



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2018 – 11:03 AM EST

PDB ID : 5NIW  
Title : Glucose oxydase mutant A2  
Authors : Hoffmann, K.; Frank, D.  
Deposited on : 2017-03-27  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

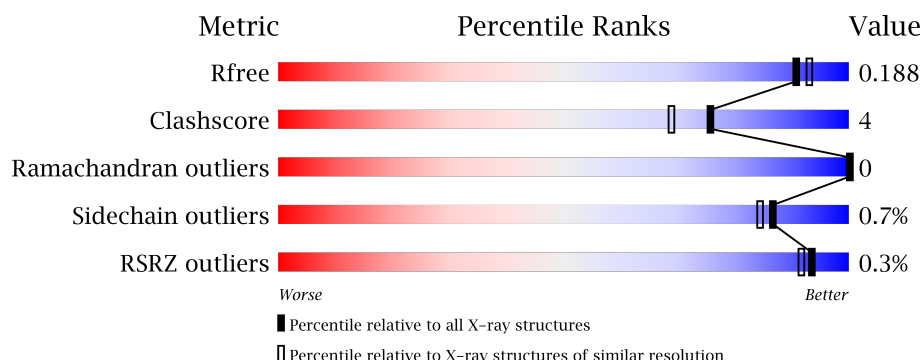
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	581	

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
4	NAG	A	606	-	-	-	X
4	NAG	A	607	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	610	-	-	-	X
6	DIO	A	611	-	-	X	-
6	DIO	A	612	-	-	-	X
6	DIO	A	613	-	-	-	X
6	DIO	A	615	-	-	-	X
6	DIO	A	617	-	-	-	X
6	DIO	A	619	-	-	-	X
6	DIO	A	620	-	-	-	X
6	DIO	A	621	-	-	-	X
6	DIO	A	622	-	-	-	X
7	PEG	A	623	-	-	-	X
7	PEG	A	624	-	-	-	X
8	P4C	A	625	-	-	-	X
8	P4C	A	626	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5085 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.

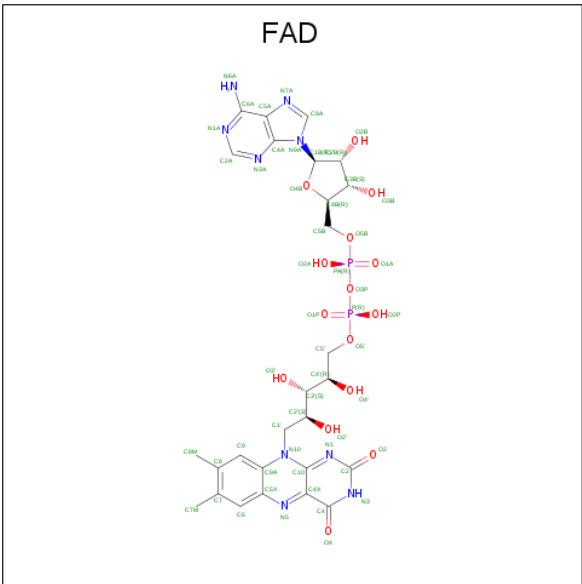
- Molecule 1 is a protein called Glucose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	4427	2792	756	867	12	2	4	0

There are 6 discrepancies between the modelled and reference sequences:

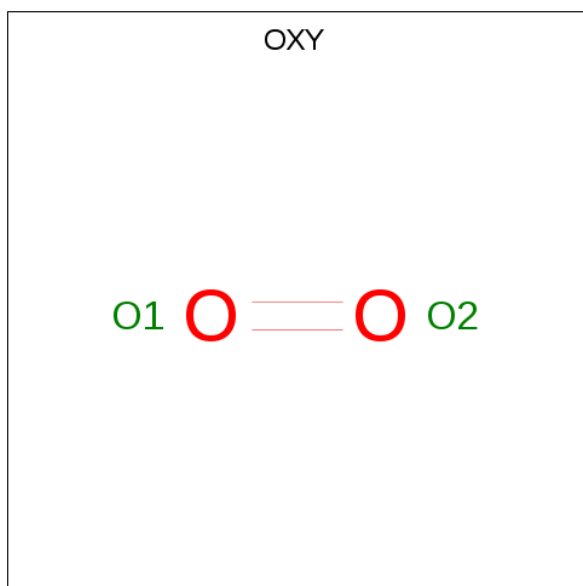
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	VAL	THR	conflict	UNP P13006
A	37	LYS	ARG	conflict	UNP P13006
A	94	VAL	ILE	conflict	UNP P13006
A	106	ILE	VAL	conflict	UNP P13006
A	162	THR	ALA	conflict	UNP P13006
A	556	VAL	MET	conflict	UNP P13006

