



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:09 PM GMT

PDB ID : 3S1C  
Title : Maize cytokinin oxidase/dehydrogenase complexed with N6-isopentenyladenosine  
Authors : Kopečný, D.; Briozzo, P.; Morera, S.  
Deposited on : 2011-05-15  
Resolution : 2.09 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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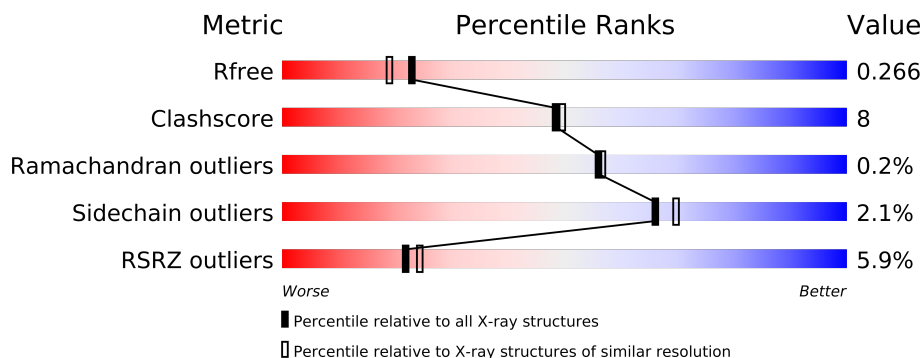
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.09 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	516	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	538	-	X
4	GOL	A	539	-	X
4	GOL	A	540	-	X
4	GOL	A	541	-	X
4	GOL	A	542	-	X
4	GOL	A	543	-	X
4	GOL	A	544	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	545	-	X
4	GOL	A	549	-	X
5	15P	A	551	-	X
5	15P	A	552	-	X
5	15P	A	553	-	X
5	15P	A	554	-	X
6	PEG	A	555	-	X
6	PEG	A	556	-	X
7	NAG	A	604	-	X

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 4414 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.

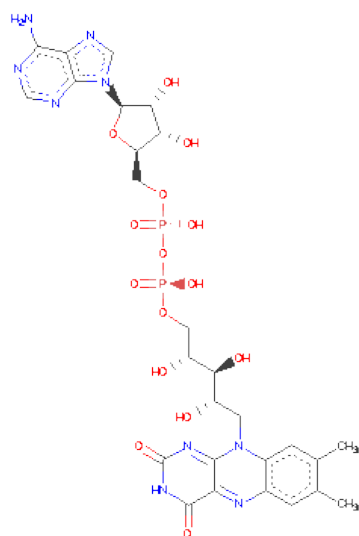
- Molecule 1 is a protein called Cytokinin dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3801	2414	667	708	12	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

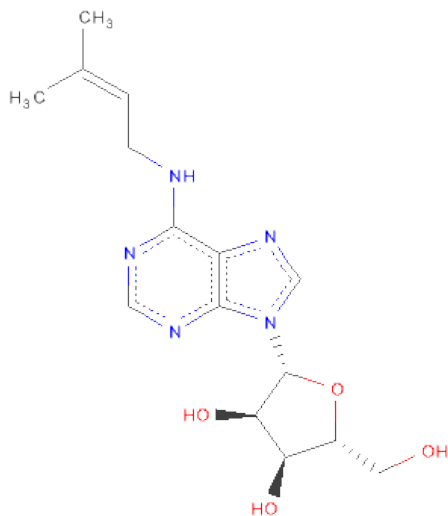
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	GLY	SEE REMARK 999	UNP Q9T0N8
A	168	THR	ASN	SEE REMARK 999	UNP Q9T0N8
A	254	LEU	PHE	SEE REMARK 999	UNP Q9T0N8

