



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:10 AM GMT

PDB ID : 2YLX  
Title : SNAPSHOTS OF ENZYMATIC BAEYER-VILLIGER CATALYSIS: OXY-  
GEN ACTIVATION AND INTERMEDIATE STABILIZATION: ASP66ALA  
MUTANT IN COMPLEX WITH NADP AND MES  
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Deposited on : 2011-06-06  
Resolution : 2.20 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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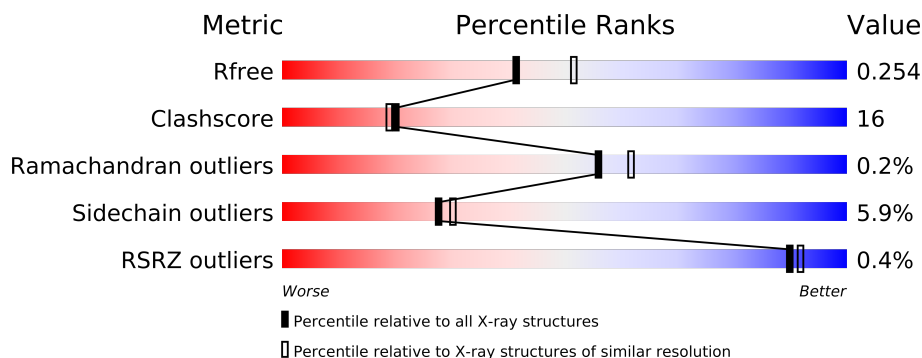
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	542	

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	MES	A	702	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4689 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.

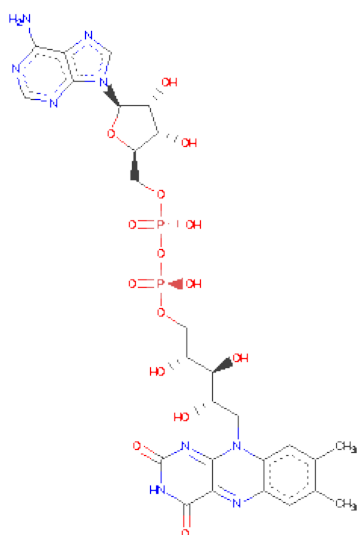
- Molecule 1 is a protein called PHENYLACETONE MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	530	4230	2698	729	794	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ALA	ASP	ENGINEERED MUTATION	UNP Q47PU3

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



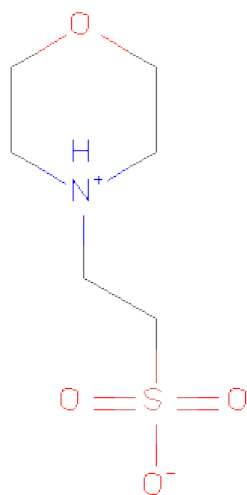
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

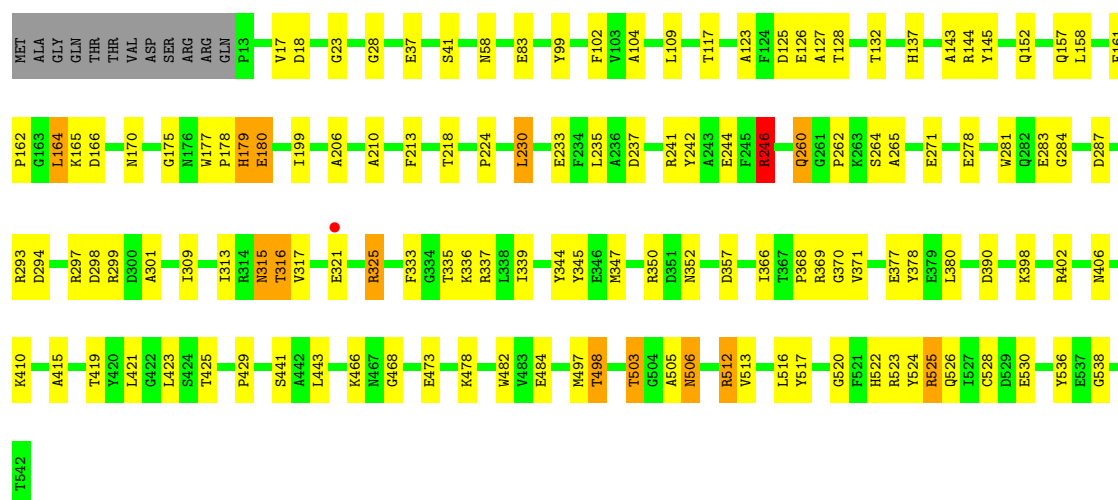
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	346	Total 346	O 346	0	0

