



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:32 AM UTC

PDB ID : 3S1D / pdb_00003s1d
Title : Glu381Ser mutant of maize cytokinin oxidase/dehydrogenase complexed with N6-isopentenyladenosine
Authors : Kopecny, D.; Briozzo, P.; Morera, S.
Deposited on : 2011-05-15
Resolution : 1.75 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

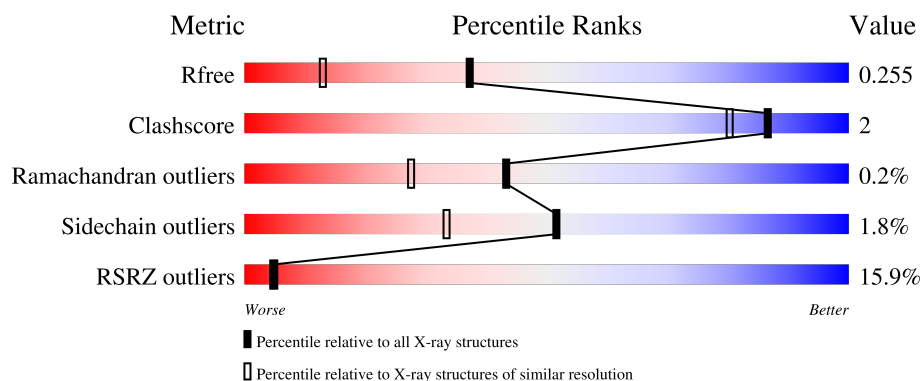
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	516	15% 90% 5% . .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4341 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.

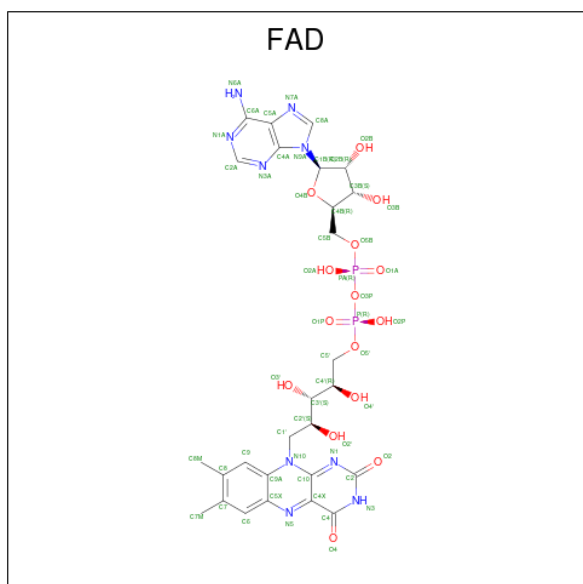
- Molecule 1 is a protein called Cytokinin dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3793	2408	667	707	11			

There are 4 discrepancies between the modelled and reference sequences:

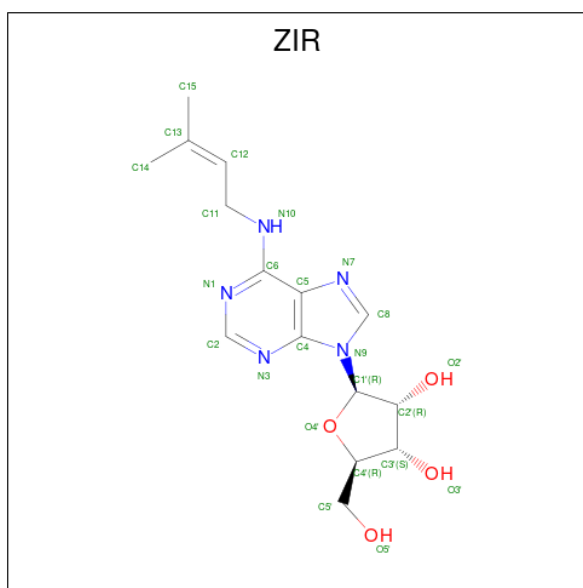
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	GLY	SEE REMARK 999	UNP Q9T0N8
A	168	THR	ASN	SEE REMARK 999	UNP Q9T0N8
A	254	LEU	PHE	SEE REMARK 999	UNP Q9T0N8
A	381	SER	GLU	engineered mutation	UNP Q9T0N8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is N-(3-methylbut-2-en-1-yl)adenosine (CCD ID: ZIR) (formula: $C_{15}H_{21}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	15	5	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

