.62
3	A	801	FAD	C4X-N5-C5X	3.23	120.48	116.76
3	A	801	FAD	C4-N3-C2	6.12	120.54	115.25
3	B	801	FAD	C4-N3-C2	7.13	121.41	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	EDO	3	0
2	A	705	EDO	1	0
2	A	707	EDO	1	0
2	A	708	EDO	1	0
3	A	801	FAD	1	0
4	A	901	URE	1	0
4	A	902	URE	1	0
4	A	904	URE	3	0
3	B	801	FAD	1	0
4	B	902	URE	2	0

## 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	472/506 (93%)	-0.02	10 (2%) 67 71	10, 22, 46, 99	0
1	B	468/506 (92%)	0.05	12 (2%) 59 64	16, 31, 63, 99	0
All	All	940/1012 (92%)	0.01	22 (2%) 64 68	10, 26, 55, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	8.9
1	B	34	GLY	6.6
1	B	35	LYS	5.2
1	B	33	GLY	3.8
1	B	308	LEU	3.7
1	B	486	SER	3.6
1	B	311	LYS	3.1
1	B	257	LYS	3.0
1	A	33	GLY	2.7
1	B	485	GLN	2.7
1	A	36	PRO	2.6
1	A	267	SER	2.6
1	A	484	GLY	2.4
1	A	489	ARG	2.3
1	A	19[A]	SER	2.3
1	A	487	LYS	2.2
1	A	488	LYS	2.2
1	B	36	PRO	2.2
1	B	105	ALA	2.2
1	A	482	LEU	2.1
1	B	263	LYS	2.1
1	B	209	VAL	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	705	4/4	0.92	0.20	18.96	28,32,33,37	0
2	EDO	A	701	4/4	0.92	0.14	10.39	25,28,29,31	0
4	URE	B	902	4/4	0.80	0.22	8.22	26,31,31,32	0
4	URE	A	902	4/4	0.77	0.20	5.51	30,35,35,36	0
4	URE	A	901	4/4	0.90	0.16	5.24	21,23,24,27	0
4	URE	A	903	4/4	0.82	0.17	4.27	49,53,53,54	0
4	URE	B	905	4/4	0.93	0.18	2.58	44,47,48,48	0
2	EDO	A	703	4/4	0.94	0.14	2.22	38,38,39,41	0
2	EDO	A	706	4/4	0.86	0.15	1.41	44,45,48,50	0
4	URE	A	905	4/4	0.94	0.11	0.80	28,33,33,34	0
4	URE	B	901	4/4	0.93	0.11	0.49	32,36,37,37	0
4	URE	A	904	4/4	0.96	0.08	0.23	18,21,22,24	0
4	URE	B	904	4/4	0.94	0.09	-0.02	26,26,27,27	0
3	FAD	A	801	53/53	0.98	0.09	-0.02	9,14,18,20	0
3	FAD	B	801	53/53	0.96	0.08	-0.16	16,23,28,30	0
2	EDO	A	708	4/4	0.79	0.22	-	51,54,57,58	0
2	EDO	A	707	4/4	0.36	0.28	-	86,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.