### 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 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: PHENYLACETONE MONOOXYGENASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.50Å 107.50Å 107.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.83 – 2.20 35.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.83-2.20) 99.5 (35.19-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.193 , 0.252 0.195 , 0.254	Depositor DCC
$R_{free}$ test set	1842 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.0	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36539 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4689	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: NAP, FAD, MES

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	1.00	5/4343 (0.1%)	0.91	6/5908 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ARG	CG-CD	8.14	1.72	1.51
1	A	244	GLU	CG-CD	6.45	1.61	1.51
1	A	336	LYS	CE-NZ	5.88	1.63	1.49
1	A	415	ALA	CA-CB	5.57	1.64	1.52
1	A	283	GLU	CD-OE1	5.04	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	A	246	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	525	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	298	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	357	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	513	VAL	CB-CA-C	-5.47	101.01	111.40

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	4230	0	4086	132	0
2	A	53	0	31	2	0
3	A	48	0	25	3	0
4	A	12	0	12	2	0
5	A	346	0	0	74	0
All	All	4689	0	4154	135	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 16.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:ARG:HH11	1:A:246:ARG:CG	1.46	1.28
1:A:246:ARG:HD2	5:A:2038:HOH:O	1.19	1.26
1:A:315:ASN:CB	5:A:2213:HOH:O	1.85	1.24
1:A:315:ASN:HB3	5:A:2213:HOH:O	1.34	1.22
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.10	1.11
1:A:246:ARG:HH11	1:A:246:ARG:HG3	1.05	1.10
1:A:293:ARG:HD2	5:A:2200:HOH:O	1.52	1.09
1:A:293:ARG:HG2	5:A:2177:HOH:O	1.53	1.06
1:A:466:LYS:HA	5:A:2298:HOH:O	1.61	1.00
1:A:246:ARG:NH1	1:A:246:ARG:CG	2.21	0.99
1:A:419:THR:HG22	5:A:2278:HOH:O	1.65	0.96
1:A:293:ARG:CG	5:A:2177:HOH:O	2.08	0.95
1:A:512:ARG:HG2	5:A:2328:HOH:O	1.66	0.94
1:A:235:LEU:HB2	5:A:2153:HOH:O	1.68	0.93
1:A:218:THR:HB	5:A:2139:HOH:O	1.66	0.93
1:A:380:LEU:HD23	5:A:2124:HOH:O	1.67	0.92
1:A:325:ARG:HG2	1:A:325:ARG:NH1	1.80	0.90
1:A:368:PRO:HA	5:A:2106:HOH:O	1.72	0.90
1:A:260:GLN:HG2	5:A:2173:HOH:O	1.72	0.88
1:A:335:THR:OG1	1:A:498:THR:HG21	1.72	0.88
1:A:402:ARG:HG3	5:A:2268:HOH:O	1.73	0.87
