



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:46 PM UTC

PDB ID : 2J08 / pdb_00002j08
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 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)
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

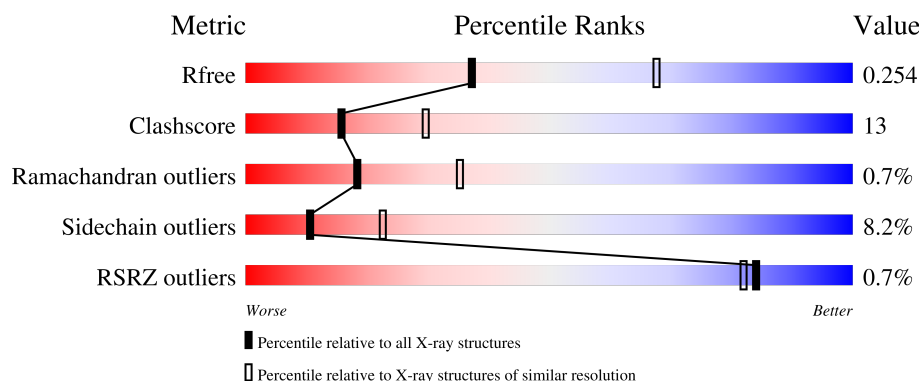
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 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	420	63% 30% 6%

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
5	PO4	A	1424	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3572 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.

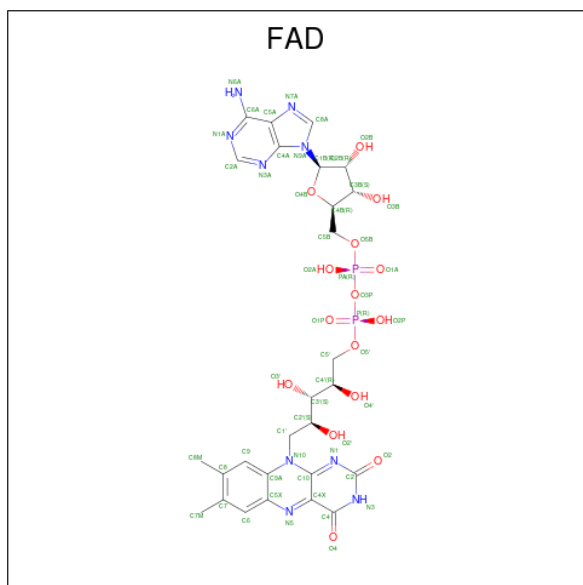
- Molecule 1 is a protein called DEOXYRIBODIPYRIMIDINE PHOTO-LYASE.

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

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

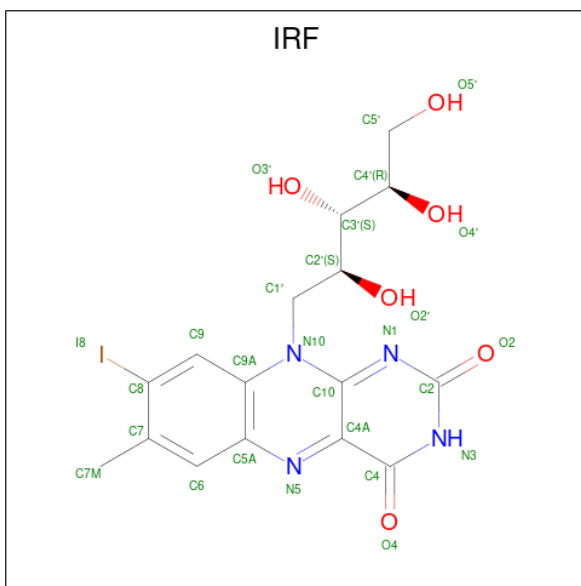
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

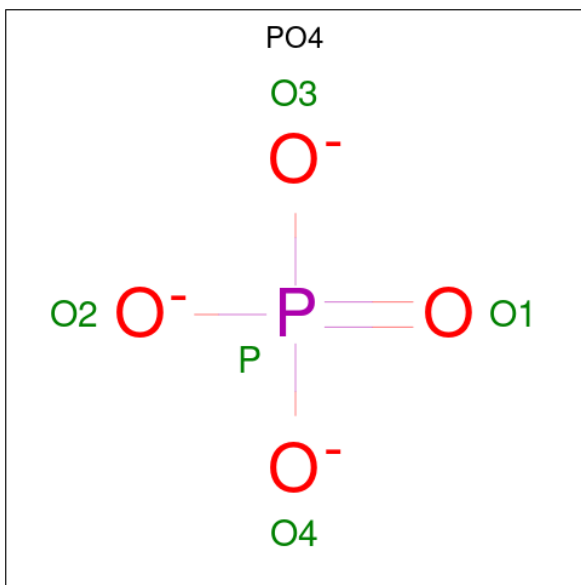
- Molecule 4 is 1-DEOXY-1-(8-IODO-7-METHYL-2,4-DIOXO-3,4-DIHYDROBENZO[G]PT

