



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:28 PM GMT

PDB ID : 4ZCC  
Title : Renalase in complex with NADH  
Authors : Silvaggi, N.R.; Moran, G.R.; Roman, J.V.  
Deposited on : 2015-04-15  
Resolution : 2.00 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

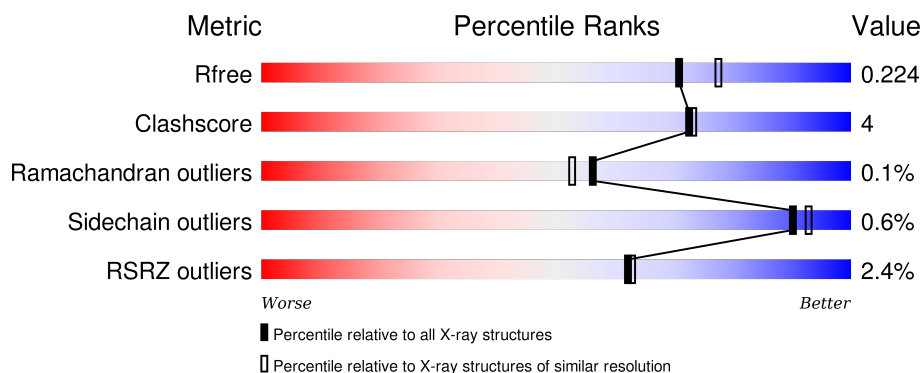
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	336	 2% 89% 6% 5%
1	B	336	 1% 88% 7% 5%
1	C	336	 4% 87% 7% . .
1	D	336	 1% 87% 11% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20810 atoms, of which 9759 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 Renalase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	H	N	O	S	0	0	0
			4828	1552	2365	449	450	12			
1	B	319	Total	C	H	N	O	S	0	0	0
			4811	1547	2357	447	448	12			
1	C	321	Total	C	H	N	O	S	0	2	0
			4861	1562	2383	451	453	12			
1	D	328	Total	C	H	N	O	S	0	0	0
			4938	1584	2418	460	464	12			

There are 36 discrepancies between the modelled and reference sequences:

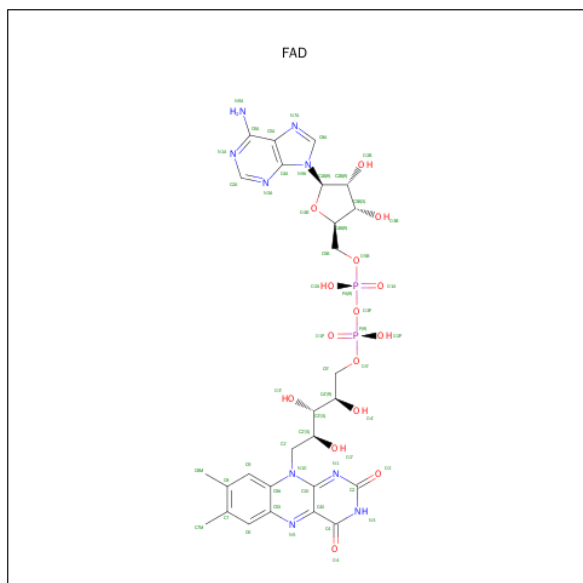
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	SER	GLY	engineered mutation	UNP Q48MT7
A	329	LEU	-	expression tag	UNP Q48MT7
A	330	GLU	-	expression tag	UNP Q48MT7
A	331	HIS	-	expression tag	UNP Q48MT7
A	332	HIS	-	expression tag	UNP Q48MT7
A	333	HIS	-	expression tag	UNP Q48MT7
A	334	HIS	-	expression tag	UNP Q48MT7
A	335	HIS	-	expression tag	UNP Q48MT7
A	336	HIS	-	expression tag	UNP Q48MT7
B	145	SER	GLY	engineered mutation	UNP Q48MT7
B	329	LEU	-	expression tag	UNP Q48MT7
B	330	GLU	-	expression tag	UNP Q48MT7
B	331	HIS	-	expression tag	UNP Q48MT7
B	332	HIS	-	expression tag	UNP Q48MT7
B	333	HIS	-	expression tag	UNP Q48MT7
B	334	HIS	-	expression tag	UNP Q48MT7
B	335	HIS	-	expression tag	UNP Q48MT7
B	336	HIS	-	expression tag	UNP Q48MT7
C	145	SER	GLY	engineered mutation	UNP Q48MT7
C	329	LEU	-	expression tag	UNP Q48MT7
C	330	GLU	-	expression tag	UNP Q48MT7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	HIS	-	expression tag	UNP Q48MT7
C	332	HIS	-	expression tag	UNP Q48MT7
C	333	HIS	-	expression tag	UNP Q48MT7
C	334	HIS	-	expression tag	UNP Q48MT7
C	335	HIS	-	expression tag	UNP Q48MT7
C	336	HIS	-	expression tag	UNP Q48MT7
D	145	SER	GLY	engineered mutation	UNP Q48MT7
D	329	LEU	-	expression tag	UNP Q48MT7
D	330	GLU	-	expression tag	UNP Q48MT7
D	331	HIS	-	expression tag	UNP Q48MT7
D	332	HIS	-	expression tag	UNP Q48MT7
D	333	HIS	-	expression tag	UNP Q48MT7
D	334	HIS	-	expression tag	UNP Q48MT7
D	335	HIS	-	expression tag	UNP Q48MT7
D	336	HIS	-	expression tag	UNP Q48MT7