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



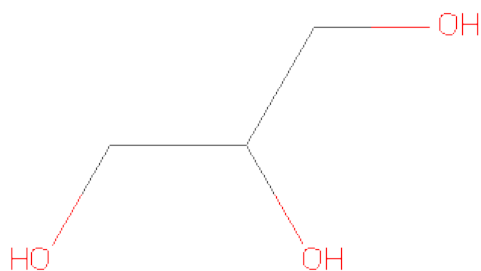
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is N-(3-METHYLBUT-2-EN-1-YL)ADENOSINE (three-letter code: ZIR) (formula:  $C_{15}H_{21}N_5O_4$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



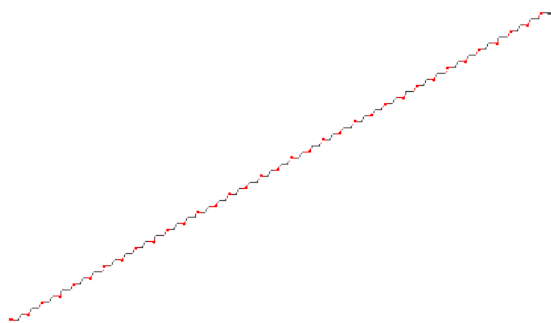
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

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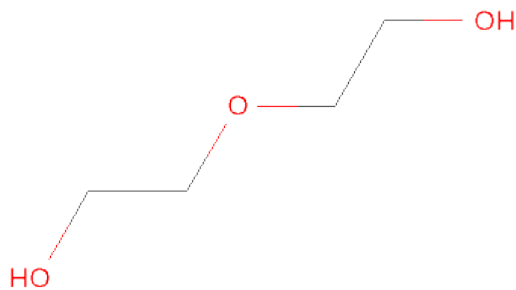
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total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

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C<sub>69</sub>H<sub>140</sub>O<sub>35</sub>).



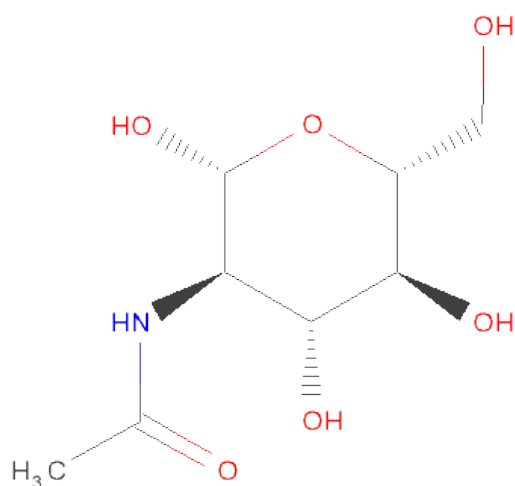
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	7	4		
5	A	1	Total	C	O	0	0
			11	7	4		
5	A	1	Total	C	O	0	0
			11	7	4		
5	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 3 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

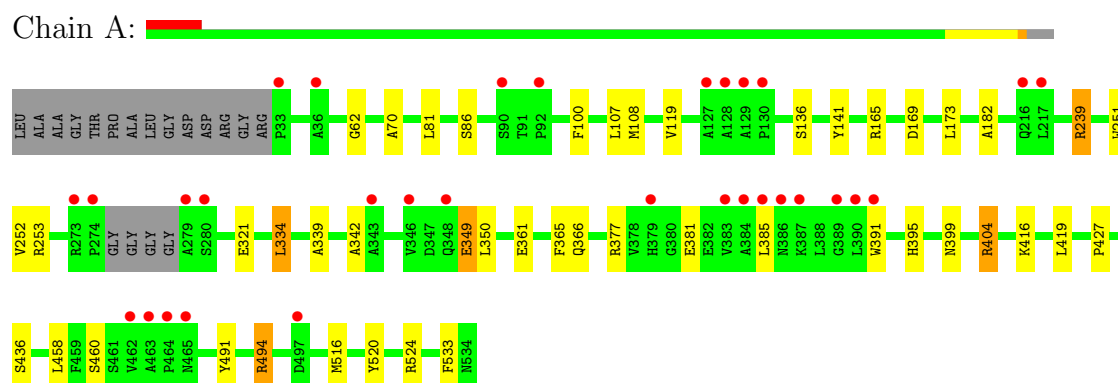
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	324	Total O 324 324	0	0