ERIDIN-10(2H)-YL)-D-RIBITOL (CCD ID: IRF) (formula: $C_{16}H_{17}IN_4O_6$).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

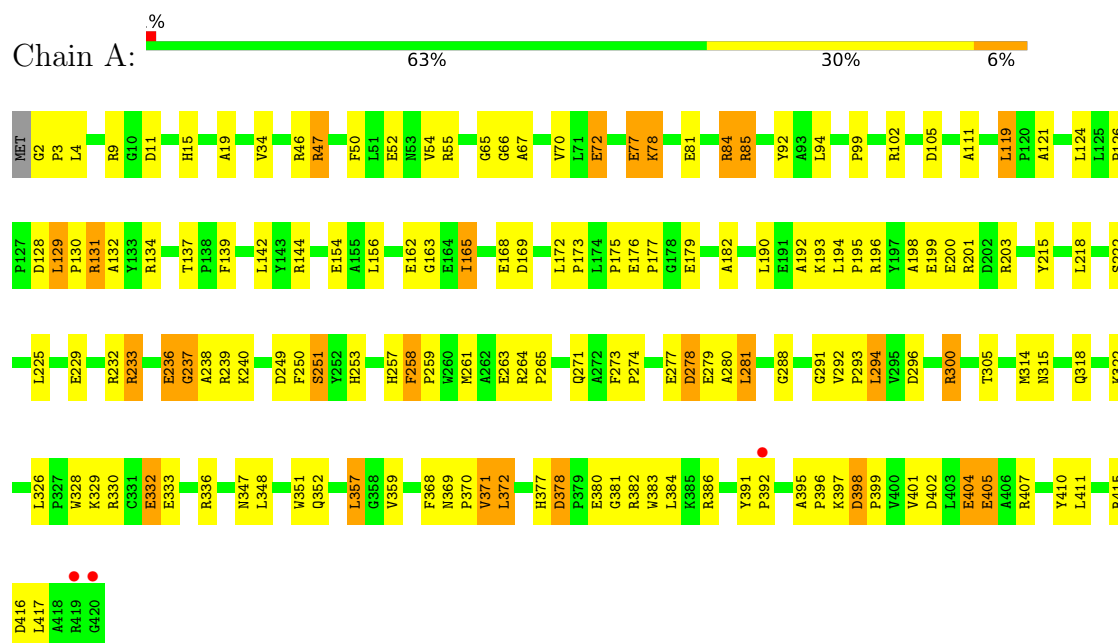
- Molecule 6 is water.