1:A:425:THR:HB	5:A:2278:HOH:O	1.73	0.87
1:A:443:LEU:O	4:A:702:MES:H81	1.78	0.83
1:A:325:ARG:NE	5:A:2218:HOH:O	2.03	0.83
1:A:179:HIS:HD2	5:A:2118:HOH:O	1.61	0.83
1:A:468:GLY:HA2	5:A:2297:HOH:O	1.78	0.81
1:A:506:ASN:HD22	1:A:506:ASN:H	1.28	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:ARG:HD3	5:A:2157:HOH:O	1.81	0.81
1:A:233:GLU:HA	5:A:2151:HOH:O	1.79	0.81
1:A:166:ASP:C	5:A:2106:HOH:O	2.20	0.80
1:A:315:ASN:HB2	5:A:2213:HOH:O	1.65	0.79
1:A:497:MET:HB2	5:A:2318:HOH:O	1.83	0.78
1:A:166:ASP:O	5:A:2106:HOH:O	2.01	0.78
1:A:246:ARG:NH1	1:A:246:ARG:HG3	1.91	0.77
1:A:316:THR:CG2	1:A:345:TYR:HB3	2.15	0.77
1:A:325:ARG:CG	1:A:325:ARG:HH11	1.96	0.77
1:A:512:ARG:HH11	1:A:512:ARG:HG2	1.51	0.76
1:A:368:PRO:CA	5:A:2106:HOH:O	2.30	0.75
1:A:278:GLU:OE1	5:A:2189:HOH:O	2.04	0.75
1:A:419:THR:HA	5:A:2278:HOH:O	1.86	0.74
1:A:246:ARG:NH1	1:A:246:ARG:HG2	2.03	0.73
1:A:206:ALA:O	1:A:350:ARG:NH2	2.21	0.73
1:A:506:ASN:HB2	5:A:2259:HOH:O	1.90	0.71
1:A:316:THR:HG21	1:A:345:TYR:HB3	1.72	0.71
1:A:262:PRO:O	5:A:2175:HOH:O	2.09	0.70
1:A:316:THR:CG2	1:A:317:VAL:HG23	2.22	0.69
1:A:126:GLU:HG2	5:A:2084:HOH:O	1.92	0.69
1:A:127:ALA:HB3	5:A:2082:HOH:O	1.93	0.69
1:A:271:GLU:OE1	5:A:2185:HOH:O	2.13	0.66
1:A:299:ARG:HD3	5:A:2204:HOH:O	1.95	0.66
1:A:237:ASP:HB3	5:A:2154:HOH:O	1.95	0.65
1:A:213:PHE:CD2	5:A:2124:HOH:O	2.49	0.64
1:A:402:ARG:HD2	1:A:406:ASN:ND2	2.13	0.63
1:A:123:ALA:HB2	5:A:2079:HOH:O	1.99	0.63
1:A:530:GLU:HB3	5:A:2344:HOH:O	1.99	0.62
1:A:180:GLU:HB3	5:A:2119:HOH:O	2.00	0.61
1:A:293:ARG:HG3	5:A:2177:HOH:O	1.86	0.61
1:A:316:THR:HG22	1:A:317:VAL:HG23	1.81	0.61
1:A:83:GLU:HB3	5:A:2053:HOH:O	2.01	0.59
1:A:380:LEU:CD2	5:A:2124:HOH:O	2.35	0.59
1:A:287:ASP:OD2	5:A:2197:HOH:O	2.17	0.58
1:A:316:THR:HG23	1:A:345:TYR:HB3	1.83	0.58
1:A:370:GLY:HA3	1:A:378:TYR:O	2.04	0.57
2:A:700:FAD:HM73	3:A:701:NAP:C5N	2.35	0.57
1:A:512:ARG:HH11	1:A:512:ARG:CG	2.18	0.55
1:A:137:HIS:CD2	5:A:2073:HOH:O	2.59	0.55
1:A:520:GLY:HA2	4:A:702:MES:H62	1.88	0.55
1:A:117:THR:HA	5:A:2073:HOH:O	2.07	0.54
1:A:441:SER:HB3	1:A:516:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:316:THR:HG23	1:A:317:VAL:HG23	1.89	0.54
1:A:137:HIS:CG	5:A:2073:HOH:O	2.61	0.53
1:A:512:ARG:HB3	5:A:2327:HOH:O	2.08	0.53
1:A:213:PHE:CE2	5:A:2124:HOH:O	2.62	0.52
3:A:701:NAP:H2A	5:A:2246:HOH:O	2.08	0.52
1:A:265:ALA:HB3	1:A:301:ALA:HB1	1.92	0.52
1:A:157:GLN:HE21	1:A:390:ASP:HB2	1.74	0.52
1:A:517:TYR:CE2	1:A:524:TYR:HB2	2.45	0.51
1:A:264:SER:HA	5:A:2177:HOH:O	2.10	0.51
1:A:497:MET:HE1	5:A:2206:HOH:O	2.10	0.51
1:A:144:ARG:HG2	1:A:145:TYR:CE2	2.45	0.51