### 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	250.95Å 50.62Å 51.40Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	32.50 – 2.09 31.32 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.50-2.09) 91.2 (31.32-2.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.213 , 0.252 0.220 , 0.266	Depositor DCC
$R_{free}$ test set	1765 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 35132 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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: GOL, ZIR, NAG, 15P, PEG, 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	0.49	0/3894	0.66	0/5306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3801	0	3724	43	0
2	A	53	0	29	3	0
3	A	24	0	21	17	0
4	A	84	0	112	12	0
5	A	44	0	48	27	0
6	A	28	0	40	2	0
7	A	28	0	26	0	0
8	A	28	0	25	0	0
9	A	324	0	0	2	0
All	All	4414	0	4025	63	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 8.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:ARG:HE	5:A:552:15P:H17	1.33	0.90
3:A:536:ZIR:H8	5:A:552:15P:H28	1.56	0.87
3:A:536:ZIR:H5'A	5:A:552:15P:H15	1.56	0.87
3:A:536:ZIR:H1'	4:A:548:GOL:C1	2.14	0.77
5:A:551:15P:C2	5:A:551:15P:H17	2.16	0.76
1:A:366:GLN:H	5:A:554:15P:H26	1.59	0.67
3:A:536:ZIR:H5'A	5:A:552:15P:C5	2.23	0.66
3:A:536:ZIR:H1'	4:A:548:GOL:O1	1.97	0.65
1:A:81:LEU:HD21	1:A:119:VAL:HG11	1.77	0.64
1:A:108[B]:MET:HG3	1:A:494:ARG:HG3	1.80	0.63
1:A:377:ARG:HE	5:A:552:15P:C7	2.10	0.62
1:A:252:VAL:HG12	1:A:366:GLN:HG2	1.80	0.62
1:A:361:GLU:HB3	5:A:551:15P:H27	1.83	0.61
3:A:536:ZIR:H14B	9:A:817:HOH:O	2.05	0.56
1:A:385:LEU:HD11	4:A:548:GOL:H2	1.88	0.56
3:A:536:ZIR:H8	5:A:552:15P:C8	2.33	0.55
1:A:251:TRP:CZ2	5:A:552:15P:H23	2.43	0.54
5:A:552:15P:C2	5:A:552:15P:H26	2.38	0.53
1:A:516:MET:CE	1:A:520:TYR:HE2	2.22	0.53
1:A:136:SER:HB3	1:A:141:TYR:CE1	2.45	0.52
3:A:536:ZIR:H1'	4:A:548:GOL:H11	1.91	0.51
5:A:552:15P:H18	9:A:740:HOH:O	2.09	0.51
1:A:404:ARG:HH11	6:A:555:PEG:H22	1.76	0.51
3:A:536:ZIR:H5'A	5:A:552:15P:C6	2.41	0.50
1:A:377:ARG:NE	5:A:552:15P:H17	2.14	0.50
1:A:381:GLU:HG2	4:A:548:GOL:C1	2.42	0.50
1:A:427:PRO:HD3	4:A:548:GOL:H32	1.94	0.49
1:A:169:ASP:HB2	3:A:536:ZIR:HN10	1.77	0.49
1:A:252:VAL:HG11	1:A:350:LEU:HD21	1.93	0.49
1:A:365:PHE:HB3	5:A:554:15P:H17	1.93	0.49
1:A:141:TYR:CE1	1:A:239:ARG:HD2	2.47	0.49
1:A:334:LEU:HD11	1:A:349:GLU:HG2	1.94	0.49
1:A:427:PRO:HD2	1:A:458:LEU:HB2	1.96	0.48
3:A:536:ZIR:H5'A	5:A:552:15P:O3	2.14	0.47
1:A:524:ARG:HG2	1:A:533:PHE:HB3	1.97	0.47
1:A:416:LYS:HB3	5:A:553:15P:H26	1.97	0.46
1:A:253:ARG:HE	5:A:552:15P:C2	2.29	0.45
1:A:436:SER:O	4:A:541:GOL:H11	2.16	0.45
3:A:536:ZIR:C5'	5:A:552:15P:O3	2.65	0.45
1:A:516:MET:HE3	1:A:520:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:GLN:HG3	5:A:554:15P:H23	1.99	0.45
1:A:366:GLN:N	5:A:554:15P:H26	2.29	0.45
3:A:536:ZIR:C8	5:A:552:15P:H28	2.39	0.44
3:A:536:ZIR:H2'	5:A:552:15P:C5	2.47	0.44
1:A:516:MET:HE3	1:A:520:TYR:CE2	2.53	0.43
1:A:377:ARG:HD2	5:A:552:15P:H16	2.01	0.43
2:A:535:FAD:N5	3:A:536:ZIR:H11A	2.34	0.43
1:A:391:TRP:O	1:A:395:HIS:HE1	2.00	0.43
1:A:427:PRO:HG2	1:A:458:LEU:HD12	2.01	0.43
1:A:70:ALA:HB1	6:A:557:PEG:H11	2.01	0.42
1:A:100:PHE:O	2:A:535:FAD:H2B	2.19	0.42
1:A:381:GLU:HG2	4:A:548:GOL:H12	2.01	0.42
1:A:165:ARG:HH22	4:A:549:GOL:H12	1.84	0.42
1:A:399:ASN:HB2	1:A:491:TYR:O	2.20	0.42
1:A:385:LEU:CD1	4:A:548:GOL:H2	2.49	0.42
1:A:321:GLU:HG3	4:A:543:GOL:H2	2.02	0.42
3:A:536:ZIR:H3'	5:A:552:15P:H15	2.01	0.41
3:A:536:ZIR:N3	4:A:548:GOL:C1	2.83	0.41
5:A:552:15P:O1	5:A:552:15P:H26	2.20	0.41
1:A:173:LEU:HD13	2:A:535:FAD:H2'	2.01	0.41
1:A:361:GLU:HB3	5:A:551:15P:H15	2.03	0.41
1:A:339:ALA:HB3	1:A:342:ALA:HB2	2.03	0.40
1:A:62:GLY:HA3	1:A:107:LEU:O	2.21	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	495/516 (96%)	481 (97%)	13 (3%)	1 (0%)	56 57