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



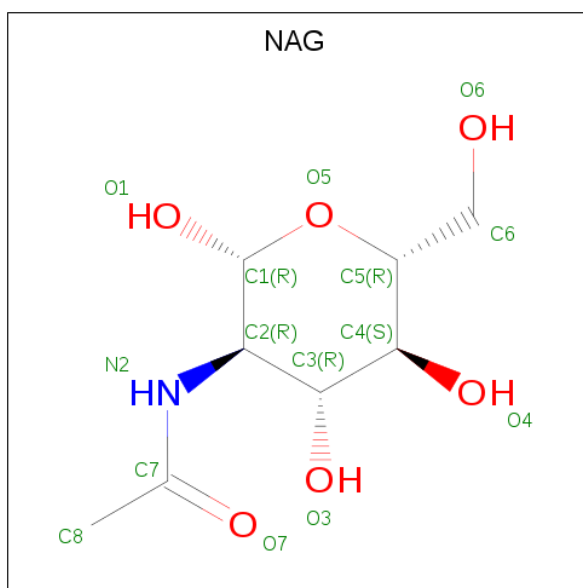
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



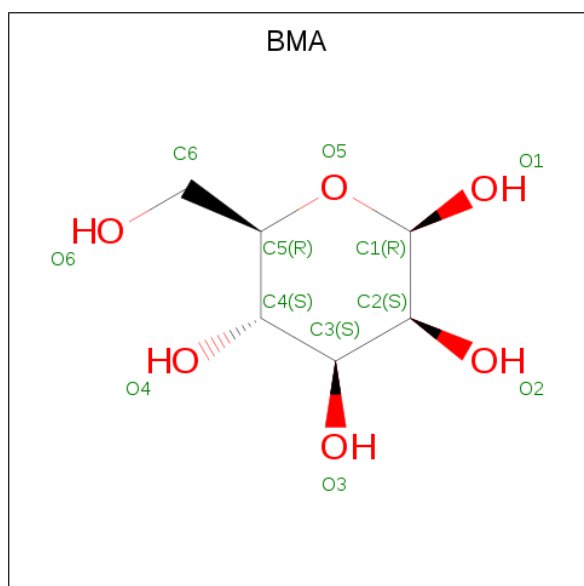
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



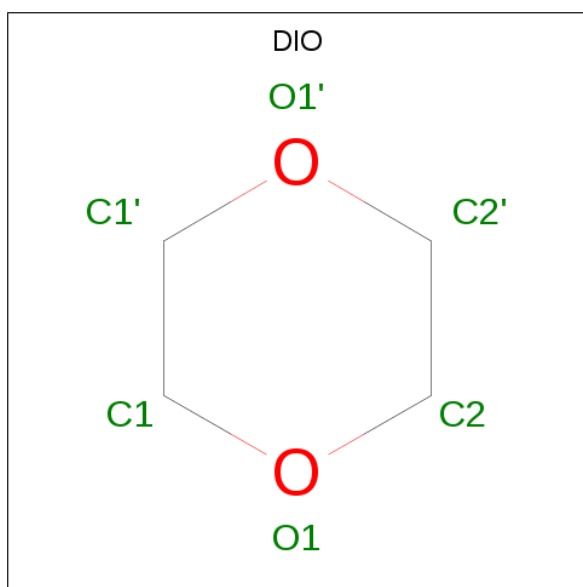
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



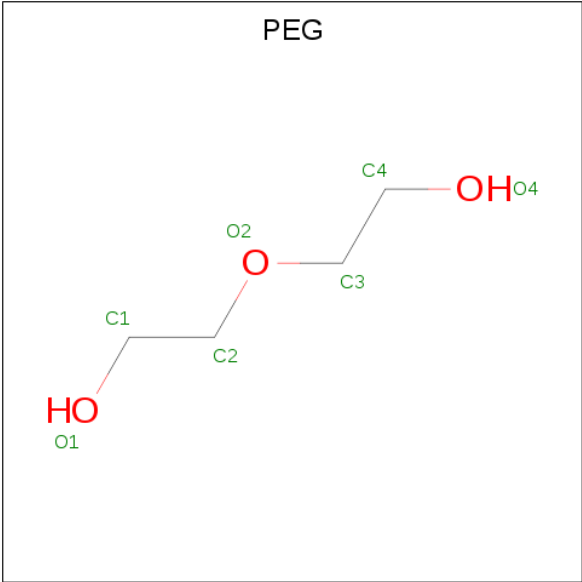
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $C_4H_8O_2$ ).