1:A:512:ARG:NH1	5:A:2328:HOH:O	2.38	0.50
1:A:128:THR:HA	5:A:2085:HOH:O	2.11	0.49
1:A:299:ARG:NH1	5:A:2205:HOH:O	2.44	0.49
1:A:506:ASN:H	1:A:506:ASN:ND2	2.04	0.49
1:A:170:ASN:HA	5:A:2108:HOH:O	2.11	0.49
1:A:366:ILE:HD12	1:A:371:VAL:HG22	1.94	0.49
3:A:701:NAP:C2A	5:A:2246:HOH:O	2.61	0.48
1:A:419:THR:CG2	5:A:2278:HOH:O	2.42	0.48
1:A:429:PRO:HB3	1:A:473:GLU:HB2	1.94	0.48
1:A:246:ARG:CD	5:A:2038:HOH:O	2.05	0.48
1:A:503:THR:HG22	1:A:505:ALA:HB2	1.96	0.48
1:A:152:GLN:HE22	2:A:700:FAD:H5'2	1.77	0.48
1:A:233:GLU:CA	5:A:2151:HOH:O	2.49	0.47
1:A:297:ARG:NH2	5:A:2203:HOH:O	2.46	0.47
1:A:309:ILE:HD13	1:A:333:PHE:CE1	2.50	0.47
1:A:164:LEU:HB2	5:A:2104:HOH:O	2.15	0.47
1:A:523:ARG:HA	1:A:526:GLN:HE21	1.79	0.47
1:A:525:ARG:HD2	5:A:2340:HOH:O	2.15	0.47
1:A:421:LEU:HA	1:A:482:TRP:CE2	2.51	0.46
1:A:58:ASN:ND2	1:A:175:GLY:HA2	2.30	0.46
1:A:144:ARG:CG	1:A:145:TYR:CE2	2.98	0.46
1:A:524:TYR:CE2	1:A:528:CYS:SG	3.08	0.46
1:A:18:ASP:HB2	1:A:41:SER:O	2.16	0.46
1:A:313:ILE:O	1:A:316:THR:HB	2.15	0.46
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.73	0.45
1:A:125:ASP:CG	5:A:2081:HOH:O	2.55	0.44
1:A:127:ALA:HB3	5:A:2081:HOH:O	2.17	0.44
1:A:177:TRP:CG	1:A:178:PRO:HD2	2.52	0.44
1:A:421:LEU:C	1:A:423:LEU:H	2.21	0.44
1:A:162:PRO:HA	5:A:2104:HOH:O	2.18	0.43
1:A:506:ASN:HD22	1:A:506:ASN:N	2.05	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:LEU:HD22	5:A:2060:HOH:O	2.18	0.43
1:A:517:TYR:OH	1:A:523:ARG:HG2	2.19	0.43
1:A:235:LEU:CB	5:A:2153:HOH:O	2.46	0.43
1:A:316:THR:HG21	1:A:345:TYR:CB	2.47	0.43
1:A:23:GLY:O	1:A:28:GLY:HA3	2.19	0.43
1:A:17:VAL:O	1:A:143:ALA:HA	2.19	0.42
1:A:419:THR:CA	5:A:2278:HOH:O	2.54	0.42
1:A:104:ALA:HA	1:A:109:LEU:HD12	2.02	0.42
1:A:166:ASP:HB3	5:A:2106:HOH:O	2.19	0.42
1:A:177:TRP:CD1	1:A:178:PRO:HD2	2.55	0.42
1:A:344:TYR:O	1:A:347:MET:HB3	2.19	0.42
1:A:161:PHE:HB2	1:A:162:PRO:HD2	2.01	0.42
1:A:235:LEU:CD1	5:A:2153:HOH:O	2.68	0.41
1:A:199:ILE:HD12	1:A:339:ILE:HD13	2.02	0.41
1:A:224:PRO:HD3	1:A:281:TRP:CH2	2.56	0.41
1:A:478:LYS:HG3	1:A:538:GLY:HA2	2.02	0.41
1:A:127:ALA:N	5:A:2081:HOH:O	2.19	0.41
1:A:99:TYR:O	1:A:102:PHE:HB3	2.21	0.41
1:A:506:ASN:ND2	5:A:2263:HOH:O	2.24	0.40
1:A:503:THR:CG2	1:A:505:ALA:HB2	2.51	0.40
1:A:210:ALA:O	1:A:352:ASN:HB2	2.21	0.40
1:A:284:GLY:HA2	5:A:2144:HOH:O	2.19	0.40
1:A:58:ASN:ND2	5:A:2019:HOH:O	2.55	0.40
1:A:294:ASP:N	1:A:294:ASP:OD1	2.55	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	528/542 (97%)	510 (97%)	17 (3%)	1 (0%)	56 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	TYR