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	388/395 (98%)	380 (98%)	8 (2%)	66 70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	239	ARG
1	A	334	LEU
1	A	349	GLU
1	A	404	ARG
1	A	419	LEU
1	A	460	SER
1	A	494	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	HIS
1	A	495	HIS

### 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 ⓘ

2 carbohydrates 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$
8	NAG	A	602	1,8	12,14,15	1.74	3 (25%)	15,19,21	1.88	3 (20%)
8	NAG	A	603	8	12,14,15	1.33	1 (8%)	15,19,21	1.17	1 (6%)

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
8	NAG	A	602	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	603	8	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	602	NAG	C2-N2	3.28	1.50	1.46
8	A	602	NAG	C3-C2	2.68	1.58	1.52
8	A	603	NAG	C3-C2	2.12	1.57	1.52
8	A	602	NAG	C4-C5	2.10	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	602	NAG	C3-C4-C5	4.08	117.49	110.20
8	A	603	NAG	O5-C5-C4	2.79	114.20	110.65
8	A	602	NAG	C2-N2-C7	2.77	127.74	123.09
8	A	602	NAG	C3-C2-N2	2.65	115.79	111.76

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

## 5.6 Ligand geometry

26 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	1.94	10 (17%)	85,89,89	1.68	13 (15%)
3	ZIR	A	536	-	26,26,26	2.21	12 (46%)	37,37,37	2.84	13 (35%)
4	GOL	A	537	-	5,5,5	0.69	0	5,5,5	1.12	0
4	GOL	A	538	-	5,5,5	0.55	0	5,5,5	0.50	0
4	GOL	A	539	-	5,5,5	0.40	0	5,5,5	0.37	0
4	GOL	A	540	-	5,5,5	0.34	0	5,5,5	0.33	0
4	GOL	A	541	-	5,5,5	0.30	0	5,5,5	0.65	0
4	GOL	A	542	-	5,5,5	0.56	0	5,5,5	0.62	0
4	GOL	A	543	-	5,5,5	0.53	0	5,5,5	0.63	0
4	GOL	A	544	-	5,5,5	0.56	0	5,5,5	0.45	0
4	GOL	A	545	-	5,5,5	0.19	0	5,5,5	0.24	0
4	GOL	A	546	-	5,5,5	0.39	0	5,5,5	0.55	0
4	GOL	A	547	-	5,5,5	0.34	0	5,5,5	0.32	0
4	GOL	A	548	-	5,5,5	0.28	0	5,5,5	0.77	0
4	GOL	A	549	-	5,5,5	0.23	0	5,5,5	0.64	0
4	GOL	A	550	-	5,5,5	1.17	0	5,5,5	1.34	1 (20%)
5	15P	A	551	-	9,10,103	0.91	0	8,9,102	0.97	0
5	15P	A	552	-	9,10,103	0.72	0	8,9,102	1.00	0
5	15P	A	553	-	9,10,103	1.23	0	8,9,102	0.74	0
5	15P	A	554	-	9,10,103	0.83	0	8,9,102	0.70	0
6	PEG	A	555	-	6,6,6	0.56	0	5,5,5	0.43	0
6	PEG	A	556	-	6,6,6	0.14	0	5,5,5	0.20	0
6	PEG	A	557	-	6,6,6	0.16	0	5,5,5	0.17	0
6	PEG	A	558	-	6,6,6	0.34	0	5,5,5	0.48	0
7	NAG	A	601	1	12,14,15	1.66	3 (25%)	15,19,21	1.46	4 (26%)
7	NAG	A	604	1	12,14,15	1.64	2 (16%)	15,19,21	1.62	4 (26%)