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

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	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) 91.5 (24.32-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.163 , 0.256 0.163 , 0.254	Depositor DCC
R_{free} test set	771 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3572	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IRF, CL, 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	1.39	11/3487 (0.3%)	1.44	39/4759 (0.8%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLY	N-CA	7.09	1.51	1.44
1	A	111	ALA	CA-CB	-6.78	1.42	1.53
1	A	54	VAL	CA-CB	6.53	1.62	1.54
1	A	176	GLU	CA-C	6.27	1.60	1.52
1	A	128	ASP	CA-C	-5.93	1.44	1.52
1	A	126	PRO	CA-C	5.61	1.57	1.52
1	A	378	ASP	CA-C	5.30	1.59	1.52
1	A	154	GLU	CA-C	-5.25	1.45	1.52
1	A	72	GLU	CG-CD	5.16	1.65	1.52
1	A	84	ARG	C-O	-5.10	1.18	1.24
1	A	305	THR	N-CA	5.09	1.52	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ILE	CA-C-N	-11.02	109.63	120.21
1	A	165	ILE	C-N-CA	-11.02	109.63	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LEU	CA-C-N	-7.89	111.62	119.90
1	A	326	LEU	C-N-CA	-7.89	111.62	119.90
1	A	121	ALA	CA-C-N	-7.87	111.63	119.90
1	A	121	ALA	C-N-CA	-7.87	111.63	119.90
1	A	222	SER	CA-C-N	-6.91	112.58	119.56
1	A	222	SER	C-N-CA	-6.91	112.58	119.56
1	A	315	ASN	N-CA-C	6.82	118.40	110.97
1	A	398	ASP	CA-C-N	6.63	126.59	119.76
1	A	398	ASP	C-N-CA	6.63	126.59	119.76
1	A	281	LEU	N-CA-C	6.58	118.24	111.14
1	A	240	LYS	N-CA-C	-6.47	104.42	112.90
1	A	84	ARG	N-CA-C	-6.33	104.30	111.14
1	A	377	HIS	N-CA-C	6.17	120.69	112.30
1	A	258	PHE	CA-C-N	6.14	126.04	119.28
1	A	258	PHE	C-N-CA	6.14	126.04	119.28
1	A	156	LEU	CA-C-N	-6.11	113.98	120.03
1	A	156	LEU	C-N-CA	-6.11	113.98	120.03
1	A	190	LEU	N-CA-C	-6.10	105.09	112.54
1	A	198	ALA	N-CA-C	-5.83	105.26	112.90
1	A	398	ASP	O-C-N	5.82	124.21	121.53
1	A	398	ASP	CB-CA-C	-5.82	107.07	111.20
1	A	65	GLY	N-CA-C	-5.74	107.18	115.27
1	A	66	GLY	N-CA-C	5.54	120.16	112.57
1	A	54	VAL	N-CA-C	-5.35	105.31	110.72
1	A	237	GLY	N-CA-C	-5.35	106.15	113.27
1	A	34	VAL	CB-CA-C	-5.34	102.72	110.63
1	A	142	LEU	N-CA-C	-5.26	106.70	113.01
1	A	193	LYS	N-CA-C	5.24	119.95	113.50
1	A	383	TRP	N-CA-C	-5.24	105.01	111.40
1	A	4	LEU	CA-C-N	-5.23	113.94	121.42
1	A	4	LEU	C-N-CA	-5.23	113.94	121.42
1	A	169	ASP	CA-C-N	-5.22	114.28	119.56
1	A	169	ASP	C-N-CA	-5.22	114.28	119.56
1	A	300	ARG	N-CA-C	5.16	118.73	112.23
1	A	251	SER	N-CA-C	5.15	117.57	111.33
1	A	233	ARG	N-CA-C	-5.10	105.80	111.36
1	A	291	GLY	N-CA-C	-5.07	108.12	115.27

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 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	3372	0	3312	90	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	91	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 13.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:HG2	1:A:232:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:NH2	1:A:165:ILE:O	2.27	0.66
1:A:72:GLU:O	1:A:78:LYS:HD2	1.95	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:369:ASN:CG	1:A:372:LEU:HB2	2.31	0.56
1:A:398:ASP:N	1:A:399:PRO:HD3	2.22	0.55
1:A:232:ARG:NH1	1:A:232:ARG:CG	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:292:VAL:O	1:A:293:PRO:C	2.48	0.53
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:46:ARG:HH12	5:A:1424:PO4:P	2.30	0.52
1:A:402:ASP:OD1	1:A:402:ASP:C	2.52	0.51
1:A:273:PHE:CD2	1:A:274:PRO:HD2	2.45	0.51
1:A:263:GLU:O	1:A:263:GLU:HG2	2.11	0.51
1:A:278:ASP:OD1	1:A:278:ASP:C	2.53	0.51
1:A:329:LYS:O	1:A:330:ARG:C	2.52	0.50
1:A:70:VAL:O	1:A:163:GLY:HA3	2.12	0.50
1:A:369:ASN:OD1	1:A:369:ASN:C	2.54	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:HD12	1:A:294:LEU:O	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:236:GLU:C	1:A:238:ALA:N	2.69	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:332:GLU:CD	1:A:332:GLU:C	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG3	6:A:2083:HOH:O	2.13	0.47
1:A:322:LYS:HG2	1:A:410:TYR:CE1	2.49	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:257:HIS:C	1:A:259:PRO:HD3	2.42	0.45
1:A:318:GLN:CD	1:A:322:LYS:HD2	2.42	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:236:GLU:O	1:A:237:GLY:C	2.60	0.44
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.80	0.44
1:A:318:GLN:OE1	1:A:368:PHE:CD2	2.70	0.44
1:A:332:GLU:HB2	1:A:351:TRP:CD1	2.53	0.44
1:A:404:GLU:O	1:A:405:GLU:C	2.61	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:279:GLU:O	1:A:280:ALA:C	2.60	0.42
1:A:131:ARG:CG	1:A:131:ARG:NH1	2.36	0.42
1:A:9:ARG:N	1:A:9:ARG:HD3	2.35	0.42
1:A:94:LEU:HA	1:A:119:LEU:O	2.19	0.42
1:A:277:GLU:HG3	1:A:278:ASP:N	2.34	0.42
1:A:253:HIS:CE1	1:A:257:HIS:CE1	3.08	0.42
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:19:ALA:HB1	1:A:92:TYR:HB3	2.03	0.41
1:A:258:PHE:N	1:A:259:PRO:HD3	2.35	0.41
1:A:194:LEU:O	1:A:237:GLY:HA3	2.21	0.41
1:A:81:GLU:O	1:A:85:ARG:HG3	2.21	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: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:132:ALA:HB1	1:A:258:PHE:CZ	2.57	0.40
1:A:381:GLY:O	1:A:382:ARG:C	2.64	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	417/420 (99%)	399 (96%)	15 (4%)	3 (1%)	18	35

