Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:44 AM GMT

PDB ID	:	3C0P
Title	:	Maize cytokinin oxidase/dehydrogenase complexed with the allenic cytokinin analog HA-8
Authors	:	Briozzo, P.; Kopecny, D.
Deposited on	:	2008-01-21
Resolution	:	1.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

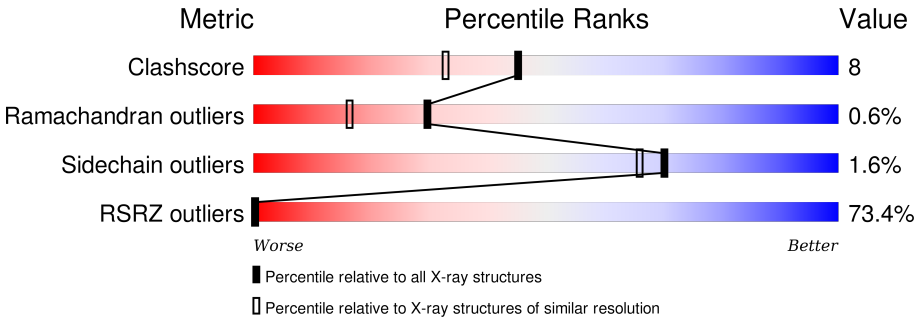
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 >=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 <=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	71%, 81%, 14%

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	NAG	A	1601	-	-	-	X
2	NAG	A	1608	X	-	-	X
3	NAG	A	1602	X	-	-	X
3	NAG	A	1605	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4336 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.

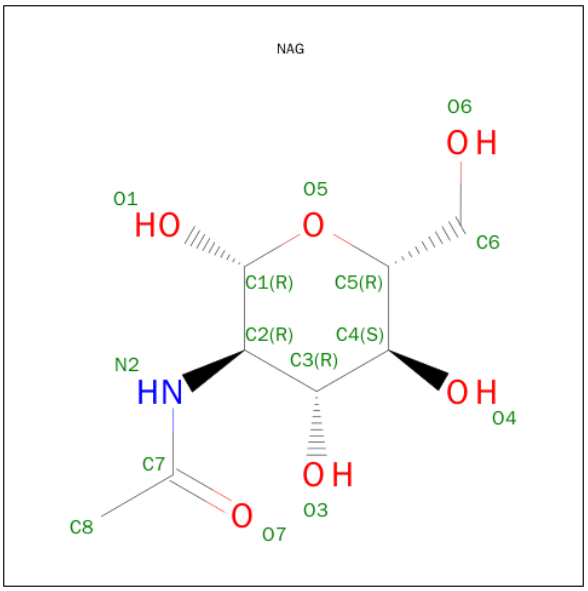
- Molecule 1 is a protein called Cytokinin dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3784	2402	665	706	11			

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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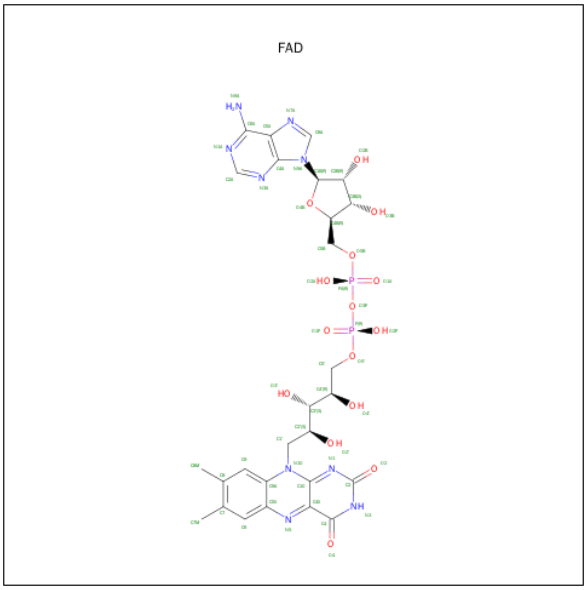
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