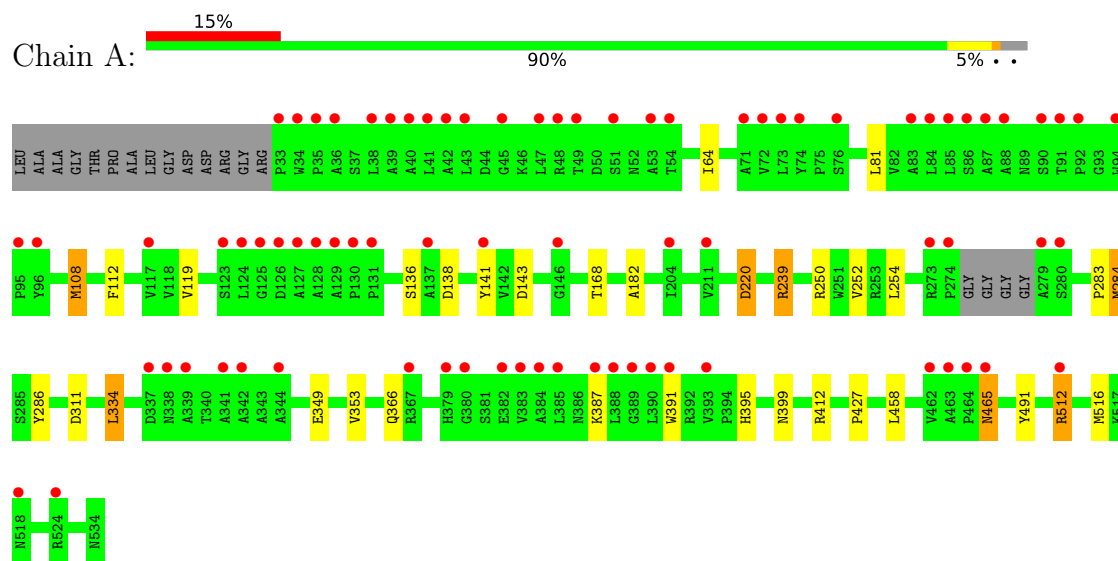
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	392	Total	O	0	0
			392	392		

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: Cytokinin dehydrogenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	251.03Å 50.40Å 51.40Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	25.62 – 1.75 25.62 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.62-1.75) 99.6 (25.62-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.215 , 0.246 0.222 , 0.255	Depositor DCC
R_{free} test set	3288 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4341	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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: GOL, ZIR, NAG, FAD, PEG

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	0.86	3/3883 (0.1%)	1.22	7/5292 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	MET	SD-CE	-9.25	1.56	1.79
1	A	516	MET	SD-CE	-6.04	1.64	1.79
1	A	284	MET	SD-CE	-5.09	1.66	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	311	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	112	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	168	THR	N-CA-C	-5.71	101.29	110.14
1	A	220	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	250	ARG	N-CA-C	-5.29	101.15	109.25
1	A	138	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3793	0	3715	16	0
2	A	53	0	30	0	0
3	A	24	0	21	0	0
4	A	30	0	40	0	0
5	A	7	0	10	1	0
6	A	42	0	39	0	0
7	A	392	0	0	1	0
All	All	4341	0	3855	16	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 2.

All (16) 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:141:TYR:CE1	1:A:239:ARG:HD2	2.37	0.59
1:A:136:SER:HB3	1:A:141:TYR:CE1	2.40	0.57
1:A:141:TYR:CD1	1:A:239:ARG:HD2	2.40	0.56
1:A:427:PRO:HG2	1:A:458:LEU:HD12	1.91	0.53
1:A:252:VAL:HG12	1:A:366:GLN:HG2	1.92	0.51
1:A:284:MET:HE3	1:A:353:VAL:HG21	1.93	0.49
1:A:108:MET:HE2	7:A:753:HOH:O	2.13	0.47
1:A:143:ASP:OD1	1:A:239:ARG:HD3	2.14	0.47
1:A:283:PRO:HG2	1:A:353:VAL:HG21	1.98	0.46
1:A:412:ARG:HG2	5:A:539:PEG:H22	1.98	0.46
1:A:334:LEU:HD11	1:A:349:GLU:HG2	1.98	0.44
1:A:64:ILE:HG21	1:A:108:MET:HE1	2.00	0.43
1:A:81:LEU:HD21	1:A:119:VAL:HG11	2.00	0.42
1:A:391:TRP:O	1:A:395:HIS:HE1	2.02	0.42
1:A:220:ASP:HB2	1:A:512:ARG:HH12	1.85	0.41
1:A:399:ASN:HB2	1:A:491:TYR:O	2.21	0.41

