wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1J9Z
Title	:	CYPOR-W677G
Authors	:	Hubbard, P.A.; Shen, A.L.; Paschke, R.; Kasper, C.B.; Kim, J.J.
Deposited on	:	2001-05-29
Resolution	:	2.70 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.70 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.
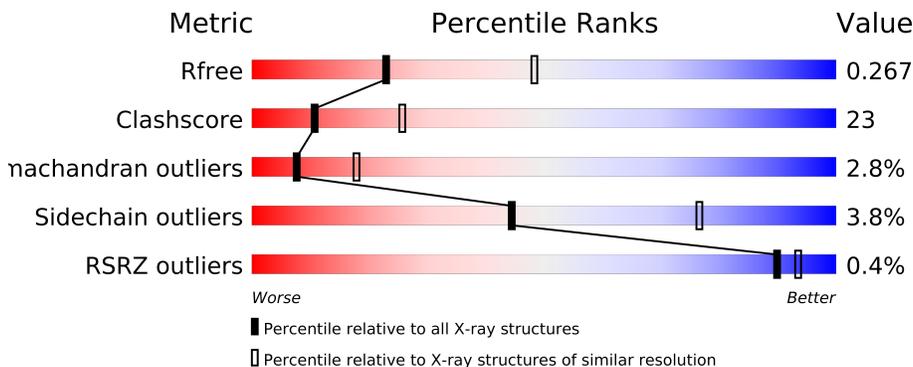
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	622	
1	B	622	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10265 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 NADPH-Cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4901	3099	844	935	23			
1	B	611	Total	C	N	O	S	0	0	0
			4890	3092	842	933	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	GLY	TRP	ENGINEERED	UNP P00388
B	677	GLY	TRP	ENGINEERED	UNP P00388

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
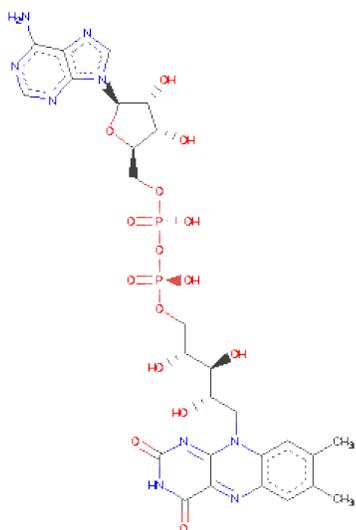
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
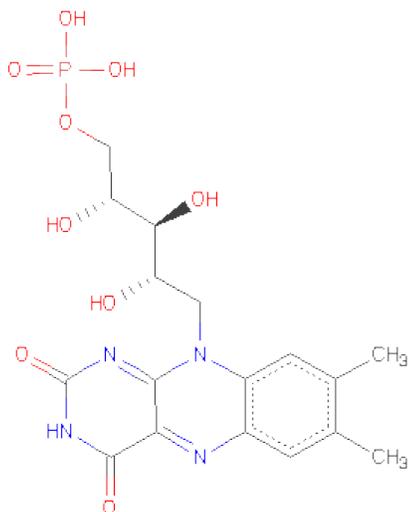
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
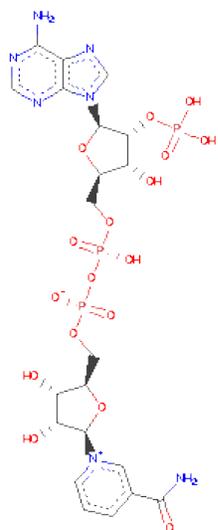
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	B	101	Total 101	O 101	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: NADPH-Cytochrome P450 reductase

Chain A:

- Molecule 1: NADPH-Cytochrome P450 reductase

Chain B:

F282 N289 L292 N293 Q294 E297 R298 H299 L300 M301 H302 L303 E304 S310 K311 I312 R313 A321 V322 Y323 P324 A329 N332 I337 L338 D341 V344 I345 M346 N349 N350 L351 D352 E353 H359 P360 F361 P362 C363 P364 T365 D376 N379 N384

V385 L386 Y387 E388 L389 A390 Q391 Y392 A393 E398 Q399 E400 H401 M405 A406 S409 K413 Y416 L417 S418 W419 V420 V421 E422 A423 L428 L431 Q432 S436 L437 R438 P439 P440 I441 D442 P449 A453 R454 Y455 Y456 S460 H470 I471 C472 A473 V474 A475

K481 R484 G488 T491 S492 W493 A500 GLY GLU ASN GLY G505 R506 F512 V513 R514 F518 R519 S524 T525 T526 P527 V528 P533 A538 E546 R547 A548 W549 L550 R551 E552 K555 E556 E559 L562 Y563 Y564 R568 E571 D572 Y573 L574 Y575

Q590 L591 N592 V593 Q599 A600 Y604 V605 Q606 R613 E614 H615 L616 W617 K618 L619 I620 G624 A625 H626 V629 C630 G631 D632 A633 R634 N635 M636 A637 K638 Q641 N642 Y645 D646 I647 V648 A649 E650 F651 M654 E655 H656 A659 V660 K664 K665 K669 G670 R671