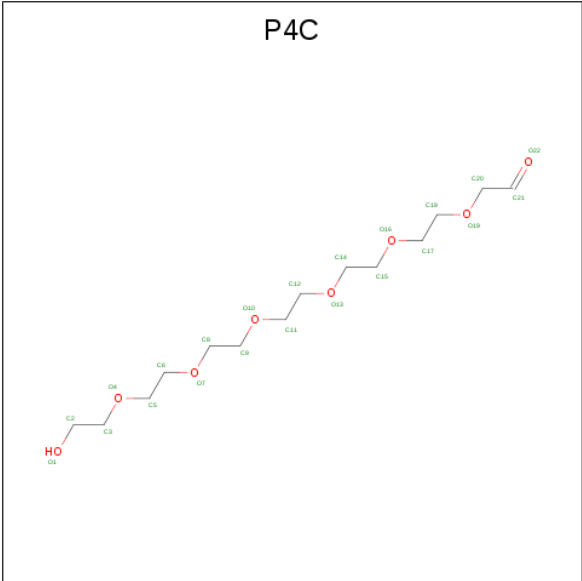
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (three-letter code: P4C) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			22	14	8		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			22	14	8		

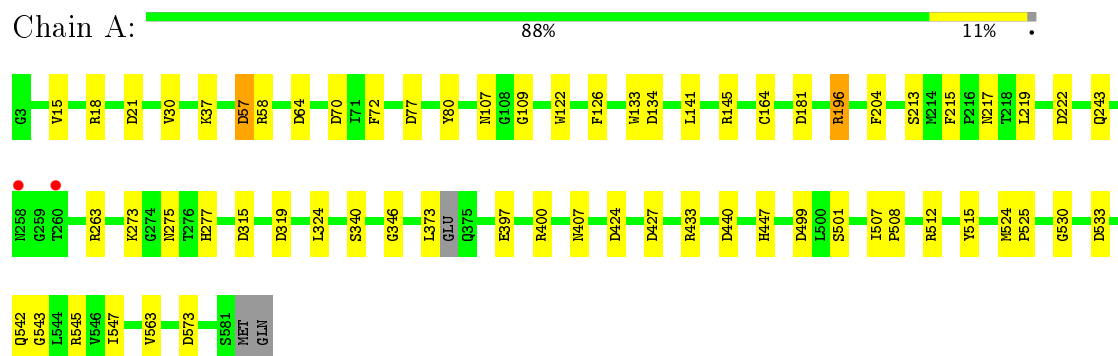
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	364	Total	O	0	0
			364	364		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Glucose oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.10 Å   128.10 Å   77.65 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	110.94 – 1.80 41.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (110.94-1.80) 99.8 (41.93-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.154 , 0.191 0.157 , 0.188	Depositor DCC
$R_{free}$ test set	3389 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, NAG, P4C, BMA, PEG, FAD, OXY

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	1.13	8/4543 (0.2%)	1.11	35/6202 (0.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	LEU	C-O	6.58	1.35	1.23
1	A	80	TYR	CG-CD1	6.29	1.47	1.39
1	A	263	ARG	CZ-NH2	5.96	1.40	1.33
1	A	340	SER	CB-OG	-5.88	1.34	1.42
1	A	501	SER	CB-OG	-5.67	1.34	1.42
1	A	346	GLY	C-O	5.44	1.32	1.23
1	A	122	TRP	CE3-CZ3	5.13	1.47	1.38
1	A	515	TYR	CE2-CZ	-5.05	1.31	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ARG	NE-CZ-NH1	-10.69	114.95	120.30
1	A	64	ASP	CB-CG-OD1	10.14	127.43	118.30
1	A	533	ASP	CB-CG-OD1	9.49	126.84	118.30
1	A	433	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	545	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	263	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	A	545	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	499	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	424	ASP	CB-CG-OD1	8.04	125.53	118.30
1	A	424	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	A	427	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	222	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	573	ASP	CB-CG-OD2	-6.53	112.42	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	433	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	57[A]	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	57[B]	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	499	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	222	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	70	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	315	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	134	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	181	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	21	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	400	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	196	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	319	ASP	CB-CG-OD1	5.22	122.99	118.30
1	A	145	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	77	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	512	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	324	LEU	CB-CG-CD2	5.16	119.77	111.00
1	A	145	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	72	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	A	533	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	440	ASP	CB-CG-OD2	5.04	122.84	118.30

