



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4AP3  
Title : Oxidized steroid monooxygenase bound to NADP  
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Deposited on : 2012-03-30  
Resolution : 2.39 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.

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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 : 1.7 (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

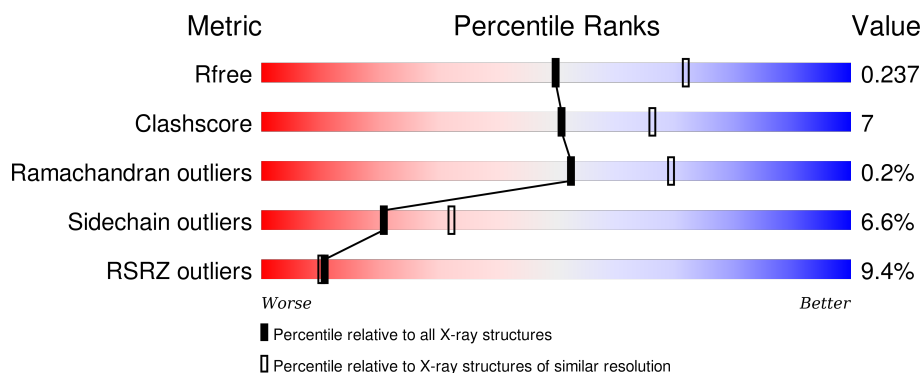
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

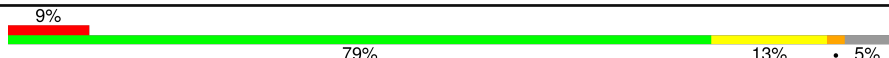
The reported resolution of this entry is 2.39 Å.

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	549	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4214 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 STEROID MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	2	0
			3987	2529	690	761	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	LEU	THR	ENGINEERED MUTATION	UNP O50641

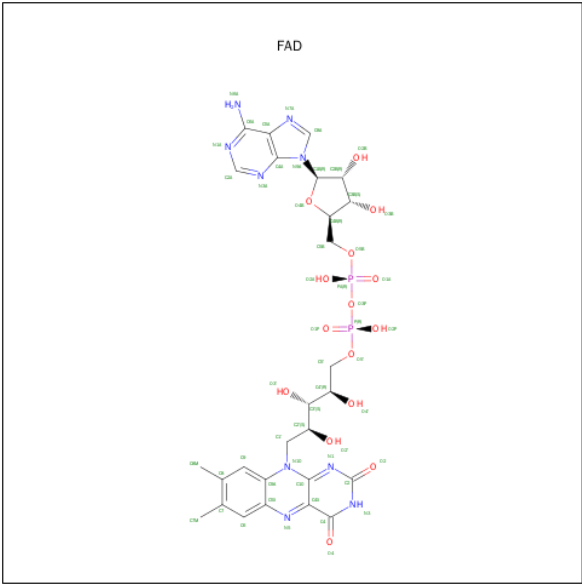
- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

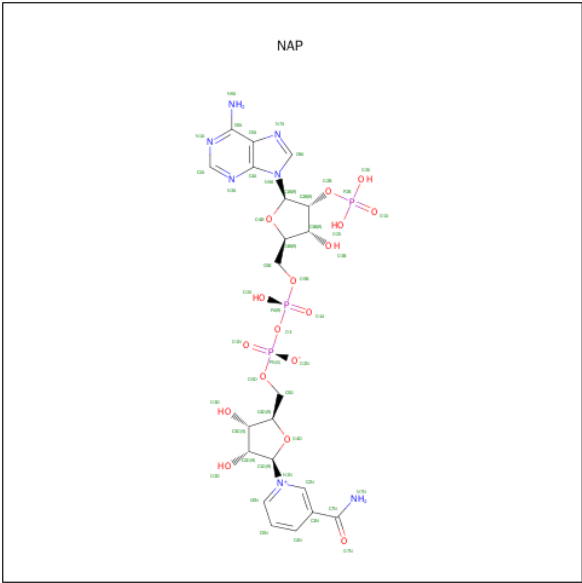
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

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
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			18	6	2	8	2		