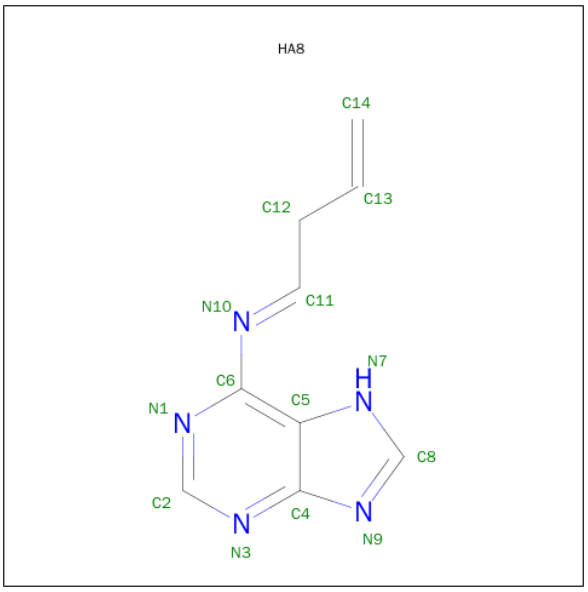
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



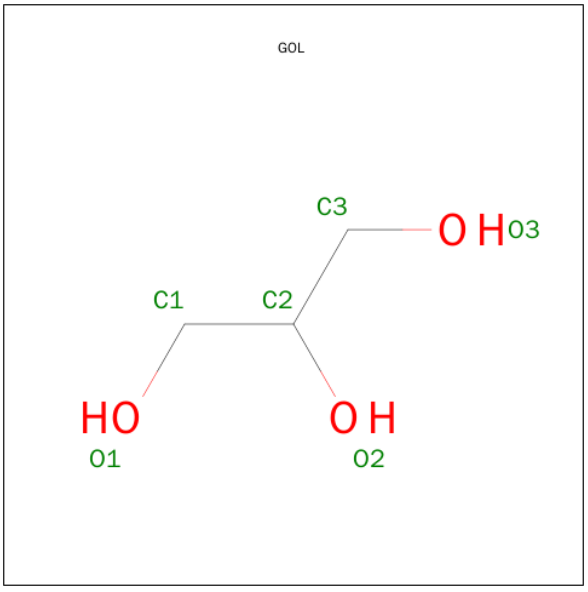
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is N6-(BUTA-2,3-DIENYL)ADENINE (three-letter code: HA8) (formula: $C_9H_9N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 14 9 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	367	Total O 367 367	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 (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

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	250.70Å 50.20Å 51.20Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 19.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.00-1.95) 81.3 (19.74-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 1.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.245 0.316 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 45729 reflections	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	4336	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HA8, GOL, NAG, 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	0.32	0/3873	0.59	0/5277

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
3	A	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1602	NAG	C1
3	A	1605	NAG	C1

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	3784	0	3700	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	26	1	0
3	A	84	0	75	7	0
4	A	53	0	29	1	0
5	A	14	0	8	0	0
6	A	6	0	8	0	0
7	A	367	0	0	8	0
All	All	4336	0	3846	61	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 8.