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	4427	0	4200	32	0
2	A	53	0	31	3	0
3	A	2	0	0	0	0
4	A	98	0	89	1	1
5	A	11	0	10	0	0
6	A	72	0	96	8	0
7	A	14	0	20	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	44	0	56	8	0
9	A	364	0	0	5	1
All	All	5085	0	4502	33	2

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 4.

All (33) 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:275:ASN:O	9:A:701:HOH:O	1.86	0.91
1:A:57[A]:ASP:OD2	9:A:702:HOH:O	1.89	0.90
1:A:275:ASN:HB3	9:A:701:HOH:O	1.77	0.83
1:A:277:HIS:ND1	9:A:704:HOH:O	2.15	0.78
1:A:107:ASN:HB2	2:A:601:FAD:C5X	2.18	0.73
1:A:273:LYS:HZ2	8:A:625:P4C:H91	1.62	0.65
1:A:542:GLN:HE22	4:A:607:NAG:C7	2.12	0.63
1:A:196:ARG:NH1	9:A:703:HOH:O	2.02	0.57
1:A:447:HIS:NE2	8:A:626:P4C:C20	2.69	0.56
1:A:447:HIS:NE2	8:A:626:P4C:H202	2.20	0.55
1:A:273:LYS:HZ3	8:A:625:P4C:H151	1.71	0.55
1:A:107:ASN:HB2	2:A:601:FAD:N5	2.22	0.54
1:A:273:LYS:HZ2	8:A:625:P4C:C9	2.21	0.53
1:A:204:PHE:CZ	1:A:213:SER:HB2	2.47	0.49
1:A:30:VAL:HG11	1:A:547:ILE:O	2.13	0.49
1:A:164:CYS:HA	6:A:611:DIO:H11	1.95	0.48
1:A:563:VAL:HG22	6:A:619:DIO:H22	1.95	0.48
8:A:625:P4C:H52	8:A:625:P4C:H91	1.96	0.48
1:A:164:CYS:HA	6:A:611:DIO:C1	2.44	0.48
1:A:141:LEU:HD21	6:A:611:DIO:H12	1.97	0.46
1:A:243:GLN:HG3	6:A:622:DIO:O1'	2.16	0.46
1:A:109:GLY:O	1:A:217:ASN:HA	2.17	0.45
1:A:273:LYS:HE2	8:A:625:P4C:O19	2.18	0.44
1:A:543:GLY:HA2	6:A:620:DIO:H1'1	1.99	0.43
1:A:126:PHE:O	1:A:525:PRO:HD3	2.19	0.42
1:A:507:ILE:N	1:A:508:PRO:CD	2.83	0.42
1:A:107:ASN:HB2	2:A:601:FAD:C4X	2.49	0.42
1:A:15:VAL:HA	1:A:18:ARG:HD2	2.02	0.42
1:A:37[A]:LYS:HD2	1:A:37[A]:LYS:HA	1.85	0.42
1:A:397:GLU:HB3	6:A:612:DIO:H2'1	2.03	0.41
1:A:273:LYS:HE2	8:A:625:P4C:C21	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:HE1	6:A:611:DIO:H2'1	1.86	0.41
1:A:524:MET:O	1:A:530:GLY:HA3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:607:NAG:O3	4:A:607:NAG:O3[6_767]	1.86	0.34
7:A:624:PEG:O2	9:A:974:HOH:O[2_774]	1.93	0.27

## 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	578/581 (100%)	559 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	461/467 (99%)	458 (99%)	3 (1%)	87	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	PHE
1	A	219	LEU
1	A	407	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	243	GLN
1	A	407	ASN
1	A	493	ASN