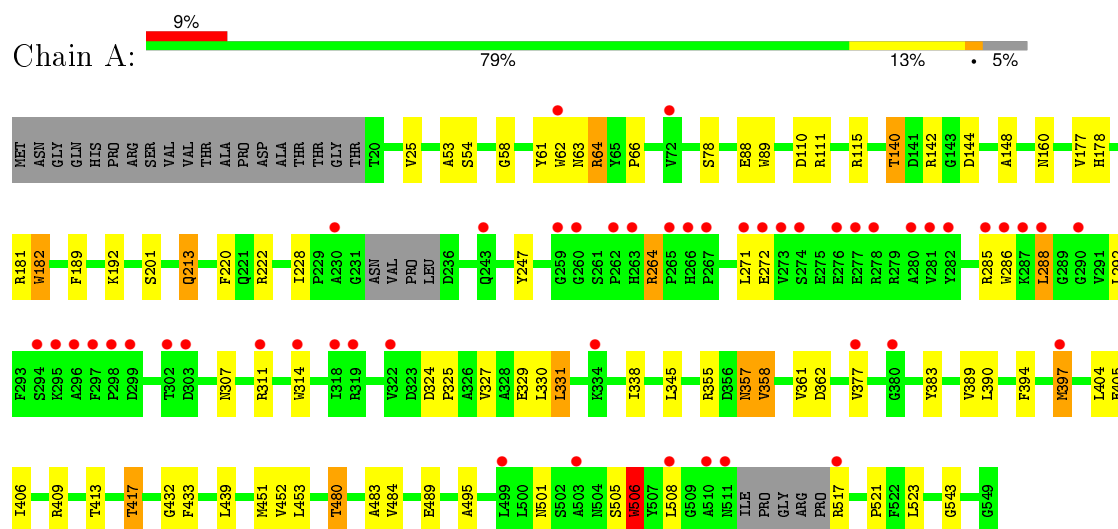
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total 146	O 146	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: STEROID MONOOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.75Å 81.75Å 228.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.44 – 2.39 66.44 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.44-2.39) 99.3 (66.44-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, $R_{free}$	0.207 , 0.239 0.205 , 0.237	Depositor DCC
$R_{free}$ test set	1577 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31316 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, SO4, 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	0.55	5/4090 (0.1%)	0.61	0/5573

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	TRP	CD2-CE2	5.25	1.47	1.41
1	A	286	TRP	CD2-CE2	5.24	1.47	1.41
1	A	506	TRP	CD2-CE2	5.07	1.47	1.41
1	A	182	TRP	CD2-CE2	5.04	1.47	1.41
1	A	314	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3987	0	3772	54	0
2	A	10	0	0	0	0
3	A	53	0	31	3	0
4	A	18	0	6	2	0
5	A	146	0	0	8	0
All	All	4214	0	3809	54	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 7.