All (61) 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	2.18	0.78
1:A:143:ASP:OD1	1:A:239:ARG:HD3	1.89	0.73
1:A:136:SER:HB3	1:A:141:TYR:CE1	2.32	0.65
1:A:123:SER:HA	1:A:126:ASP:OD2	1.97	0.65
1:A:441:GLY:HA2	1:A:512:ARG:HH12	1.63	0.63
1:A:48:ARG:HD3	1:A:74:TYR:CE2	2.33	0.63
1:A:465:ASN:HB2	7:A:1913:HOH:O	2.01	0.60
1:A:382:GLU:HG3	1:A:391:TRP:CE2	2.37	0.59
1:A:427:PRO:HG2	1:A:458:LEU:HD12	1.84	0.58
1:A:141:TYR:CD1	1:A:239:ARG:HD2	2.38	0.58
1:A:524:ARG:HG3	1:A:533:PHE:HB3	1.86	0.57
1:A:509:LYS:HE3	7:A:1945:HOH:O	2.04	0.57
1:A:41:LEU:HB3	1:A:47:LEU:HD23	1.88	0.56
1:A:90:SER:O	1:A:92:PRO:HD3	2.05	0.56
1:A:143:ASP:CB	3:A:1602:NAG:H81	2.35	0.55
1:A:463:ALA:O	1:A:464:PRO:O	2.24	0.55
1:A:254:LEU:N	1:A:254:LEU:HD22	2.22	0.54
1:A:134:ASN:ND2	3:A:1602:NAG:H82	2.24	0.53
1:A:143:ASP:HB3	3:A:1602:NAG:H81	1.89	0.53
1:A:464:PRO:O	1:A:466:ASP:N	2.42	0.52
1:A:460:SER:HB3	1:A:462:VAL:HG13	1.92	0.52
1:A:252:VAL:HG12	1:A:366:GLN:HG2	1.90	0.52
1:A:73:LEU:HG	1:A:75:PRO:HD3	1.92	0.51
1:A:199:LEU:N	1:A:199:LEU:HD12	2.26	0.50
1:A:58:SER:HB3	1:A:68:LEU:HD23	1.95	0.49
1:A:392:ARG:HG3	1:A:392:ARG:HH11	1.78	0.48
1:A:284:MET:HE2	1:A:334:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ARG:NH2	7:A:1880:HOH:O	2.46	0.48
1:A:88:ALA:HA	1:A:94:TRP:CD2	2.47	0.48
1:A:50:ASP:OD2	1:A:52:ASN:HB2	2.13	0.47
1:A:382:GLU:HG3	1:A:391:TRP:CD2	2.50	0.47
3:A:1604:NAG:H5	3:A:1605:NAG:H83	1.96	0.47
1:A:97:THR:HB	1:A:528:PRO:HG3	1.97	0.47
1:A:41:LEU:HB3	1:A:47:LEU:CD2	2.45	0.47
1:A:412:ARG:HD2	7:A:1960:HOH:O	2.13	0.47
2:A:1608:NAG:H5	7:A:1934:HOH:O	2.14	0.46
3:A:1604:NAG:H5	3:A:1605:NAG:C8	2.47	0.45
1:A:462:VAL:HG23	1:A:463:ALA:N	2.31	0.45
1:A:524:ARG:CG	1:A:533:PHE:HB3	2.46	0.45
1:A:388:LEU:HG	7:A:1625:HOH:O	2.16	0.45
1:A:465:ASN:C	7:A:1857:HOH:O	2.56	0.44
1:A:191:HIS:C	1:A:437:MET:HE2	2.38	0.44
1:A:398:LEU:HG	1:A:400:MET:HE3	1.99	0.44
1:A:73:LEU:HD22	1:A:84:LEU:HD22	1.99	0.44
3:A:1607:NAG:O3	3:A:1607:NAG:H83	2.17	0.44
1:A:344:ALA:O	1:A:348:GLN:HG3	2.18	0.43
1:A:41:LEU:CB	1:A:47:LEU:HD23	2.49	0.42
1:A:65:THR:HG22	7:A:1657:HOH:O	2.19	0.42
1:A:273:ARG:HB2	1:A:280:SER:OG	2.19	0.42
1:A:491:TYR:CD2	1:A:492:LEU:HG	2.55	0.42
1:A:48:ARG:HB3	1:A:50:ASP:OD1	2.20	0.42
1:A:284:MET:HE3	1:A:353:VAL:HG21	2.01	0.41
1:A:65:THR:HG23	1:A:112:PHE:HE2	1.85	0.41
1:A:57:ALA:HB1	1:A:118:VAL:HG11	2.02	0.41
1:A:143:ASP:C	3:A:1602:NAG:H81	2.41	0.41
1:A:47:LEU:HD22	1:A:73:LEU:HD13	2.02	0.41
1:A:515:GLU:HG2	1:A:516:MET:CE	2.51	0.41
1:A:501:TRP:CE2	1:A:532:ILE:HG12	2.55	0.41
1:A:61:PHE:CD2	4:A:1535:FAD:HM82	2.57	0.40
1:A:398:LEU:HD21	1:A:400:MET:HE1	2.03	0.40
1:A:293:VAL:HG21	1:A:424:ILE:HD12	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	492/516 (95%)	476 (97%)	13 (3%)	3 (1%)	30 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	PRO
1	A	182	ALA
1	A	465	ASN

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	386/395 (98%)	380 (98%)	6 (2%)	70 66

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	220	ASP
1	A	239	ARG
1	A	349	GLU
1	A	419	LEU
1	A	494	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