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



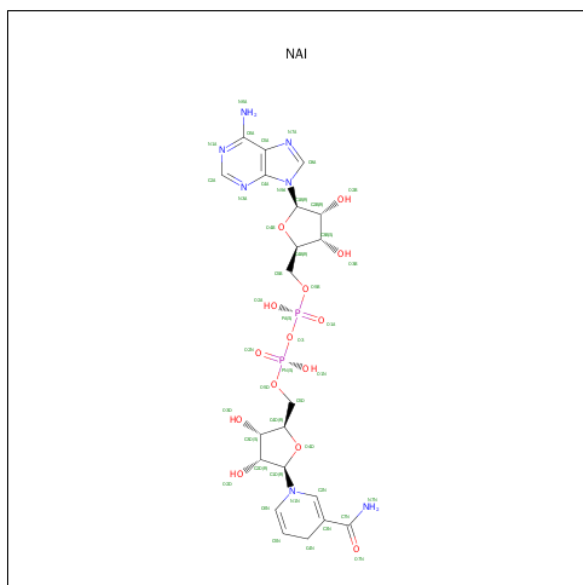
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

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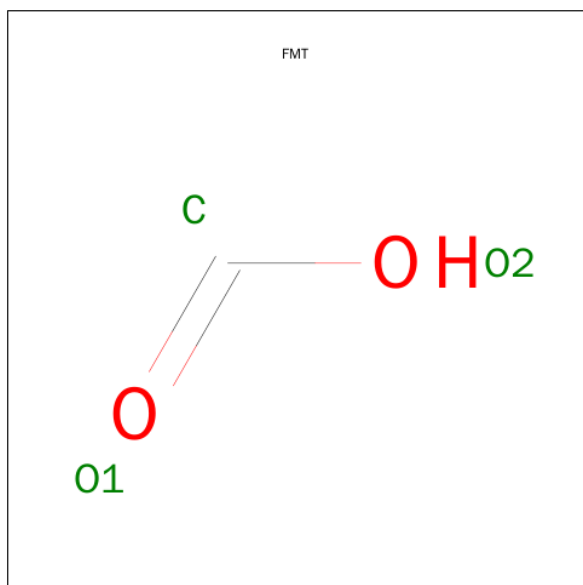
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	C	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	D	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			4	1	1	2		
4	B	1	Total	C	H	O	0	0
			4	1	1	2		
4	C	1	Total	C	H	O	0	0
			4	1	1	2		
4	D	1	Total	C	H	O	0	0
			4	1	1	2		

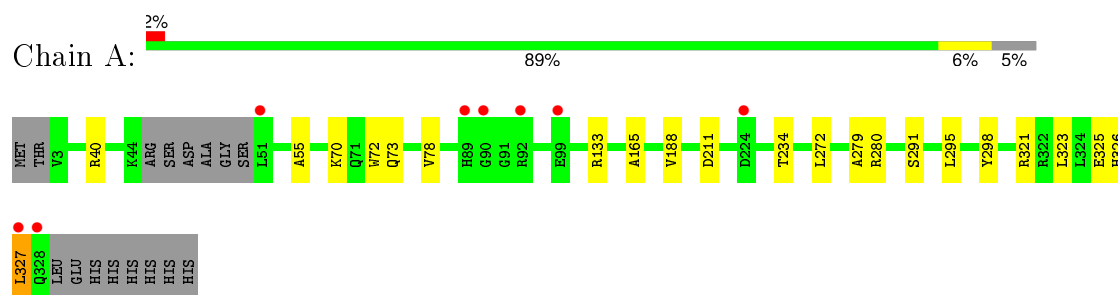
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	0
			198	198		
5	B	191	Total	O	0	0
			191	191		
5	C	167	Total	O	0	0
			167	167		
5	D	180	Total	O	0	0
			180	180		