### 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	442/452 (98%)	416 (94%)	26 (6%)	28	30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	132	THR
1	A	158	LEU
1	A	164	LEU
1	A	165	LYS
1	A	179	HIS
1	A	180	GLU
1	A	230	LEU
1	A	242	TYR
1	A	246	ARG
1	A	260	GLN
1	A	315	ASN
1	A	316	THR
1	A	321	GLU
1	A	325	ARG
1	A	337	ARG
1	A	369	ARG
1	A	377	GLU
1	A	398	LYS
1	A	410	LYS
1	A	484	GLU
1	A	498	THR
1	A	503	THR
1	A	506	ASN
1	A	512	ARG
1	A	522	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	129	ASN
1	A	152	GLN
1	A	157	GLN
1	A	406	ASN
1	A	506	ASN
1	A	526	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

3 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	700	-	58,58,58	1.29	7 (12%)	85,89,89	1.73	10 (11%)
3	NAP	A	701	-	52,52,52	1.46	10 (19%)	80,80,80	1.91	18 (22%)
4	MES	A	702	-	12,12,12	2.12	1 (8%)	16,16,16	3.03	8 (50%)

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	700	-	-	0/34/50/50	0/1/6/6
3	NAP	A	701	-	-	0/35/67/67	0/3/5/5
4	MES	A	702	-	-	0/6/14/14	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	MES	C8-S	-6.71	1.66	1.78
2	A	700	FAD	C2A-N3A	3.68	1.39	1.32
2	A	700	FAD	C1'-N10	3.30	1.51	1.48
2	A	700	FAD	C5X-N5	3.12	1.40	1.35
3	A	701	NAP	P2B-O1X	3.09	1.61	1.51
3	A	701	NAP	C4A-N3A	-3.01	1.31	1.35
3	A	701	NAP	C2D-C1D	2.88	1.57	1.53
3	A	701	NAP	C2B-C1B	2.87	1.57	1.52
3	A	701	NAP	PN-O1N	2.80	1.55	1.48
2	A	700	FAD	C2A-N1A	2.75	1.39	1.33
3	A	701	NAP	O4D-C1D	2.48	1.45	1.41
3	A	701	NAP	P2B-O2B	2.48	1.67	1.59
2	A	700	FAD	C10-N1	2.40	1.40	1.35
2	A	700	FAD	PA-O3P	2.39	1.64	1.59
2	A	700	FAD	C4-C4X	-2.32	1.37	1.41
3	A	701	NAP	P2B-O3X	2.21	1.62	1.54
3	A	701	NAP	C4N-C3N	2.19	1.43	1.39
3	A	701	NAP	PA-O3	2.10	1.63	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	FAD	N3A-C2A-N1A	-10.96	119.54	128.71
3	A	701	NAP	C3N-C7N-N7N	6.62	125.31	117.77
4	A	702	MES	C8-C7-N4	-6.42	101.46	112.44
4	A	702	MES	C5-N4-C3	5.91	121.47	109.75