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	601	-	51,58,58	2.04	14 (27%)	54,89,89	2.70	17 (31%)
3	OXY	A	602	-	1,1,1	0.03	0	0,0,0	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	603	1,4	14,14,15	1.00	0	15,19,21	1.76	5 (33%)
4	NAG	A	604	5,4	14,14,15	1.04	1 (7%)	15,19,21	1.67	3 (20%)
5	BMA	A	605	4	11,11,12	1.59	2 (18%)	13,15,17	2.00	4 (30%)
4	NAG	A	606	1	14,14,15	1.18	1 (7%)	15,19,21	2.23	4 (26%)
4	NAG	A	607	1	14,14,15	0.78	1 (7%)	15,19,21	2.19	7 (46%)
4	NAG	A	608	1	14,14,15	0.94	0	15,19,21	2.12	8 (53%)
4	NAG	A	609	1	14,14,15	1.43	2 (14%)	15,19,21	2.01	3 (20%)
4	NAG	A	610	1	14,14,15	0.66	0	15,19,21	1.46	1 (6%)
6	DIO	A	611	-	6,6,6	0.52	0	6,6,6	1.16	0
6	DIO	A	612	-	6,6,6	0.47	0	6,6,6	2.13	2 (33%)
6	DIO	A	613	-	6,6,6	0.69	0	6,6,6	0.56	0
6	DIO	A	614	-	6,6,6	0.76	0	6,6,6	0.89	0
6	DIO	A	615	-	6,6,6	0.51	0	6,6,6	1.15	0
6	DIO	A	616	-	6,6,6	0.48	0	6,6,6	0.79	0
6	DIO	A	617	-	6,6,6	0.94	0	6,6,6	1.31	0
6	DIO	A	618	-	6,6,6	0.78	0	6,6,6	1.07	0
6	DIO	A	619	-	6,6,6	0.76	0	6,6,6	1.39	1 (16%)
6	DIO	A	620	-	6,6,6	0.57	0	6,6,6	1.06	1 (16%)
6	DIO	A	621	-	6,6,6	0.48	0	6,6,6	0.63	0
6	DIO	A	622	-	6,6,6	0.52	0	6,6,6	0.37	0
7	PEG	A	623	-	6,6,6	0.41	0	5,5,5	1.22	1 (20%)
7	PEG	A	624	-	6,6,6	0.41	0	5,5,5	0.84	0
8	P4C	A	625	-	21,21,21	0.65	0	20,20,20	1.09	1 (5%)
8	P4C	A	626	-	21,21,21	0.90	0	20,20,20	2.00	7 (35%)