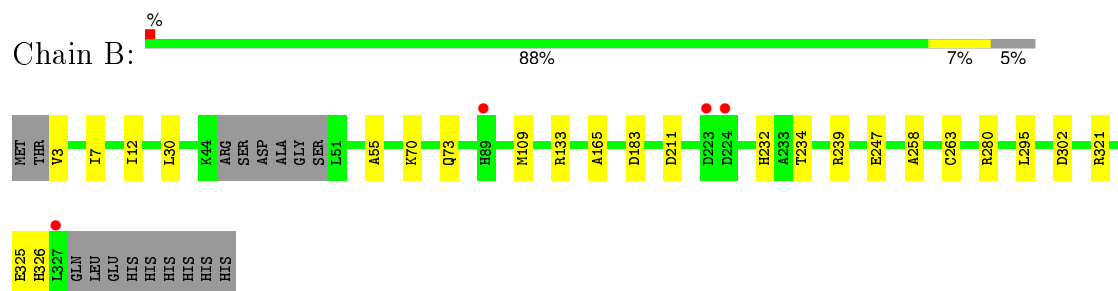
### 3 Residue-property plots [i](#)

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.

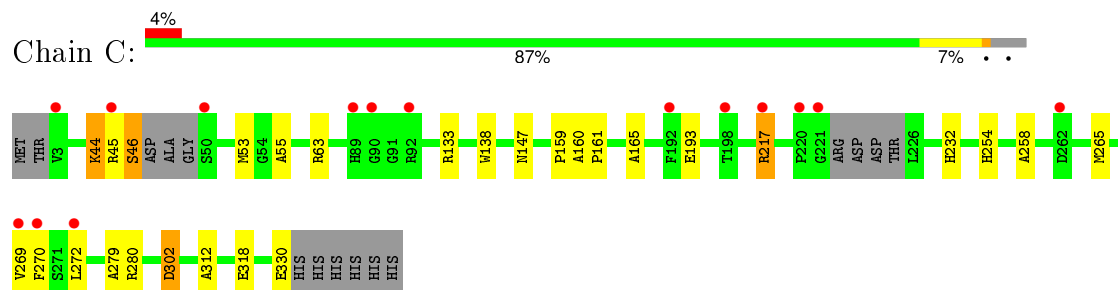
#### • Molecule 1: Renalase



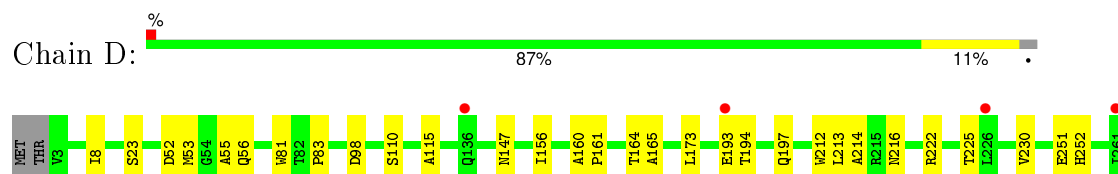
#### • Molecule 1: Renalase



#### • Molecule 1: Renalase



#### • Molecule 1: Renalase



Y269	F270	S271	L272	H276	A279	E310	E330	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.50Å 71.50Å 143.80Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	46.22 – 2.00 46.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.22-2.00) 88.7 (46.22-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1965)	Depositor
R, $R_{free}$	0.170 , 0.215 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	3000 reflections (4.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 83618 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.24 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8329e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: FMT, NAI, 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	0.69	0/2531	0.76	1/3446 (0.0%)
1	B	0.69	0/2522	0.74	1/3434 (0.0%)
1	C	0.64	0/2556	0.77	1/3477 (0.0%)
1	D	0.66	1/2589 (0.0%)	0.75	0/3525
All	All	0.67	1/10198 (0.0%)	0.75	3/13882 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	276	TRP	CB-CG	6.21	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	302	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	40	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	2463	2365	2378	19	0
1	B	2454	2357	2370	18	0
1	C	2478	2383	2388	22	1
1	D	2520	2418	2431	28	1
2	A	53	31	31	3	0
2	B	53	31	31	3	0
2	C	53	31	31	5	0
2	D	53	31	31	3	0
3	A	44	27	27	2	0
3	B	44	27	27	3	0
3	C	44	27	27	2	0
3	D	44	27	27	0	0
4	A	3	1	1	0	0
4	B	3	1	1	0	0
4	C	3	1	1	0	0
4	D	3	1	1	1	0
5	A	198	0	0	5	0
5	B	191	0	0	4	0
5	C	167	0	0	4	0
5	D	180	0	0	11	0
All	All	11051	9759	9803	85	1