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	-	0/34/50/50	0/1/6/6
3	ZIR	A	536	-	-	0/12/28/28	0/1/3/3
4	GOL	A	537	-	-	0/4/4/4	0/0/0/0
4	GOL	A	538	-	-	0/4/4/4	0/0/0/0
4	GOL	A	539	-	-	0/4/4/4	0/0/0/0
4	GOL	A	540	-	-	0/4/4/4	0/0/0/0
4	GOL	A	541	-	-	0/4/4/4	0/0/0/0
4	GOL	A	542	-	-	0/4/4/4	0/0/0/0
4	GOL	A	543	-	-	0/4/4/4	0/0/0/0
4	GOL	A	544	-	-	0/4/4/4	0/0/0/0
4	GOL	A	545	-	-	0/4/4/4	0/0/0/0
4	GOL	A	546	-	-	0/4/4/4	0/0/0/0
4	GOL	A	547	-	-	0/4/4/4	0/0/0/0
4	GOL	A	548	-	-	0/4/4/4	0/0/0/0
4	GOL	A	549	-	-	0/4/4/4	0/0/0/0
4	GOL	A	550	-	-	0/4/4/4	0/0/0/0
5	15P	A	551	-	-	0/8/8/101	0/0/0/0
5	15P	A	552	-	-	0/8/8/101	0/0/0/0
5	15P	A	553	-	-	0/8/8/101	0/0/0/0
5	15P	A	554	-	-	0/8/8/101	0/0/0/0
6	PEG	A	555	-	-	0/4/4/4	0/0/0/0
6	PEG	A	556	-	-	0/4/4/4	0/0/0/0
6	PEG	A	557	-	-	0/4/4/4	0/0/0/0
6	PEG	A	558	-	-	0/4/4/4	0/0/0/0
7	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	NAG	A	604	1	-	0/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	535	FAD	C4X-C10	7.69	1.54	1.40
3	A	536	ZIR	C11-C12	-6.26	1.37	1.50
2	A	535	FAD	C4-C4X	6.21	1.51	1.41
3	A	536	ZIR	C4-N9	-4.11	1.31	1.37
2	A	535	FAD	C5X-N5	3.87	1.41	1.35
2	A	535	FAD	C9A-N10	3.56	1.44	1.38
2	A	535	FAD	C1'-N10	-3.54	1.44	1.48
3	A	536	ZIR	C8-N9	-3.28	1.31	1.36
2	A	535	FAD	C2A-N3A	3.21	1.38	1.32
7	A	604	NAG	C3-C2	3.19	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	536	ZIR	O4'-C1'	2.95	1.45	1.41
7	A	601	NAG	C3-C2	2.88	1.58	1.52
7	A	604	NAG	C2-N2	2.78	1.49	1.46
7	A	601	NAG	C4-C3	2.78	1.59	1.52
2	A	535	FAD	O4B-C1B	2.78	1.45	1.41
3	A	536	ZIR	C8-N7	-2.77	1.29	1.34
3	A	536	ZIR	C6-N10	-2.63	1.30	1.34
3	A	536	ZIR	C1'-N9	2.57	1.56	1.48
7	A	601	NAG	C4-C5	2.55	1.58	1.53
3	A	536	ZIR	C2-N1	-2.51	1.29	1.33
2	A	535	FAD	PA-O3P	2.50	1.64	1.59
2	A	535	FAD	C8A-N9A	2.37	1.40	1.36
3	A	536	ZIR	C6-C5	-2.16	1.39	1.44
2	A	535	FAD	C2A-N1A	2.08	1.38	1.33
3	A	536	ZIR	C5-N7	-2.06	1.32	1.40
3	A	536	ZIR	C12-C13	2.04	1.38	1.32
3	A	536	ZIR	C5-C4	-2.01	1.36	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	536	ZIR	N3-C2-N1	-10.36	120.05	128.71
2	A	535	FAD	C4X-C10-N10	-8.41	116.31	120.51
2	A	535	FAD	C2-N1-C10	6.54	121.56	114.98