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	601	-	-	0/28/50/50	0/6/6/6
3	OXY	A	602	-	-	0/0/0/0	0/0/0/0
4	NAG	A	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	605	4	-	0/2/19/22	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	607	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	608	1	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	609	1	-	0/6/23/26	0/1/1/1
4	NAG	A	610	1	-	0/6/23/26	0/1/1/1
6	DIO	A	611	-	-	0/0/6/6	0/1/1/1
6	DIO	A	612	-	-	0/0/6/6	0/1/1/1
6	DIO	A	613	-	-	0/0/6/6	0/1/1/1
6	DIO	A	614	-	-	0/0/6/6	0/1/1/1
6	DIO	A	615	-	-	0/0/6/6	0/1/1/1
6	DIO	A	616	-	-	0/0/6/6	0/1/1/1
6	DIO	A	617	-	-	0/0/6/6	0/1/1/1
6	DIO	A	618	-	-	0/0/6/6	0/1/1/1
6	DIO	A	619	-	-	0/0/6/6	0/1/1/1
6	DIO	A	620	-	-	0/0/6/6	0/1/1/1
6	DIO	A	621	-	-	0/0/6/6	0/1/1/1
6	DIO	A	622	-	-	0/0/6/6	0/1/1/1
7	PEG	A	623	-	-	0/4/4/4	0/0/0/0
7	PEG	A	624	-	-	0/4/4/4	0/0/0/0
8	P4C	A	625	-	-	0/18/19/19	0/0/0/0
8	P4C	A	626	-	-	0/18/19/19	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-N10	-6.60	1.41	1.48
4	A	609	NAG	O5-C1	-4.28	1.36	1.43
2	A	601	FAD	O2'-C2'	-2.42	1.38	1.43
4	A	609	NAG	C2-N2	-2.41	1.42	1.46
2	A	601	FAD	C2B-C1B	-2.34	1.49	1.53
4	A	604	NAG	O5-C1	-2.18	1.40	1.43
4	A	606	NAG	O5-C5	-2.16	1.38	1.43
4	A	607	NAG	C1-C2	2.17	1.55	1.52
2	A	601	FAD	C5X-N5	2.22	1.38	1.35
5	A	605	BMA	O5-C5	2.29	1.48	1.43
2	A	601	FAD	C4X-N5	2.36	1.36	1.33
2	A	601	FAD	C5A-C4A	2.51	1.46	1.40
2	A	601	FAD	C9A-N10	2.59	1.42	1.38
2	A	601	FAD	C2-N1	3.14	1.44	1.38
2	A	601	FAD	C4-C4X	3.23	1.47	1.41
2	A	601	FAD	C8-C7	3.43	1.49	1.41
2	A	601	FAD	C9A-C5X	3.83	1.50	1.42
2	A	601	FAD	C2A-N3A	3.83	1.38	1.32
5	A	605	BMA	C2-C3	3.98	1.57	1.52
2	A	601	FAD	C4X-C10	4.56	1.49	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4B-C1B	5.02	1.48	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	NAG	C4-C3-C2	-6.64	101.29	111.02
2	A	601	FAD	C4-C4X-C10	-6.32	114.85	119.96
2	A	601	FAD	N3A-C2A-N1A	-5.23	124.31	128.86
2	A	601	FAD	C1B-N9A-C4A	-4.50	118.86	126.64
2	A	601	FAD	C4X-C10-N10	-4.50	117.40	120.52
4	A	609	NAG	C4-C3-C2	-4.44	104.51	111.02
2	A	601	FAD	C4X-C4-N3	-4.21	117.49	123.48
4	A	609	NAG	C1-C2-N2	-4.09	103.50	110.49
4	A	604	NAG	O7-C7-C8	-4.04	114.70	122.06
6	A	612	DIO	O1-C2-C2'	-3.60	92.99	110.89
4	A	603	NAG	O5-C1-C2	-3.42	106.72	111.47
4	A	609	NAG	C2-N2-C7	-3.07	118.46	122.94
4	A	608	NAG	C1-C2-N2	-3.07	105.24	110.49
4	A	603	NAG	C4-C3-C2	-2.97	106.67	111.02
4	A	608	NAG	C6-C5-C4	-2.97	106.06	113.00
4	A	603	NAG	C1-C2-N2	-2.90	105.53	110.49
4	A	608	NAG	C3-C4-C5	-2.90	105.11	110.22
8	A	626	P4C	O22-C21-C20	-2.83	117.04	126.38
4	A	606	NAG	O5-C1-C2	-2.81	107.56	111.47
4	A	608	NAG	O6-C6-C5	-2.76	102.06	111.34
4	A	606	NAG	O6-C6-C5	-2.72	102.19	111.34
2	A	601	FAD	C4'-C3'-C2'	-2.67	107.67	113.41
5	A	605	BMA	O5-C1-C2	-2.43	106.98	110.79
2	A	601	FAD	C4B-O4B-C1B	-2.38	107.24	109.77
4	A	606	NAG	C2-N2-C7	-2.30	119.58	122.94
2	A	601	FAD	C6-C7-C8	-2.27	115.91	119.95
4	A	604	NAG	O4-C4-C5	-2.24	103.63	109.28
4	A	607	NAG	C3-C4-C5	-2.22	106.30	110.22
2	A	601	FAD	O2'-C2'-C1'	-2.13	104.87	109.79
4	A	608	NAG	O4-C4-C5	-2.10	103.99	109.28
4	A	603	NAG	O4-C4-C3	-2.07	105.84	110.36
4	A	607	NAG	C6-C5-C4	2.01	117.70	113.00
8	A	625	P4C	O10-C9-C8	2.06	119.86	110.41
8	A	626	P4C	O4-C3-C2	2.06	119.68	110.15
6	A	620	DIO	C2-O1-C1	2.16	117.18	109.89