All (54) 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:110:ASP:OD1	1:A:115:ARG:NH2	2.16	0.78
1:A:140:THR:CG2	1:A:142:ARG:H	2.00	0.74
1:A:480:THR:HG22	1:A:483:ALA:H	1.54	0.72
1:A:355:ARG:HE	1:A:357:ASN:HD21	1.40	0.70
1:A:220:PHE:CE1	5:A:2110:HOH:O	2.42	0.70
1:A:307:ASN:HD21	1:A:338:ILE:H	1.41	0.68
1:A:383:TYR:CE1	5:A:2110:HOH:O	2.47	0.68
1:A:140:THR:HG22	1:A:142:ARG:H	1.59	0.67
1:A:285:ARG:HD3	1:A:288:LEU:HD11	1.77	0.67
1:A:383:TYR:CZ	5:A:2110:HOH:O	2.47	0.66
1:A:361:VAL:HG11	5:A:2110:HOH:O	1.98	0.63
1:A:220:PHE:HE1	5:A:2110:HOH:O	1.79	0.62
1:A:25:VAL:HG23	1:A:148:ALA:HB2	1.80	0.61
1:A:181:ARG:NH1	5:A:2076:HOH:O	2.33	0.61
1:A:88[A]:GLU:CD	1:A:111:ARG:HH12	2.04	0.59
1:A:64:ARG:NH1	5:A:2025:HOH:O	2.37	0.57
1:A:201:SER:OG	4:A:1553:NAP:H6N	2.04	0.57
1:A:361:VAL:HG21	5:A:2110:HOH:O	2.05	0.56
1:A:140:THR:HG21	1:A:144:ASP:OD2	2.05	0.56
1:A:62[A]:TRP:HZ3	1:A:160:ASN:HD21	1.52	0.56
1:A:140:THR:HB	1:A:144:ASP:HB2	1.87	0.55
1:A:63:ASN:HD21	1:A:394:PHE:HZ	1.53	0.54
1:A:140:THR:HG23	1:A:142:ARG:H	1.73	0.54
1:A:53:ALA:HB2	1:A:62[B]:TRP:CZ2	2.44	0.53
1:A:177:VAL:CG2	1:A:389:VAL:HG22	2.40	0.52
1:A:355:ARG:HB2	1:A:358:VAL:HG13	1.92	0.51
1:A:140:THR:HG22	1:A:142:ARG:N	2.26	0.50
1:A:480:THR:HB	1:A:543:GLY:O	2.12	0.50
1:A:495:ALA:HA	1:A:523:LEU:HD23	1.94	0.50
1:A:54:SER:HB2	1:A:61:TYR:OH	2.12	0.50
1:A:330:LEU:HD21	1:A:362:ASP:HB2	1.95	0.48
1:A:397:MET:CE	1:A:521:PRO:HG3	2.43	0.47
1:A:404:LEU:HD11	3:A:1552:FAD:N6A	2.30	0.46
1:A:417:THR:HG21	1:A:433:PHE:HE1	1.80	0.46
1:A:285:ARG:HA	1:A:288:LEU:HD12	1.96	0.46
1:A:264:ARG:HH21	1:A:285:ARG:HH21	1.64	0.46
1:A:357:ASN:H	1:A:357:ASN:HD22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD22	1:A:292:LEU:HD13	1.99	0.45
1:A:404:LEU:HD11	3:A:1552:FAD:H61A	1.82	0.45
1:A:178:HIS:CE1	1:A:390:LEU:HD12	2.51	0.45
1:A:58:GLY:HA2	3:A:1552:FAD:O3B	2.17	0.44
1:A:406:ILE:O	1:A:413:THR:HA	2.18	0.44
1:A:409:ARG:HG3	1:A:432:GLY:HA2	2.01	0.42
1:A:505:SER:HB3	1:A:508:LEU:HG	2.00	0.42
1:A:417:THR:HG21	1:A:433:PHE:CE1	2.55	0.41
1:A:324:ASP:HA	1:A:325:PRO:HD2	1.94	0.41
1:A:506:TRP:CH2	4:A:1553:NAP:H2N	2.56	0.41
1:A:189:PHE:HB2	1:A:213:GLN:CG	2.51	0.41
1:A:271:LEU:HD12	1:A:272:GLU:HG3	2.02	0.41
1:A:66:PRO:HD3	1:A:182:TRP:CE2	2.56	0.41
1:A:53:ALA:HB2	1:A:62[B]:TRP:CE2	2.56	0.40
1:A:501:ASN:ND2	1:A:508:LEU:HD21	2.36	0.40
1:A:78:SER:C	1:A:452:VAL:HG11	2.42	0.40
1:A:327:VAL:HG12	1:A:331:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

## 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	517/549 (94%)	502 (97%)	14 (3%)	1 (0%)	52	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	MET

### 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	395/436 (91%)	369 (93%)	26 (7%)	21	32

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

Mol	Chain	Res	Type
1	A	64	ARG
1	A	140	THR
1	A	192	LYS
1	A	213	GLN
1	A	222	ARG
1	A	228	ILE
1	A	247	TYR
1	A	264	ARG
1	A	288	LEU
1	A	311	ARG
1	A	329	GLU
1	A	331	LEU
1	A	345	LEU
1	A	357	ASN
1	A	358	VAL
1	A	377	VAL
1	A	405	GLU
1	A	417	THR
1	A	439	LEU
1	A	451	MET
1	A	453	LEU
1	A	480	THR
1	A	484	VAL
1	A	489	GLU
1	A	506	TRP
1	A	517	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	98	GLN
1	A	178	HIS
1	A	205	GLN
1	A	216	GLN
1	A	221	GLN
1	A	225	ASN
1	A	307	ASN
1	A	357	ASN
1	A	382	HIS
1	A	501	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	SO4	A	1550	-	4,4,4	0.36	0	6,6,6	0.24	0
2	SO4	A	1551	-	4,4,4	0.44	0	6,6,6	0.17	0
3	FAD	A	1552	-	48,58,58	1.39	7 (14%)	54,89,89	2.13	10 (18%)
4	NAP	A	1553	-	16,17,52	1.06	1 (6%)	22,24,80	1.16	2 (9%)