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	494/516 (96%)	485 (98%)	8 (2%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ALA

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	387/395 (98%)	380 (98%)	7 (2%)	51	33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ARG
1	A	254	LEU
1	A	286	TYR
1	A	334	LEU
1	A	387	LYS
1	A	465	ASN
1	A	512	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	134	ASN
1	A	181	ASN
1	A	218	ASN
1	A	295	GLN
1	A	473	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	487	GLN
1	A	495	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	FAD	A	535	1	58,58,58	1.68	17 (29%)	85,89,89	1.27	8 (9%)
3	ZIR	A	536	-	26,26,26	1.48	4 (15%)	36,37,37	2.36	15 (41%)
4	GOL	A	540	-	5,5,5	0.43	0	5,5,5	0.39	0
6	NAG	A	545	1	14,14,15	1.61	3 (21%)	17,19,21	1.11	1 (5%)
4	GOL	A	541	-	5,5,5	0.68	0	5,5,5	0.45	0
4	GOL	A	537	-	5,5,5	0.63	0	5,5,5	0.53	0
5	PEG	A	539	-	6,6,6	0.31	0	5,5,5	0.53	0
4	GOL	A	542	-	5,5,5	0.48	0	5,5,5	0.91	0
6	NAG	A	543	1	14,14,15	1.51	4 (28%)	17,19,21	1.18	1 (5%)
4	GOL	A	538	-	5,5,5	0.47	0	5,5,5	0.63	0
6	NAG	A	544	1	14,14,15	1.54	2 (14%)	17,19,21	1.26	2 (11%)