3	A	536	ZIR	N3-C4-N9	5.66	135.65	125.43
3	A	536	ZIR	C5-C4-N3	-4.42	116.08	125.70
3	A	536	ZIR	C2-N3-C4	3.90	125.12	114.01
3	A	536	ZIR	O4'-C1'-C2'	-3.65	101.18	106.77
3	A	536	ZIR	C2'-C1'-N9	3.52	122.30	113.27
3	A	536	ZIR	C5'-C4'-C3'	-3.50	106.50	115.06
3	A	536	ZIR	C11-C12-C13	-3.47	120.14	127.00
7	A	604	NAG	C3-C4-C5	-3.38	104.17	110.20
3	A	536	ZIR	C2-N1-C6	3.33	118.78	116.69
7	A	604	NAG	O5-C5-C6	3.22	110.36	106.98
3	A	536	ZIR	C4-C5-N7	-3.22	106.77	109.52
2	A	535	FAD	C1'-C2'-C3'	-3.15	100.81	109.82
3	A	536	ZIR	C4'-O4'-C1'	3.09	113.10	109.75
3	A	536	ZIR	C15-C13-C14	2.85	121.89	114.62
2	A	535	FAD	C1'-N10-C9A	2.85	121.64	118.87
2	A	535	FAD	N1-C10-N10	2.81	123.35	115.97
3	A	536	ZIR	C3'-C2'-C1'	2.68	105.11	100.91
2	A	535	FAD	O2P-P-O3P	2.61	117.50	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	535	FAD	N3A-C2A-N1A	-2.56	126.57	128.71
4	A	550	GOL	O3-C3-C2	2.51	121.96	109.71
2	A	535	FAD	C10-C4X-N5	2.47	123.46	120.45
7	A	601	NAG	O5-C5-C6	2.41	109.51	106.98
2	A	535	FAD	C4X-C10-N1	-2.39	120.34	122.73
2	A	535	FAD	C4'-C3'-C2'	2.39	118.65	113.25
7	A	601	NAG	C4-C3-C2	2.37	117.13	111.32
2	A	535	FAD	O4B-C1B-N9A	2.36	110.64	108.44
7	A	604	NAG	C3-C2-N2	2.28	115.24	111.76
7	A	601	NAG	O5-C5-C4	2.23	113.48	110.65
2	A	535	FAD	O3'-C3'-C4'	2.20	114.28	108.74
7	A	601	NAG	C3-C4-C5	2.08	113.92	110.20
7	A	604	NAG	O4-C4-C5	2.01	114.59	109.28
2	A	535	FAD	C4A-C5A-N7A	2.00	111.24	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	498/516 (96%)	0.37	31 (6%) 20 22	14, 26, 52, 72	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	10.6
1	A	128	ALA	7.0
1	A	279	ALA	6.7
1	A	390	LEU	6.7
1	A	462	VAL	6.1
1	A	274	PRO	5.5
1	A	127	ALA	5.0
1	A	389	GLY	4.4
1	A	465	ASN	3.6
1	A	391	TRP	3.4
1	A	383	VAL	3.1
1	A	216	GLN	3.0
1	A	387	LYS	3.0
1	A	273	ARG	2.9
1	A	463	ALA	2.8
1	A	280	SER	2.8
1	A	92	PRO	2.7
1	A	130	PRO	2.7
1	A	386	ASN	2.5
1	A	385	LEU	2.5
1	A	346	VAL	2.4
1	A	343	ALA	2.4
1	A	497	ASP	2.4
1	A	348	GLN	2.3
1	A	217	LEU	2.3
1	A	90	SER	2.2
1	A	384	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	379	HIS	2.2
1	A	36	ALA	2.2
1	A	464	PRO	2.0
1	A	33	PRO	2.0