6 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	$\#\|Z\| > 2$
3	NAG	A	1602	1,3	14,14,15	0.67	0	15,19,21	0.75	1 (6%)
3	NAG	A	1603	3	14,14,15	0.48	0	15,19,21	0.73	1 (6%)
3	NAG	A	1604	1,3	14,14,15	0.56	0	15,19,21	0.93	1 (6%)
3	NAG	A	1605	3	14,14,15	0.56	0	15,19,21	0.73	1 (6%)
3	NAG	A	1606	1,3	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
3	NAG	A	1607	3	14,14,15	0.51	0	15,19,21	0.69	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
3	NAG	A	1602	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1603	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1605	3	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1606	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1607	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1606	NAG	C2-N2-C7	-2.65	119.64	123.04
3	A	1603	NAG	C2-N2-C7	-2.29	120.09	123.04
3	A	1604	NAG	C2-N2-C7	-2.25	120.15	123.04
3	A	1607	NAG	C2-N2-C7	-2.11	120.33	123.04
3	A	1605	NAG	C2-N2-C7	-2.09	120.36	123.04
3	A	1602	NAG	C2-N2-C7	-2.06	120.39	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1605	NAG	C1
3	A	1602	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	NAG	4	0
3	A	1604	NAG	2	0
3	A	1605	NAG	2	0
3	A	1607	NAG	1	0

5.6 Ligand geometry (i)

5 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	$\#\|Z\|>2$
4	FAD	A	1535	1,5	48,58,58	2.35	10 (20%)	54,89,89	3.21	5 (9%)
5	HA8	A	1536	4	11,15,15	1.42	2 (18%)	5,19,19	4.95	4 (80%)
2	NAG	A	1601	1	14,14,15	0.45	0	15,19,21	0.72	1 (6%)
2	NAG	A	1608	1	14,14,15	0.48	0	15,19,21	0.80	1 (6%)
6	GOL	A	718	-	5,5,5	0.28	0	5,5,5	0.24	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
4	FAD	A	1535	1,5	-	0/30/50/50	0/6/6/6
5	HA8	A	1536	4	-	0/2/5/5	0/2/2/2
2	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1608	1	1/1/5/7	0/6/23/26	0/1/1/1
6	GOL	A	718	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1535	FAD	C1'-N10	-2.44	1.45	1.48
4	A	1535	FAD	C5A-C4A	-2.11	1.35	1.40
5	A	1536	HA8	C12-C13	-2.06	1.39	1.51
5	A	1536	HA8	C11-N10	2.32	1.32	1.26
4	A	1535	FAD	O4B-C1B	2.39	1.44	1.41
4	A	1535	FAD	C5X-N5	2.64	1.39	1.35
4	A	1535	FAD	C9-C8	3.05	1.46	1.37
4	A	1535	FAD	C4A-N3A	3.41	1.40	1.35
4	A	1535	FAD	C9A-N10	4.77	1.45	1.38
4	A	1535	FAD	C4-N3	5.32	1.43	1.33
4	A	1535	FAD	C4X-N5	7.09	1.44	1.33
4	A	1535	FAD	C4X-C10	9.08	1.58	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1535	FAD	C4-C4X-C10	-19.06	107.75	119.94
5	A	1536	HA8	N3-C2-N1	-9.43	121.67	128.89
4	A	1535	FAD	C4-C4X-N5	-7.14	110.05	118.72
4	A	1535	FAD	C4X-C4-N3	-5.96	115.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1608	NAG	C2-N2-C7	-2.54	119.77	123.04
2	A	1601	NAG	C2-N2-C7	-2.24	120.17	123.04
5	A	1536	HA8	C4-C5-N7	-2.13	107.52	109.48
4	A	1535	FAD	C4X-N5-C5X	3.34	120.60	116.76
5	A	1536	HA8	C2-N1-C6	3.34	121.05	113.56
5	A	1536	HA8	C13-C12-C11	4.21	124.80	112.22
4	A	1535	FAD	C4-N3-C2	7.52	121.74	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1608	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1535	FAD	1	0
2	A	1608	NAG	1	0

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

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^{th} 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	496/516 (96%)	3.29	364 (73%)	0	0	11, 25, 46, 61	15 (3%)