L674 D675 V676 G677 S678

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.63Å 116.06Å 118.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.80 – 2.71	Depositor EDS
% Data completeness (in resolution range)	79.6 (30.00-2.70) 79.6 (29.80-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188 , 0.270 0.187 , 0.267	Depositor DCC
R_{free} test set	1535 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 7.3	EDS
Estimated twinning fraction	0.034 for -h,l,k	Xtriage
L-test for twinning	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Outliers	1 of 30972 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: FMN, NAP, 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	0.38	0/5016	0.61	0/6784
1	B	0.37	0/5004	0.61	0/6768
All	All	0.38	0/10020	0.61	0/13552

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	456	TYR	Sidechain

5.2 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 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	4901	0	4748	222	0
1	B	4890	0	4737	231	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	19	3	0
3	B	31	0	19	1	0
4	A	48	0	25	0	0
4	B	48	0	25	3	0
5	A	109	0	0	6	0
5	B	101	0	0	2	0
All	All	10265	0	9635	451	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 23.

The worst 5 of 451 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.30	1.14
1:B:527:PRO:HB2	1:B:625:ALA:HB2	1.33	1.09
1:B:78:ARG:HH22	1:B:352:ASP:HB2	1.26	1.00
1:B:163:LEU:HB2	1:B:196:GLY:HA3	1.44	0.96
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.27	0.96

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	609/622 (98%)	536 (88%)	61 (10%)	12 (2%)	11	28
1	B	607/622 (98%)	516 (85%)	69 (11%)	22 (4%)	5	11
All	All	1216/1244 (98%)	1052 (86%)	130 (11%)	34 (3%)	8	18

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLU
1	B	159	THR
1	B	160	ASP
1	B	202	GLU
1	B	234	GLU

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	523/530 (99%)	500 (96%)	23 (4%)	39	71
1	B	522/530 (98%)	505 (97%)	17 (3%)	50	81
All	All	1045/1060 (99%)	1005 (96%)	40 (4%)	44	76

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	572	ASP
1	A	672	TYR
1	B	573	TYR
1	A	613	ARG
1	B	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	B	79	ASN
1	B	599	GLN
1	A	553	GLN
1	A	590	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 ⓘ

6 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	750	-	58,58,58	2.50	24 (41%)	85,89,89	2.16	15 (17%)
3	FMN	A	751	-	33,33,33	2.20	12 (36%)	46,50,50	2.18	10 (21%)
4	NAP	A	752	-	52,52,52	3.49	21 (40%)	80,80,80	1.86	15 (18%)
2	FAD	B	850	-	58,58,58	2.69	23 (39%)	85,89,89	2.38	19 (22%)
3	FMN	B	851	-	33,33,33	2.44	15 (45%)	46,50,50	2.31	12 (26%)
4	NAP	B	852	-	52,52,52	3.45	19 (36%)	80,80,80	1.73	14 (17%)

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	750	-	-	0/34/50/50	0/1/6/6
3	FMN	A	751	-	-	0/18/18/18	0/0/3/3
4	NAP	A	752	-	-	0/35/67/67	0/3/5/5
2	FAD	B	850	-	-	0/34/50/50	0/1/6/6
3	FMN	B	851	-	-	0/18/18/18	0/0/3/3
4	NAP	B	852	-	-	0/35/67/67	0/3/5/5

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	752	NAP	C2N-N1N	13.02	1.52	1.35
4	B	852	NAP	C2N-N1N	12.83	1.51	1.35
4	B	852	NAP	C4N-C3N	10.48	1.57	1.39
4	A	752	NAP	C4N-C3N	9.98	1.56	1.39
4	A	752	NAP	C4A-N3A	9.51	1.50	1.35

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	850	FAD	C2'-C1'-N10	-13.11	95.06	112.45
2	A	750	FAD	C2'-C1'-N10	-9.87	99.36	112.45
3	A	751	FMN	C4A-C10-N10	-9.26	115.89	120.51
3	B	851	FMN	C4A-C10-N10	-8.93	116.05	120.51
2	B	850	FAD	C2-N1-C10	7.64	122.68	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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, 95th 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	613/622 (98%)	-0.57	0	100	100	16, 36, 57, 87	0
1	B	611/622 (98%)	-0.35	4 (0%)	84	89	16, 44, 92, 107	0
All	All	1224/1244 (98%)	-0.46	4 (0%)	90	95	16, 38, 85, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	3.1
1	B	178	TYR	2.6
1	B	136	CYS	2.5
1	B	240	SER	2.1

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, 95th 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^2)	Q<0.9
3	FMN	B	851	31/31	0.28	1.33	75,91,94,94	0
4	NAP	B	852	48/48	0.13	0.81	26,34,72,74	0
3	FMN	A	751	31/31	0.16	0.53	37,55,58,58	0
2	FAD	A	750	53/53	0.14	0.19	24,30,35,35	0
4	NAP	A	752	48/48	0.13	0.15	26,40,70,74	0
2	FAD	B	850	53/53	0.12	0.10	16,21,24,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.