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 [i](#)

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%)	302 (92%)	27 (8%)	10	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	77	GLU
1	A	78	LYS
1	A	119	LEU
1	A	129	LEU
1	A	131	ARG
1	A	134	ARG
1	A	137	THR

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	201	ARG
1	A	229	GLU
1	A	236	GLU
1	A	251	SER
1	A	281	LEU
1	A	294	LEU
1	A	314	MET
1	A	332	GLU
1	A	333	GLU
1	A	348	LEU
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

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	271	GLN
1	A	276	GLN
1	A	283	GLN
1	A	347	ASN
1	A	349	GLN
1	A	373	GLN
1	A	377	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	IRF	A	1422	-	29,29,29	2.03	4 (13%)	41,43,43	2.13	17 (41%)
5	PO4	A	1423	-	4,4,4	0.80	0	6,6,6	1.78	1 (16%)
5	PO4	A	1424	-	4,4,4	0.74	0	6,6,6	1.02	1 (16%)
3	FAD	A	1421	-	58,58,58	1.32	7 (12%)	85,89,89	2.24	24 (28%)

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
4	IRF	A	1422	-	-	13/14/14/14	0/3/3/3
3	FAD	A	1421	-	-	5/34/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1422	IRF	C7-C8	7.86	1.50	1.39
3	A	1421	FAD	C4X-N5	4.01	1.39	1.30
4	A	1422	IRF	C9A-C5A	3.68	1.47	1.41
3	A	1421	FAD	C8A-N7A	3.24	1.37	1.31
3	A	1421	FAD	O4-C4	2.75	1.28	1.23
4	A	1422	IRF	C1'-C2'	-2.58	1.49	1.52
4	A	1422	IRF	C4-N3	-2.54	1.34	1.38
3	A	1421	FAD	O2-C2	-2.51	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1421	FAD	C2A-N1A	2.39	1.38	1.33
3	A	1421	FAD	C8A-N9A	2.33	1.41	1.37
3	A	1421	FAD	C9A-N10	-2.28	1.37	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1421	FAD	O2-C2-N1	-6.72	110.65	121.80
3	A	1421	FAD	C4X-C10-N10	5.96	125.02	116.48
3	A	1421	FAD	N9A-C8A-N7A	-5.47	106.18	113.94
3	A	1421	FAD	N3A-C2A-N1A	-5.21	120.69	128.58
3	A	1421	FAD	C4-N3-C2	-4.81	117.10	125.64
3	A	1421	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
3	A	1421	FAD	O3'-C3'-C2'	4.28	118.66	108.93
3	A	1421	FAD	C5A-N7A-C8A	4.22	110.08	103.45
3	A	1421	FAD	C10-C4X-N5	-4.03	116.58	124.81
3	A	1421	FAD	C5X-C9A-N10	3.84	121.44	117.97
3	A	1421	FAD	C2B-C1B-N9A	-3.84	103.78	113.30
4	A	1422	IRF	O2'-C2'-C3'	3.83	118.21	109.25
3	A	1421	FAD	C2A-N3A-C4A	3.71	120.88	111.83
4	A	1422	IRF	O5'-C5'-C4'	-3.58	103.64	111.16
4	A	1422	IRF	C4A-C10-N1	-3.55	115.88	124.59
3	A	1421	FAD	C9A-N10-C10	-3.48	115.45	120.75
3	A	1421	FAD	C4-C4X-C10	3.45	122.85	116.93
4	A	1422	IRF	C5A-N5-C4A	3.42	123.61	118.09
4	A	1422	IRF	C1'-N10-C9A	-3.40	114.02	120.63
5	A	1423	PO4	O2-P-O1	-3.38	99.00	110.95
4	A	1422	IRF	C4-N3-C2	-3.25	119.88	125.64
4	A	1422	IRF	C7-C8-I8	-3.19	118.19	120.69
3	A	1421	FAD	N3A-C4A-N9A	3.12	132.48	127.17
4	A	1422	IRF	O4'-C4'-C3'	-3.06	102.09	109.25
4	A	1422	IRF	C5'-C4'-C3'	-3.05	105.96	112.17
3	A	1421	FAD	C9-C9A-N10	-3.04	117.77	121.85
4	A	1422	IRF	C10-C4A-N5	-2.95	118.79	124.81
3	A	1421	FAD	C4'-C3'-C2'	-2.87	108.79	113.57
4	A	1422	IRF	O2-C2-N1	-2.85	117.07	121.80
3	A	1421	FAD	O2-C2-N3	2.84	124.03	118.58
3	A	1421	FAD	C4A-N9A-C8A	2.80	108.67	105.74
3	A	1421	FAD	N3-C2-N1	2.71	125.27	119.50
4	A	1422	IRF	C4A-C10-N10	2.69	120.34	116.48
4	A	1422	IRF	O3'-C3'-C2'	2.65	114.96	108.93
3	A	1421	FAD	C4X-C10-N1	-2.58	118.27	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1422	IRF	C9A-C5A-N5	-2.49	119.81	122.45
3	A	1421	FAD	C4A-C5A-N7A	-2.47	107.76	110.58
4	A	1422	IRF	C10-N1-C2	2.38	122.01	116.85
3	A	1421	FAD	O3B-C3B-C4B	2.37	117.88	111.08
3	A	1421	FAD	C1'-C2'-C3'	2.29	115.86	109.66
4	A	1422	IRF	C4-C4A-N5	2.27	121.35	118.21
5	A	1424	PO4	O4-P-O1	-2.09	103.55	110.95
4	A	1422	IRF	O4-C4-C4A	-2.04	121.14	126.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1421	FAD	C5B-O5B-PA-O1A
4	A	1422	IRF	N10-C1'-C2'-O2'
4	A	1422	IRF	N10-C1'-C2'-C3'
4	A	1422	IRF	C1'-C2'-C3'-O3'
4	A	1422	IRF	C1'-C2'-C3'-C4'
4	A	1422	IRF	C2'-C3'-C4'-O4'
4	A	1422	IRF	O3'-C3'-C4'-O4'
4	A	1422	IRF	O3'-C3'-C4'-C5'
4	A	1422	IRF	O4'-C4'-C5'-O5'
4	A	1422	IRF	C3'-C4'-C5'-O5'
3	A	1421	FAD	O3'-C3'-C4'-O4'
4	A	1422	IRF	C2'-C3'-C4'-C5'
4	A	1422	IRF	O2'-C2'-C3'-O3'
4	A	1422	IRF	O2'-C2'-C3'-C4'
3	A	1421	FAD	O3'-C3'-C4'-C5'
3	A	1421	FAD	C5B-O5B-PA-O2A
3	A	1421	FAD	C5B-O5B-PA-O3P
4	A	1422	IRF	C2'-C1'-N10-C10