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	SO4	A	1550	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1551	-	-	0/0/0/0	0/0/0/0
3	FAD	A	1552	-	-	0/30/50/50	0/6/6/6
4	NAP	A	1553	-	-	0/10/10/67	0/1/1/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1552	FAD	C10-N10	2.27	1.41	1.39
3	A	1552	FAD	C5A-C4A	2.73	1.46	1.40
3	A	1552	FAD	C9A-N10	2.92	1.42	1.38
3	A	1552	FAD	C8-C7	3.13	1.49	1.41
4	A	1553	NAP	PA-O1A	3.24	1.61	1.51
3	A	1552	FAD	C4-C4X	3.46	1.48	1.41
3	A	1552	FAD	C9A-C5X	3.57	1.49	1.42
3	A	1552	FAD	C4X-C10	3.99	1.48	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1552	FAD	N3A-C2A-N1A	-7.55	123.11	128.89
3	A	1552	FAD	C4-C4X-C10	-5.32	116.54	119.94
3	A	1552	FAD	C4X-C4-N3	-3.47	118.84	123.59
3	A	1552	FAD	C4A-C5A-N7A	-3.17	106.56	109.48
3	A	1552	FAD	O2'-C2'-C1'	-2.05	104.90	109.94
3	A	1552	FAD	C4-C4X-N5	2.18	121.36	118.72
4	A	1553	NAP	C6N-N1N-C2N	2.22	120.94	116.84
3	A	1552	FAD	C5X-C9A-N10	2.79	119.74	117.62
3	A	1552	FAD	C4X-N5-C5X	3.14	120.38	116.76
4	A	1553	NAP	O5B-PA-O2A	3.26	119.81	107.38
3	A	1552	FAD	C1'-N10-C9A	4.05	123.41	118.86
3	A	1552	FAD	C4-N3-C2	7.89	122.07	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1552	FAD	3	0
4	A	1553	NAP	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 ⓘ

### 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	521/549 (94%)	0.76	49 (9%) 11 10	28, 50, 109, 165	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	PRO	6.9
1	A	267	PRO	6.3
1	A	288	LEU	5.7
1	A	503	ALA	5.7
1	A	273	VAL	5.1
1	A	271	LEU	5.0
1	A	510	ALA	4.5
1	A	298	PRO	4.4
1	A	297	PHE	3.9
1	A	266	HIS	3.7
1	A	511	ASN	3.5
1	A	259	GLY	3.4
1	A	280	ALA	3.4
1	A	274	SER	3.2
1	A	499	LEU	3.2
1	A	281	VAL	3.2
1	A	285	ARG	3.1
1	A	508	LEU	3.1
1	A	299	ASP	3.1
1	A	290	GLY	3.0
1	A	243	GLN	3.0
1	A	263	HIS	3.0
1	A	334	LYS	2.9
1	A	277	GLU	2.9
1	A	62[A]	TRP	2.9
1	A	296	ALA	2.8
1	A	397	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	2.7
1	A	260	GLY	2.6
1	A	318	ILE	2.6
1	A	319	ARG	2.6
1	A	278	ARG	2.6
1	A	295	LYS	2.5
1	A	276	GLU	2.5
1	A	282	TYR	2.5
1	A	287	LYS	2.4
1	A	314	TRP	2.4
1	A	517	ARG	2.4
1	A	262	PRO	2.3
1	A	380	GLY	2.2
1	A	302	THR	2.2
1	A	303	ASP	2.2
1	A	72	VAL	2.2
1	A	311	ARG	2.2
1	A	286	TRP	2.1
1	A	230	ALA	2.1
1	A	322	VAL	2.1
1	A	294	SER	2.1
1	A	377	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
4	NAP	A	1553	18/48	0.88	0.23	1.18	62,71,79,81	4
3	FAD	A	1552	53/53	0.97	0.16	-0.33	25,32,40,43	0
2	SO4	A	1550	5/5	0.97	0.16	-	51,52,57,58	0
2	SO4	A	1551	5/5	0.86	0.26	-	95,103,106,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.