## 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 ⓘ

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
8	NAG	A	602	14/15	0.16	7.56	39,43,46,46	0
8	NAG	A	603	14/15	0.28	-	54,58,60,61	0

## 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
6	PEG	A	555	7/7	0.31	10.83	30,33,34,43	0
4	GOL	A	542	6/6	0.28	9.98	52,53,53,54	0
4	GOL	A	541	6/6	0.24	9.22	57,58,58,59	0
5	15P	A	551	11/104	0.34	9.01	40,41,44,45	0
4	GOL	A	543	6/6	0.26	8.45	43,43,44,45	0
4	GOL	A	544	6/6	0.34	7.60	62,63,63,64	0
4	GOL	A	540	6/6	0.24	7.06	62,63,63,63	0
4	GOL	A	545	6/6	0.26	6.99	53,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	604	14/15	0.18	6.88	40,44,47,47	0
6	PEG	A	556	7/7	0.29	6.62	73,74,77,78	0
5	15P	A	552	11/104	0.30	6.23	40,41,44,44	0
4	GOL	A	539	6/6	0.21	5.89	39,40,40,41	0
5	15P	A	553	11/104	0.29	5.50	49,51,53,54	0
5	15P	A	554	11/104	0.26	5.32	55,57,59,60	0
4	GOL	A	549	6/6	0.21	2.75	69,70,70,71	0
4	GOL	A	538	6/6	0.18	2.55	29,32,33,34	0
3	ZIR	A	536	24/24	0.20	1.95	29,34,47,52	0
4	GOL	A	548	6/6	0.28	1.90	66,67,67,69	0
4	GOL	A	550	6/6	0.20	1.66	28,31,31,32	0
7	NAG	A	601	14/15	0.23	1.60	38,42,45,45	0
4	GOL	A	547	6/6	0.19	0.86	52,53,54,54	0
6	PEG	A	557	7/7	0.16	0.59	53,54,57,58	0
6	PEG	A	558	7/7	0.18	0.36	59,60,62,64	0
4	GOL	A	537	6/6	0.16	0.00	44,45,46,46	0
2	FAD	A	535	53/53	0.14	-0.36	19,20,21,22	0
4	GOL	A	546	6/6	0.20	-	65,66,67,67	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.