3	A	701	NAP	N3A-C2A-N1A	-5.71	123.94	128.71
3	A	701	NAP	N3A-C4A-N9A	4.64	133.81	125.43
2	A	700	FAD	C5X-C9A-N10	4.14	120.88	116.80
3	A	701	NAP	O7N-C7N-N7N	-4.02	116.78	122.59
4	A	702	MES	O1-C6-C5	-3.70	106.93	111.34
3	A	701	NAP	C2D-C1D-N1N	-3.59	107.78	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAP	O2N-PN-O3	-3.59	99.12	108.79
3	A	701	NAP	O2X-P2B-O1X	3.47	121.78	110.44
4	A	702	MES	C2-C3-N4	-3.44	105.54	109.96
3	A	701	NAP	C3B-C2B-C1B	-3.36	96.19	102.73
2	A	700	FAD	C9A-N10-C10	-3.25	118.57	121.77
3	A	701	NAP	O3X-P2B-O1X	-3.15	100.14	110.44
4	A	702	MES	O1-C2-C3	-3.12	107.62	111.34
3	A	701	NAP	C2B-C1B-N9A	-3.12	101.91	113.74
3	A	701	NAP	C4A-C5A-N7A	-3.10	106.87	109.52
4	A	702	MES	C7-N4-C3	2.98	119.45	111.66
4	A	702	MES	O3S-S-C8	2.97	113.66	105.99
2	A	700	FAD	N3A-C4A-N9A	2.88	130.63	125.43
2	A	700	FAD	C1'-N10-C9A	2.82	121.62	118.87
3	A	701	NAP	O3-PN-O5D	2.79	112.53	101.36
4	A	702	MES	C7-N4-C5	2.78	118.93	111.66
3	A	701	NAP	C5A-C4A-N3A	-2.72	119.78	125.70
2	A	700	FAD	C1B-N9A-C4A	-2.63	122.10	126.64
2	A	700	FAD	C2'-C1'-N10	2.50	115.77	112.45
3	A	701	NAP	PN-O3-PA	-2.48	122.29	132.95
2	A	700	FAD	O2'-C2'-C1'	-2.43	103.69	109.71
2	A	700	FAD	C3B-C2B-C1B	2.31	104.52	100.91
3	A	701	NAP	O2X-P2B-O2B	2.28	113.67	107.09
2	A	700	FAD	C8A-N9A-C1B	2.23	130.78	126.38
3	A	701	NAP	O5B-C5B-C4B	-2.13	101.11	108.94
3	A	701	NAP	P2B-O2B-C2B	-2.12	117.48	121.96
3	A	701	NAP	C2A-N3A-C4A	2.04	119.82	114.01

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	530/542 (97%)	-0.45	1 (0%) 93 94	19, 33, 48, 60	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	GLU	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 ⓘ

There are no carbohydrates in this entry.

### 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
4	MES	A	702	12/12	0.44	7.95	21,28,34,35	12
3	NAP	A	701	48/48	0.12	-0.06	16,27,35,37	0
2	FAD	A	700	53/53	0.10	-0.07	17,24,33,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.