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	FAD	A	535	1	-	2/34/50/50	0/6/6/6
3	ZIR	A	536	-	-	4/12/28/28	0/3/3/3
4	GOL	A	540	-	-	4/4/4/4	-
6	NAG	A	545	1	-	2/6/23/26	0/1/1/1
4	GOL	A	541	-	-	4/4/4/4	-
4	GOL	A	537	-	-	0/4/4/4	-
5	PEG	A	539	-	-	3/4/4/4	-
4	GOL	A	542	-	-	2/4/4/4	-
6	NAG	A	543	1	-	0/6/23/26	0/1/1/1
4	GOL	A	538	-	-	0/4/4/4	-
6	NAG	A	544	1	-	0/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	535	FAD	C2A-N3A	3.94	1.40	1.33
2	A	535	FAD	O4-C4	-3.56	1.16	1.23
3	A	536	ZIR	C5-N7	-3.42	1.32	1.39
2	A	535	FAD	C10-N10	3.37	1.44	1.37
6	A	545	NAG	C1-C2	3.15	1.56	1.52
2	A	535	FAD	C6-C7	3.13	1.43	1.39
6	A	544	NAG	C1-C2	2.94	1.56	1.52
3	A	536	ZIR	C2-N3	-2.93	1.28	1.33
2	A	535	FAD	C5X-N5	2.90	1.44	1.39
3	A	536	ZIR	C4-N9	-2.79	1.31	1.37
6	A	543	NAG	C4-C5	2.76	1.58	1.53
6	A	545	NAG	C3-C2	2.70	1.58	1.52
2	A	535	FAD	C2-N3	-2.70	1.33	1.39
6	A	544	NAG	O5-C5	2.66	1.48	1.43
2	A	535	FAD	C6-C5X	2.62	1.44	1.40
2	A	535	FAD	C4X-N5	2.56	1.36	1.30
2	A	535	FAD	PA-O3P	2.53	1.62	1.59
2	A	535	FAD	C4X-C4	2.48	1.53	1.44
2	A	535	FAD	C9-C9A	2.44	1.43	1.39
2	A	535	FAD	C2B-C3B	2.37	1.59	1.53
6	A	543	NAG	C4-C3	2.36	1.58	1.52
2	A	535	FAD	C4X-C10	2.32	1.51	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	543	NAG	C3-C2	2.31	1.57	1.52
2	A	535	FAD	C2'-C3'	2.28	1.57	1.53
2	A	535	FAD	C1'-N10	-2.27	1.42	1.47
2	A	535	FAD	C9A-N10	2.22	1.45	1.41
3	A	536	ZIR	O2'-C2'	-2.20	1.37	1.43
2	A	535	FAD	C2-N1	2.09	1.41	1.36
6	A	545	NAG	C4-C3	2.08	1.57	1.52
6	A	543	NAG	O5-C5	2.03	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	536	ZIR	C5-C4-N3	-5.57	119.05	126.72
2	A	535	FAD	O2P-P-O3P	5.19	121.30	107.27
3	A	536	ZIR	N3-C2-N1	-5.05	120.94	128.58
3	A	536	ZIR	N3-C4-N9	4.57	134.93	127.17
3	A	536	ZIR	O4'-C1'-N9	-4.12	100.18	108.09
3	A	536	ZIR	C2-N3-C4	4.03	121.68	111.83
6	A	545	NAG	C4-C3-C2	3.71	116.45	111.02
3	A	536	ZIR	C11-C12-C13	-3.44	120.83	127.01
3	A	536	ZIR	O4'-C1'-C2'	-2.88	100.45	106.62
2	A	535	FAD	C5'-C4'-C3'	2.85	117.60	112.22
3	A	536	ZIR	N10-C6-N1	2.82	123.00	118.47
6	A	544	NAG	C2-N2-C7	2.74	126.57	122.90
3	A	536	ZIR	C2'-C3'-C4'	-2.71	97.38	102.61
2	A	535	FAD	C10-N1-C2	2.58	122.43	116.85
2	A	535	FAD	C8M-C8-C9	-2.57	115.05	119.57
6	A	543	NAG	C4-C3-C2	2.48	114.65	111.02
3	A	536	ZIR	C14-C13-C12	-2.42	115.41	122.66
3	A	536	ZIR	C5'-C4'-C3'	-2.41	109.40	115.10
3	A	536	ZIR	C15-C13-C14	2.40	120.11	114.59
2	A	535	FAD	O3B-C3B-C4B	-2.38	104.24	111.08
3	A	536	ZIR	C4-C5-C6	2.32	118.71	116.78
2	A	535	FAD	C4-C4X-N5	2.23	121.28	118.21
2	A	535	FAD	O2-C2-N1	-2.19	118.17	121.80
2	A	535	FAD	C5X-C9A-N10	2.12	119.88	117.97
3	A	536	ZIR	C5-N7-C8	2.11	106.77	103.45
6	A	544	NAG	C1-O5-C5	2.01	114.88	112.19
3	A	536	ZIR	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (21) torsion outliers are listed below:

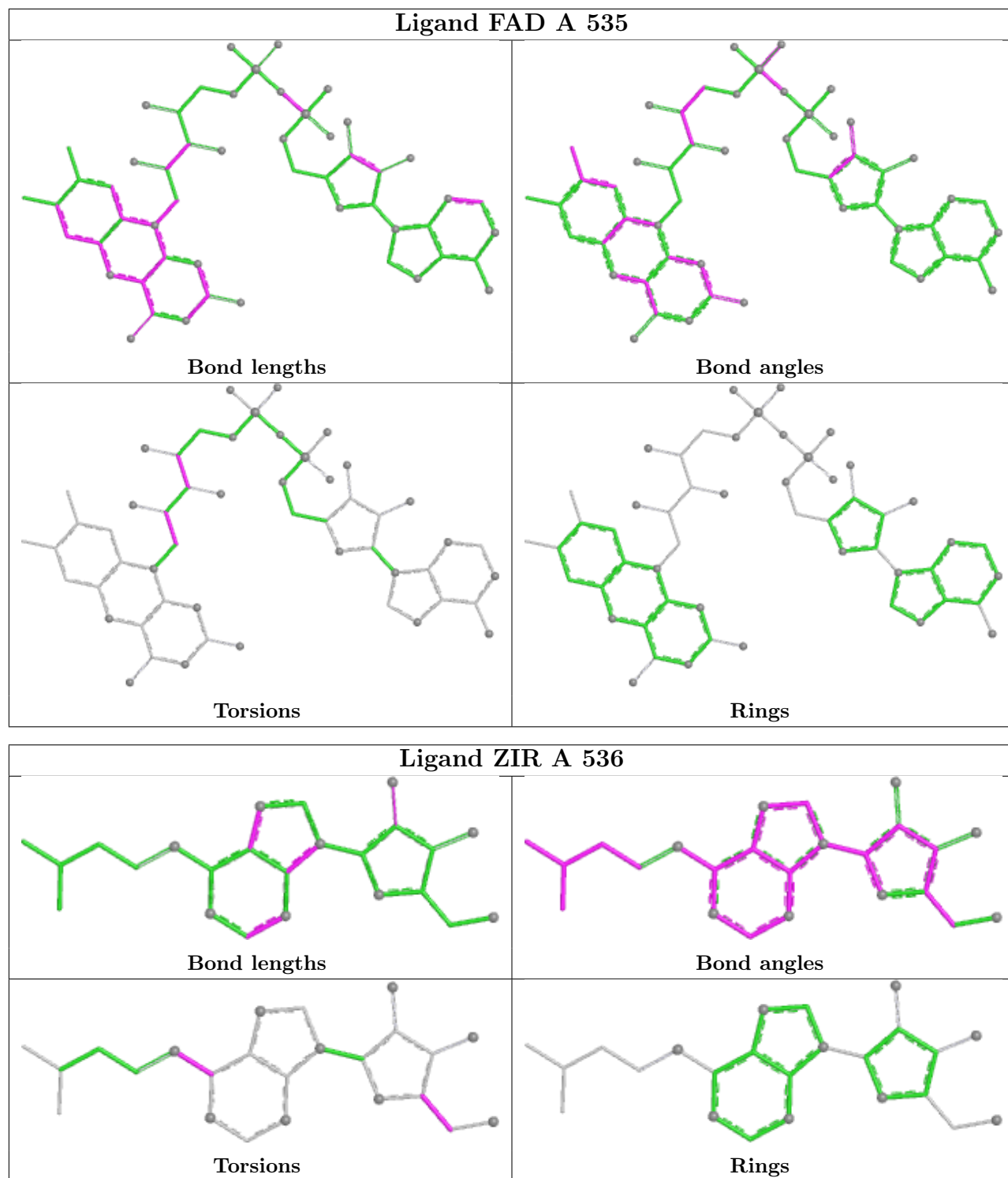
Mol	Chain	Res	Type	Atoms
3	A	536	ZIR	C5-C6-N10-C11
4	A	541	GOL	O1-C1-C2-C3
4	A	542	GOL	O1-C1-C2-C3
3	A	536	ZIR	O4'-C4'-C5'-O5'
3	A	536	ZIR	C3'-C4'-C5'-O5'
4	A	541	GOL	O1-C1-C2-O2
4	A	541	GOL	C1-C2-C3-O3
5	A	539	PEG	O2-C3-C4-O4
6	A	545	NAG	C4-C5-C6-O6
3	A	536	ZIR	N1-C6-N10-C11
4	A	542	GOL	O1-C1-C2-O2
5	A	539	PEG	O1-C1-C2-O2
4	A	540	GOL	O1-C1-C2-O2
6	A	545	NAG	O5-C5-C6-O6
5	A	539	PEG	C4-C3-O2-C2
4	A	541	GOL	O2-C2-C3-O3
2	A	535	FAD	C2'-C3'-C4'-C5'
4	A	540	GOL	O1-C1-C2-C3
4	A	540	GOL	O2-C2-C3-O3
2	A	535	FAD	N10-C1'-C2'-O2'
4	A	540	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	539	PEG	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/516 (96%)	0.82	79 (15%) 5 5	13, 28, 53, 68	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ALA	6.0
1	A	36	ALA	5.9
1	A	129	ALA	5.6
1	A	274	PRO	5.2
1	A	127	ALA	4.7
1	A	390	LEU	4.5
1	A	95	PRO	4.2
1	A	85	LEU	3.9
1	A	41	LEU	3.9
1	A	128	ALA	3.7
1	A	124	LEU	3.7
1	A	462	VAL	3.7
1	A	463	ALA	3.7
1	A	342	ALA	3.6
1	A	211	VAL	3.6
1	A	96	TYR	3.6
1	A	40	ALA	3.6
1	A	39	ALA	3.5
1	A	88	ALA	3.5
1	A	38	LEU	3.5
1	A	130	PRO	3.5
1	A	273	ARG	3.4
1	A	385	LEU	3.3
1	A	84	LEU	3.3
1	A	42	ALA	3.3
1	A	86	SER	3.3
1	A	49	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	90	SER	3.1
1	A	87	ALA	3.1
1	A	389	GLY	3.1
1	A	339	ALA	3.1
1	A	391	TRP	3.0
1	A	43	LEU	3.0
1	A	383	VAL	3.0
1	A	465	ASN	2.9
1	A	33	PRO	2.9
1	A	280	SER	2.9
1	A	388	LEU	2.9
1	A	35	PRO	2.8
1	A	384	ALA	2.8
1	A	45	GLY	2.7
1	A	512	ARG	2.7
1	A	393	VAL	2.6
1	A	72	VAL	2.6
1	A	74	TYR	2.6
1	A	34	TRP	2.5
1	A	126	ASP	2.4
1	A	387	LYS	2.4
1	A	125	GLY	2.4
1	A	337	ASP	2.4
1	A	131	PRO	2.4
1	A	367	ARG	2.4
1	A	76	SER	2.3
1	A	382	GLU	2.3
1	A	47	LEU	2.3
1	A	54	THR	2.3
1	A	380	GLY	2.3
1	A	123	SER	2.3
1	A	92	PRO	2.2
1	A	91	THR	2.2
1	A	518	ASN	2.2
1	A	53	ALA	2.2
1	A	73	LEU	2.2
1	A	379	HIS	2.2
1	A	464	PRO	2.2
1	A	341	ALA	2.2
1	A	117	VAL	2.1
1	A	137	ALA	2.1
1	A	524	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	338	ASN	2.1
1	A	71	ALA	2.1
1	A	83	ALA	2.1
1	A	146	GLY	2.1
1	A	51	SER	2.1
1	A	94	TRP	2.1
1	A	204	ILE	2.1
1	A	344	ALA	2.0
1	A	48	ARG	2.0
1	A	141	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