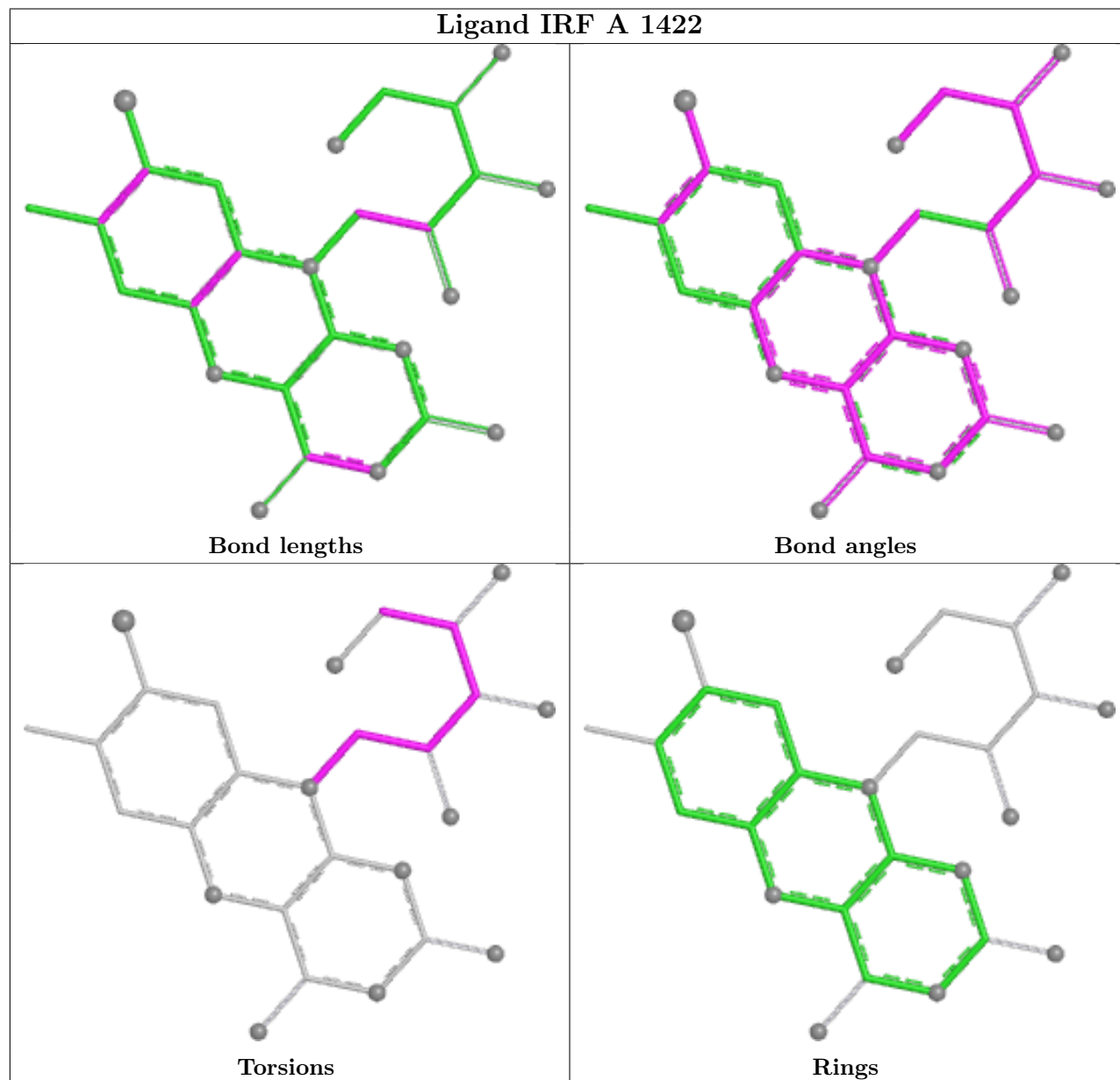
There are no ring outliers.