2	A	601	FAD	C7-C6-C5X	2.17	124.44	121.08
8	A	626	P4C	C11-O10-C9	2.17	122.71	113.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	607	NAG	O7-C7-N2	2.19	126.13	121.92
2	A	601	FAD	C6-C5X-N5	2.22	121.58	118.97
8	A	626	P4C	O7-C8-C9	2.25	120.74	110.41
7	A	623	PEG	O2-C3-C4	2.28	120.69	110.15
2	A	601	FAD	O2P-P-O1P	2.30	124.20	112.28
4	A	608	NAG	C4-C3-C2	2.33	114.43	111.02
4	A	607	NAG	C1-O5-C5	2.33	115.38	112.17
5	A	605	BMA	C1-O5-C5	2.39	115.46	112.17
4	A	607	NAG	C4-C3-C2	2.40	114.53	111.02
4	A	608	NAG	O3-C3-C4	2.45	115.69	110.36
2	A	601	FAD	C4-C4X-N5	2.56	121.49	118.68
8	A	626	P4C	O10-C9-C8	2.57	122.20	110.41
2	A	601	FAD	C10-C4X-N5	2.67	123.66	120.59
6	A	619	DIO	C2-O1-C1	2.68	118.97	109.89
4	A	603	NAG	O3-C3-C2	2.80	115.38	109.39
6	A	612	DIO	C2'-O1'-C1'	3.17	120.60	109.89
4	A	604	NAG	O7-C7-N2	3.17	128.01	121.92
2	A	601	FAD	O2'-C2'-C3'	3.31	117.31	109.09
4	A	607	NAG	C2-N2-C7	3.41	127.91	122.94
4	A	610	NAG	O3-C3-C4	3.58	118.16	110.36
4	A	608	NAG	C1-O5-C5	3.60	117.13	112.17
2	A	601	FAD	C1'-N10-C9A	3.79	121.82	118.35
5	A	605	BMA	O3-C3-C2	3.80	116.94	110.02
5	A	605	BMA	O2-C2-C3	3.83	117.70	110.17
8	A	626	P4C	O7-C6-C5	4.09	129.20	110.41
8	A	626	P4C	O16-C15-C14	4.33	130.30	110.41
4	A	607	NAG	C1-C2-N2	5.11	119.21	110.49
2	A	601	FAD	C4-N3-C2	12.64	126.22	115.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	607	NAG	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	3	0
4	A	607	NAG	1	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	611	DIO	4	0
6	A	612	DIO	1	0
6	A	619	DIO	1	0
6	A	620	DIO	1	0
6	A	622	DIO	1	0
7	A	624	PEG	0	1
8	A	625	P4C	6	0
8	A	626	P4C	2	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 [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, 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	578/581 (99%)	-0.50	2 (0%) 93 92	17, 23, 35, 66	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	THR	4.0
1	A	258	ASN	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	PEG	A	623	7/7	0.87	0.66	36.49	31,31,32,33	7
6	DIO	A	612	6/6	0.90	0.15	6.23	41,43,46,49	0
4	NAG	A	610	14/15	0.70	0.25	6.11	51,58,68,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	DIO	A	621	6/6	0.85	0.24	5.82	64,68,70,71	0
6	DIO	A	617	6/6	0.78	0.18	5.74	42,46,48,48	0
6	DIO	A	619	6/6	0.91	0.16	4.99	38,40,41,42	0
6	DIO	A	620	6/6	0.84	0.20	4.67	62,64,65,66	0
7	PEG	A	624	7/7	0.89	0.19	4.65	43,55,59,61	0
6	DIO	A	615	6/6	0.90	0.15	4.02	49,52,53,53	0
8	P4C	A	625	22/22	0.89	0.17	3.97	36,50,77,84	0
6	DIO	A	613	6/6	0.93	0.12	3.87	29,32,37,40	0
8	P4C	A	626	22/22	0.84	0.17	3.79	32,51,58,60	0
6	DIO	A	622	6/6	0.92	0.29	3.23	59,60,61,64	0
4	NAG	A	606	14/15	0.93	0.09	2.76	19,22,31,32	0
4	NAG	A	604	14/15	0.91	0.14	1.17	29,30,35,39	0
4	NAG	A	609	14/15	0.91	0.09	0.62	32,37,48,52	0
4	NAG	A	603	14/15	0.96	0.09	0.17	25,27,31,33	0
6	DIO	A	611	6/6	0.94	0.07	0.08	37,40,45,45	0
2	FAD	A	601	53/53	0.98	0.09	-0.07	16,18,22,22	0
4	NAG	A	608	14/15	0.93	0.10	-0.13	37,44,48,50	0
6	DIO	A	614	6/6	0.86	0.13	-	44,47,52,54	0
4	NAG	A	607	14/15	0.66	0.41	-	69,79,86,87	0
6	DIO	A	616	6/6	0.98	0.16	-	35,36,37,37	6
6	DIO	A	618	6/6	0.66	0.22	-	49,51,56,56	0
5	BMA	A	605	11/12	0.50	0.29	-	47,51,65,65	0
3	OXY	A	602	2/2	0.96	0.21	-	28,28,28,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.