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	PRO	21.0
1	A	390	LEU	12.7
1	A	128	ALA	12.0
1	A	465	ASN	10.5
1	A	343	ALA	9.6
1	A	383	VAL	9.5
1	A	127	ALA	9.5
1	A	95	PRO	9.4
1	A	124	LEU	9.4
1	A	129	ALA	9.3
1	A	514	VAL	9.1
1	A	33	PRO	8.8
1	A	281	PHE	8.4
1	A	34	TRP	7.7
1	A	41	LEU	7.7
1	A	38	LEU	7.6
1	A	94	TRP	7.5
1	A	463	ALA	7.5
1	A	336	TYR	7.4
1	A	53	ALA	7.2
1	A	92	PRO	7.1
1	A	353	VAL	7.1
1	A	52	ASN	6.9
1	A	43	LEU	6.9
1	A	111	ALA	6.9
1	A	384	ALA	6.8
1	A	90	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	6.8
1	A	55	ALA	6.7
1	A	67	ALA	6.7
1	A	84	LEU	6.7
1	A	211	VAL	6.6
1	A	85	LEU	6.5
1	A	462	VAL	6.5
1	A	73	LEU	6.5
1	A	273	ARG	6.5
1	A	280	SER	6.5
1	A	373	ALA	6.5
1	A	96	TYR	6.5
1	A	216	GLN	6.3
1	A	391	TRP	6.2
1	A	39	ALA	6.1
1	A	99	ALA	6.0
1	A	339	ALA	5.9
1	A	153	VAL	5.9
1	A	88	ALA	5.9
1	A	130	PRO	5.8
1	A	158	LEU	5.7
1	A	71	ALA	5.7
1	A	510	TRP	5.7
1	A	72	VAL	5.7
1	A	47	LEU	5.7
1	A	172	TYR	5.6
1	A	367	ARG	5.6
1	A	392	ARG	5.5
1	A	503	ARG	5.5
1	A	126	ASP	5.5
1	A	149	VAL	5.3
1	A	159	ALA	5.3
1	A	179	LEU	5.3
1	A	520	TYR	5.2
1	A	225	VAL	5.2
1	A	388	LEU	5.2
1	A	210	MET	5.2
1	A	42	ALA	5.2
1	A	118	VAL	5.1
1	A	122	ALA	5.1
1	A	155	ARG	5.1
1	A	512	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	370	ALA	5.1
1	A	506	GLY	5.1
1	A	154	LEU	5.0
1	A	48	ARG	5.0
1	A	165	ARG	5.0
1	A	100	PHE	4.9
1	A	232	PHE	4.9
1	A	460	SER	4.9
1	A	44	ASP	4.9
1	A	221	LEU	4.9
1	A	87	ALA	4.8
1	A	82	VAL	4.8
1	A	119	VAL	4.8
1	A	209	GLU	4.8
1	A	272	PRO	4.7
1	A	141	TYR	4.7
1	A	344	ALA	4.7
1	A	224	ALA	4.6
1	A	337	ASP	4.6
1	A	201	MET	4.5
1	A	208	GLY	4.5
1	A	113	ALA	4.5
1	A	54	THR	4.5
1	A	498	ARG	4.5
1	A	491	TYR	4.5
1	A	98	ILE	4.5
1	A	217	LEU	4.5
1	A	518	ASN	4.5
1	A	380	GLY	4.5
1	A	46	LYS	4.5
1	A	178	THR	4.5
1	A	146	GLY	4.5
1	A	425	VAL	4.5
1	A	49	THR	4.4
1	A	342	ALA	4.4
1	A	56	ALA	4.3
1	A	526	LEU	4.3
1	A	134	ASN	4.3
1	A	504	HIS	4.3
1	A	389	GLY	4.3
1	A	203	VAL	4.3
1	A	51	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASN	4.3
1	A	454	ALA	4.2
1	A	519	LYS	4.2
1	A	386	ASN	4.2
1	A	466	ASP	4.2
1	A	79	ALA	4.2
1	A	160	ARG	4.2
1	A	144	ALA	4.1
1	A	307	PHE	4.1
1	A	515	GLU	4.1
1	A	346	VAL	4.1
1	A	200	GLU	4.1
1	A	524	ARG	4.1
1	A	492	LEU	4.1
1	A	81	LEU	4.1
1	A	483	LEU	4.1
1	A	77	SER	4.1
1	A	496	THR	4.0
1	A	175	VAL	4.0
1	A	104	GLY	4.0
1	A	424	ILE	4.0
1	A	91	THR	4.0
1	A	283	PRO	3.9
1	A	135	VAL	3.9
1	A	37	SER	3.9
1	A	414	VAL	3.9
1	A	138	ASP	3.9
1	A	452	PHE	3.9