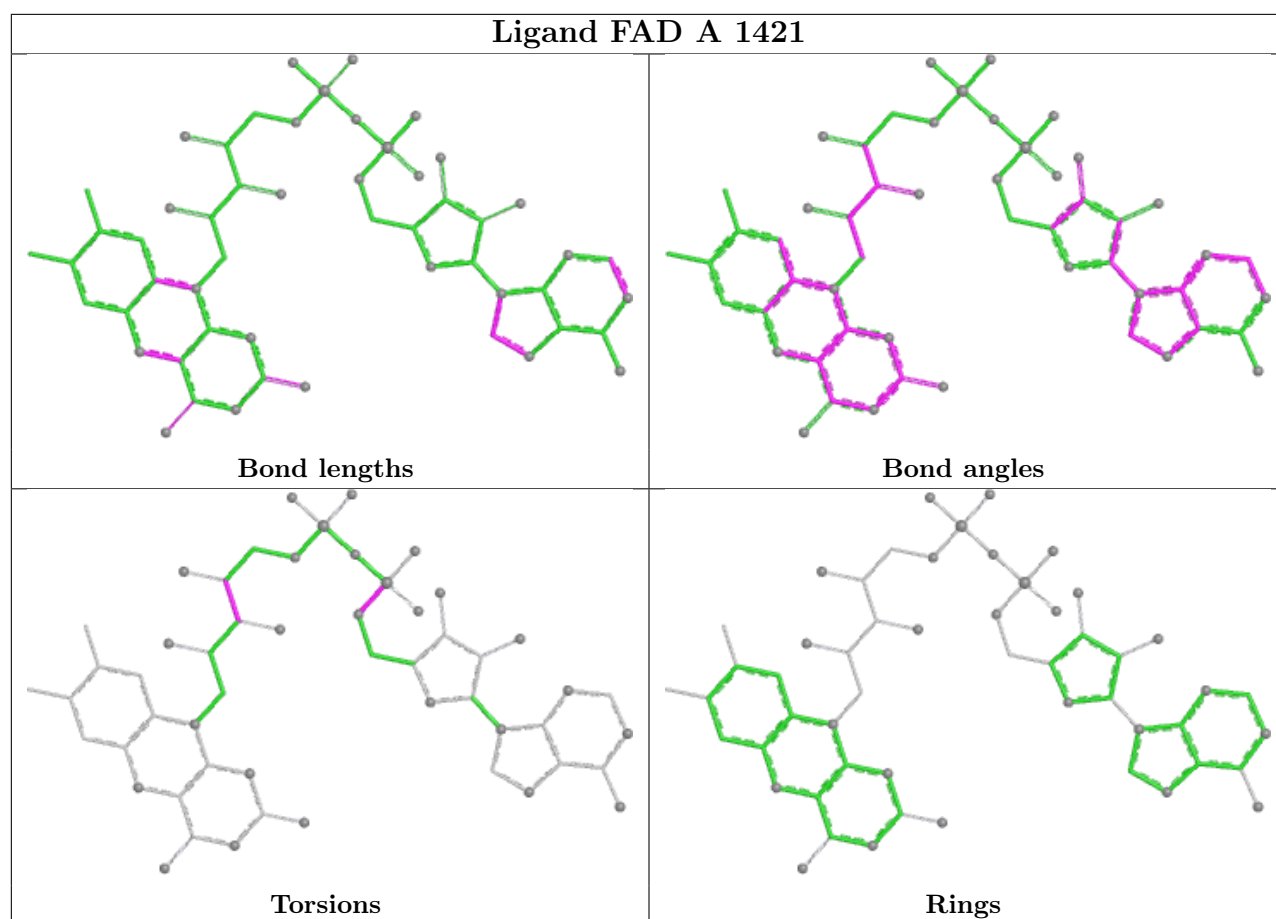
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1422	IRF	1	0
5	A	1424	PO4	3	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 [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, 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	419/420 (99%)	-0.41	3 (0%) 84 82	10, 25, 43, 62	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ARG	2.4
1	A	392	PRO	2.2
1	A	420	GLY	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