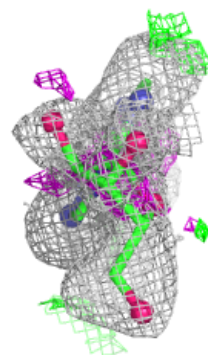
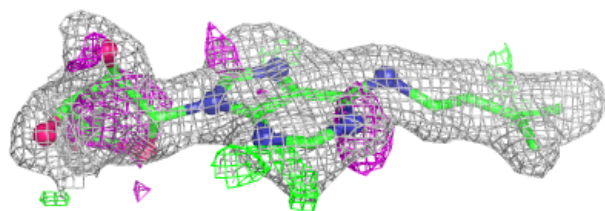
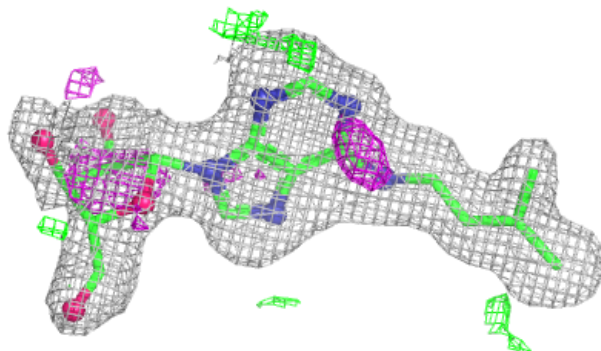
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	539	7/7	0.72	0.28	72,72,74,76	0
4	GOL	A	541	6/6	0.78	0.19	58,59,59,59	0
4	GOL	A	542	6/6	0.78	0.15	53,54,54,54	0
3	ZIR	A	536	24/24	0.78	0.14	29,38,53,54	0
4	GOL	A	538	6/6	0.79	0.15	53,55,55,55	0
4	GOL	A	540	6/6	0.80	0.16	64,65,65,66	0
6	NAG	A	545	14/15	0.80	0.12	40,44,46,46	0
6	NAG	A	544	14/15	0.83	0.12	40,44,47,47	0
4	GOL	A	537	6/6	0.84	0.12	35,37,38,40	0
6	NAG	A	543	14/15	0.84	0.13	40,44,46,47	0
2	FAD	A	535	53/53	0.95	0.07	19,21,22,23	0