1	A	57	ALA	3.9
1	A	523	LYS	3.9
1	A	121	MET	3.9
1	A	75	PRO	3.9
1	A	340	THR	3.9
1	A	173	LEU	3.8
1	A	151	ILE	3.8
1	A	479	ARG	3.8
1	A	381	GLU	3.8
1	A	334	LEU	3.8
1	A	365	PHE	3.8
1	A	374	PHE	3.8
1	A	486	ILE	3.8
1	A	112	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	3.8
1	A	378	VAL	3.8
1	A	132	ARG	3.7
1	A	233	GLY	3.7
1	A	76	SER	3.7
1	A	397	TRP	3.7
1	A	301	LEU	3.7
1	A	115	GLY	3.7
1	A	230	GLY	3.7
1	A	345	ALA	3.7
1	A	248	ARG	3.7
1	A	213	CYS	3.6
1	A	324	ALA	3.6
1	A	493	ALA	3.6
1	A	170	TYR	3.6
1	A	418	ILE	3.6
1	A	338	ASN	3.6
1	A	80	ASP	3.6
1	A	350	LEU	3.6
1	A	441	GLY	3.6
1	A	341	ALA	3.5
1	A	133	ILE	3.5
1	A	385	LEU	3.5
1	A	61	PHE	3.5
1	A	516	MET	3.5
1	A	318	LEU	3.5
1	A	489	LYS	3.5
1	A	478	LEU	3.5
1	A	352	SER	3.5
1	A	212	THR	3.5
1	A	40	ALA	3.5
1	A	354	LEU	3.5
1	A	59	THR	3.4
1	A	495	HIS	3.4
1	A	259	PHE	3.4
1	A	410	PHE	3.4
1	A	348	GLN	3.4
1	A	327	VAL	3.4
1	A	86	SER	3.4
1	A	105	HIS	3.4
1	A	83	ALA	3.4
1	A	228	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	220	ASP	3.3
1	A	36	ALA	3.3
1	A	369	VAL	3.3
1	A	470	LEU	3.3
1	A	500	ASP	3.3
1	A	286	TYR	3.3
1	A	422	THR	3.3
1	A	357	LEU	3.2
1	A	332	ALA	3.2
1	A	304	THR	3.2
1	A	442	MET	3.2
1	A	198	VAL	3.2
1	A	143	ASP	3.2
1	A	156	ALA	3.2
1	A	214	SER	3.2
1	A	398	LEU	3.2
1	A	240	ILE	3.2
1	A	446	THR	3.2
1	A	522	PRO	3.2
1	A	145	GLY	3.2
1	A	166	SER	3.1
1	A	393	VAL	3.1
1	A	229	LEU	3.1
1	A	262	PHE	3.1
1	A	533	PHE	3.1
1	A	430	VAL	3.1
1	A	532	ILE	3.1
1	A	387	LYS	3.1
1	A	50	ASP	3.1
1	A	488	TYR	3.1
1	A	142	VAL	3.1
1	A	458	LEU	3.1
1	A	501	TRP	3.1
1	A	245	ALA	3.0
1	A	394	PRO	3.0
1	A	525	LEU	3.0
1	A	222	PHE	3.0
1	A	117	VAL	3.0
1	A	244	PRO	3.0
1	A	70	ALA	3.0
1	A	74	TYR	3.0
1	A	291	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	152	ASP	3.0
1	A	235	ILE	3.0
1	A	306	PHE	3.0
1	A	476	ARG	2.9
1	A	513	PHE	2.9
1	A	451	VAL	2.9
1	A	508	ALA	2.9
1	A	68	LEU	2.9
1	A	226	LEU	2.9
1	A	371	TYR	2.9
1	A	328	TYR	2.9
1	A	372	ALA	2.9
1	A	431	TYR	2.8
1	A	481	CYS	2.8
1	A	362	GLY	2.8
1	A	69	PRO	2.8
1	A	264	ALA	2.8
1	A	237	ARG	2.8
1	A	438	TRP	2.8
1	A	131	PRO	2.8
1	A	359	TYR	2.8
1	A	66	SER	2.8
1	A	294	ASN	2.7
1	A	123	SER	2.7
1	A	290	SER	2.7
1	A	507	ALA	2.7
1	A	125	GLY	2.7
1	A	375	LEU	2.7
1	A	419	LEU	2.7
1	A	455	VAL	2.7
1	A	231	GLN	2.7
1	A	45	GLY	2.7
1	A	320	GLY	2.7
1	A	310	ALA	2.7
1	A	190	ARG	2.7
1	A	497	ASP	2.7
1	A	64	ILE	2.7
1	A	184	ILE	2.7
1	A	521	ASP	2.7
1	A	189	PHE	2.7
1	A	78	THR	2.6