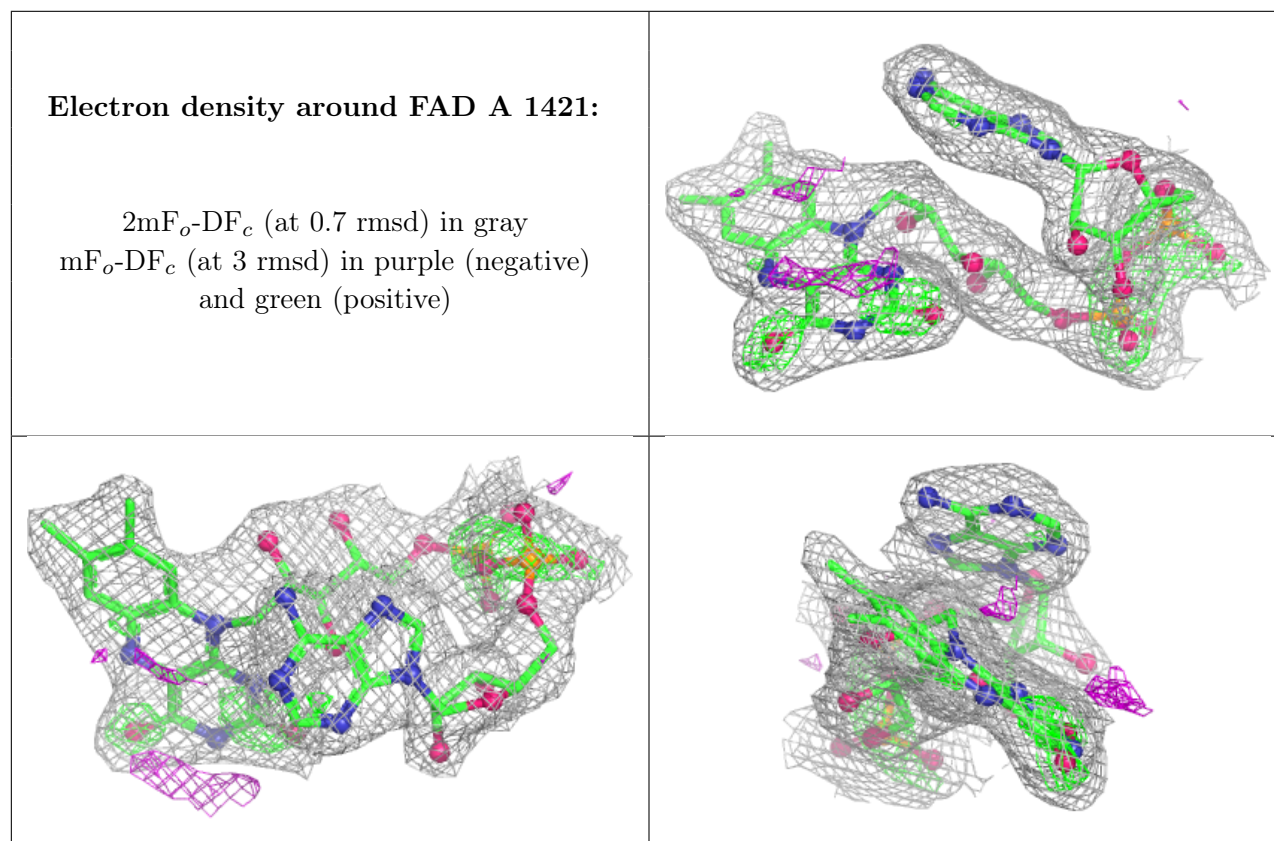
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	901	1/1	0.94	0.07	57,57,57,57	0
2	CL	A	902	1/1	0.94	0.06	50,50,50,50	0
5	PO4	A	1423	5/5	0.94	0.13	32,35,48,50	0
3	FAD	A	1421	53/53	0.95	0.10	12,25,30,32	0