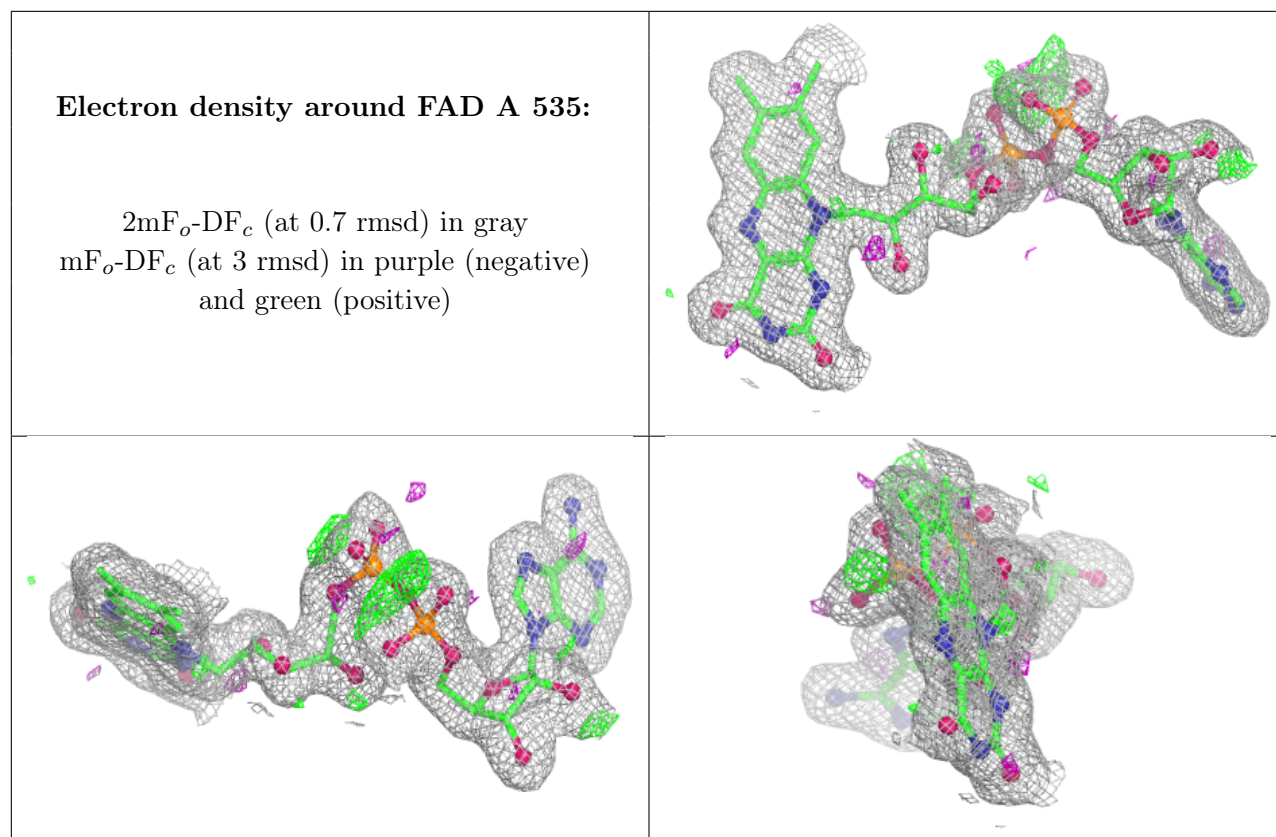
The following is a graphical depiction of the model fit to experimental electron density of all

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

Electron density around ZIR A 536:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.