1	A	219	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	313	ALA	2.6
1	A	268	ARG	2.6
1	A	453	TYR	2.6
1	A	62	GLY	2.6
1	A	176	GLY	2.6
1	A	254	LEU	2.6
1	A	356	THR	2.6
1	A	468	ALA	2.6
1	A	295	GLN	2.6
1	A	108	MET	2.6
1	A	247	ALA	2.6
1	A	396	PRO	2.6
1	A	204	ILE	2.6
1	A	448	SER	2.6
1	A	103	ARG	2.5
1	A	426	GLY	2.5
1	A	161	GLY	2.5
1	A	251	TRP	2.5
1	A	363	PHE	2.5
1	A	300	ASP	2.5
1	A	191	HIS	2.4
1	A	223	ASP	2.4
1	A	174	THR	2.4
1	A	296	SER	2.4
1	A	163	ALA	2.4
1	A	271	ALA	2.4
1	A	205	THR	2.4
1	A	136	SER	2.4
1	A	297	LEU	2.4
1	A	400	MET	2.4
1	A	437	MET	2.4
1	A	429	ILE	2.3
1	A	246	PRO	2.3
1	A	106	SER	2.3
1	A	499	SER	2.3
1	A	401	PHE	2.3
1	A	494	ARG	2.3
1	A	150	TRP	2.3
1	A	403	PRO	2.3
1	A	58	SER	2.3
1	A	249	ALA	2.3
1	A	234	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	253	ARG	2.3
1	A	423	ASP	2.3
1	A	459	PHE	2.3
1	A	157	SER	2.3
1	A	207	HIS	2.3
1	A	89	ASN	2.3
1	A	528	PRO	2.3
1	A	65	THR	2.3
1	A	148	GLN	2.3
1	A	323	ASN	2.3
1	A	377	ARG	2.3
1	A	531	ASP	2.3
1	A	428	LEU	2.2
1	A	330	ILE	2.2
1	A	408	ALA	2.2
1	A	164	PRO	2.2
1	A	93	GLY	2.2
1	A	239	ARG	2.2
1	A	480	PHE	2.2
1	A	473	GLN	2.2
1	A	447	PRO	2.2
1	A	406	ARG	2.2
1	A	109	GLY	2.1
1	A	97	THR	2.1
1	A	461	SER	2.1
1	A	402	VAL	2.1
1	A	409	ASP	2.1
1	A	511	ASN	2.1
1	A	255	VAL	2.1
1	A	285	SER	2.1
1	A	308	THR	2.1
1	A	315	ILE	2.1
1	A	137	ALA	2.1
1	A	250	ARG	2.1
1	A	116	GLY	2.1
1	A	379	HIS	2.1
1	A	303	ASN	2.0
1	A	107	LEU	2.0
1	A	474	ASN	2.0
1	A	364	ALA	2.0
1	A	382	GLU	2.0
1	A	490	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	319	ALA	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)

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^{th} 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^2)	Q<0.9
3	NAG	A	1602	14/15	0.40	0.88	10.79	43,44,46,47	14
3	NAG	A	1605	14/15	0.23	0.87	-	40,42,43,44	14
3	NAG	A	1604	14/15	0.63	0.39	-	28,31,35,37	14
3	NAG	A	1606	14/15	0.42	0.55	-	35,38,40,45	14
3	NAG	A	1603	14/15	0.26	0.88	-	49,50,52,53	14
3	NAG	A	1607	14/15	0.15	0.81	-	49,51,52,53	14

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^{th} 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^2)	Q<0.9
2	NAG	A	1601	14/15	0.47	0.52	2.49	24,31,34,35	14
2	NAG	A	1608	14/15	0.14	0.88	0.96	55,55,56,57	14
4	FAD	A	1535	53/53	0.82	0.21	-0.72	18,21,25,27	0
5	HA8	A	1536	14/14	0.83	0.18	-1.02	18,19,26,28	0
6	GOL	A	718	6/6	0.53	0.39	-	31,34,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.