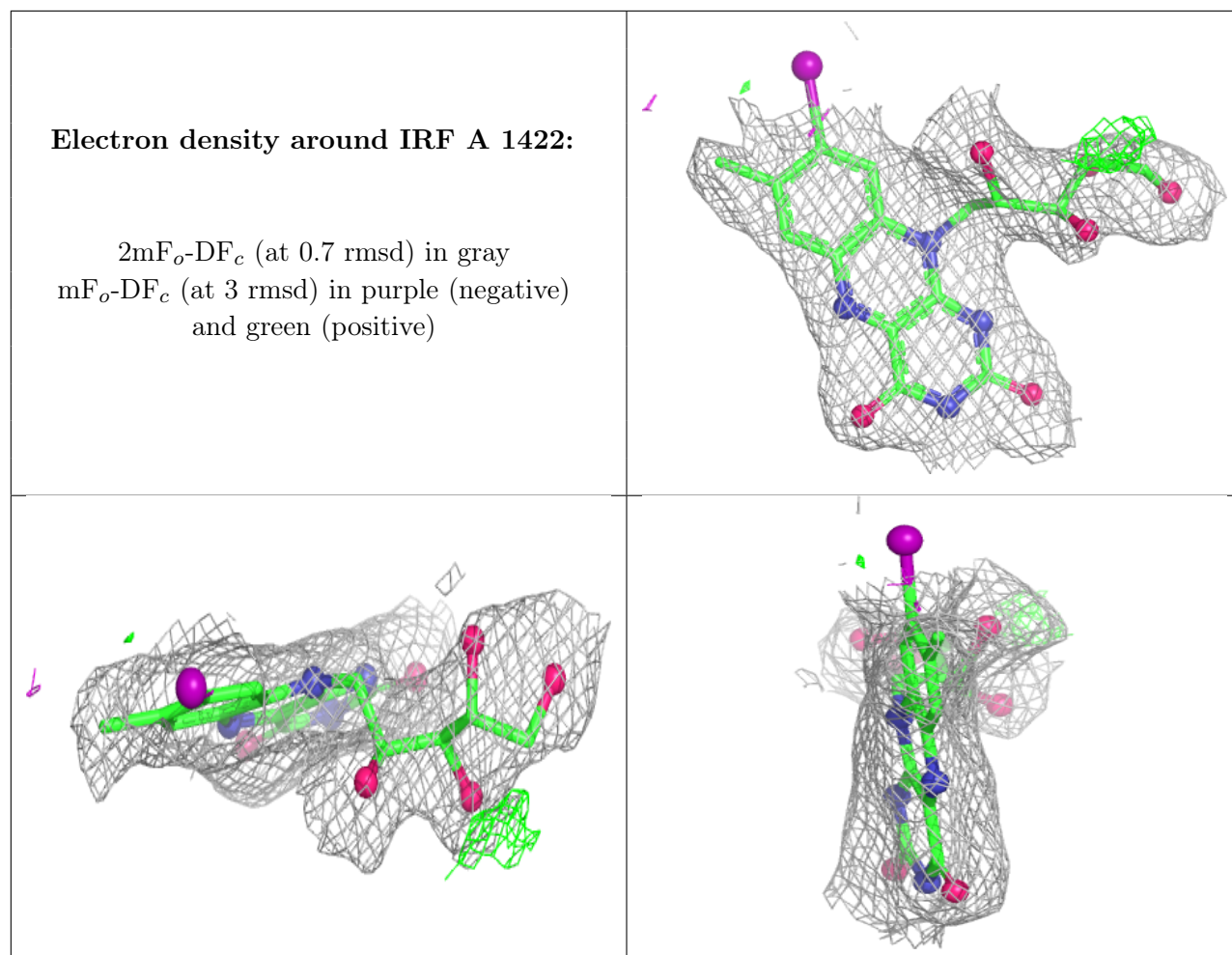
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	A	1424	5/5	0.95	0.11	44,48,52,58	0
4	IRF	A	1422	27/27	0.99	0.06	13,22,35,43	0

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.