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 (85) 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:B:3:VAL:N	5:B:501:HOH:O	1.85	1.06
1:D:147:ASN:ND2	5:D:501:HOH:O	1.92	1.01
1:B:239:ARG:NH1	5:B:502:HOH:O	2.01	0.91
1:B:280:ARG:HB3	3:B:402:NAI:H42N	1.63	0.80
1:D:23:SER:OG	5:D:503:HOH:O	2.00	0.79
1:B:247:GLU:OE1	5:B:503:HOH:O	2.03	0.77
1:D:310:GLU:OE2	5:D:505:HOH:O	2.08	0.71
1:D:52:ASP:O	1:D:56:GLN:NE2	2.20	0.70
1:D:147:ASN:ND2	5:D:502:HOH:O	1.97	0.70
1:A:326:HIS:ND1	5:A:504:HOH:O	2.28	0.67
1:C:46:SER:O	1:C:46:SER:OG	2.13	0.67
1:A:280:ARG:HB3	3:A:402:NAI:H42N	1.77	0.65
1:B:183:ASP:OD1	1:B:239:ARG:NH2	2.25	0.64
1:B:70:LYS:HD3	1:B:73:GLN:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ARG:NH2	1:B:325:GLU:OE2	2.36	0.58
1:A:280:ARG:HD3	3:A:402:NAI:H42N	1.85	0.57
1:B:326:HIS:ND1	5:B:505:HOH:O	2.32	0.57
1:D:194:THR:O	5:D:506:HOH:O	2.18	0.55
1:A:280:ARG:NH2	5:A:509:HOH:O	2.41	0.54
1:C:63:ARG:NE	5:C:508:HOH:O	2.41	0.53
1:A:291:SER:OG	5:A:502:HOH:O	2.18	0.53
1:B:258:ALA:O	1:D:252:HIS:HD2	1.93	0.51
1:D:193:GLU:HB2	1:D:269:VAL:HG11	1.93	0.51
1:C:53:MET:HB2	5:C:551:HOH:O	2.11	0.50
1:D:216:ASN:OD1	1:D:222:ARG:HG2	2.12	0.50
1:D:53:MET:HB2	5:D:579:HOH:O	2.11	0.50
1:D:8:ILE:HD12	1:D:156:ILE:CD1	2.43	0.49
1:C:254:HIS:CD2	1:C:265:MET:CE	2.95	0.49
1:D:279:ALA:HB1	2:D:401:FAD:HM83	1.96	0.48
1:B:165:ALA:HB2	1:C:165:ALA:HB2	1.95	0.48
1:A:70:LYS:HD3	1:A:73:GLN:OE1	2.14	0.48
1:A:211:ASP:HB3	1:A:234:THR:HG22	1.95	0.47
1:D:212:TRP:CZ2	1:D:214:ALA:HB2	2.50	0.47
1:C:280:ARG:NH2	5:C:510:HOH:O	2.45	0.47
1:D:115:ALA:HB3	5:D:614:HOH:O	2.14	0.46
1:D:55:ALA:HA	2:D:401:FAD:N5	2.30	0.46
1:C:55:ALA:HA	2:C:401:FAD:N5	2.30	0.46
1:D:147:ASN:HB2	5:D:502:HOH:O	2.15	0.46
1:D:164:THR:HG21	5:D:626:HOH:O	2.15	0.46
1:A:133:ARG:NH1	1:A:295:LEU:O	2.45	0.46
1:A:321:ARG:NH1	1:A:325:GLU:OE1	2.48	0.46
1:A:165:ALA:HB2	1:D:165:ALA:HB2	1.98	0.45
1:D:98:ASP:OD1	5:D:507:HOH:O	2.21	0.45
1:D:160:ALA:HB3	1:D:161:PRO:HD3	1.99	0.44
1:B:55:ALA:O	1:B:109:MET:HG3	2.17	0.44
1:C:302:ASP:HB3	1:C:312:ALA:HB2	2.00	0.44
2:A:401:FAD:H2B	5:A:520:HOH:O	2.18	0.44
1:B:280:ARG:CB	3:B:402:NAI:H42N	2.41	0.44
1:C:280:ARG:HD3	3:C:402:NAI:C5N	2.48	0.44
1:D:81:TRP:CG	1:D:83:PRO:HD3	2.51	0.44
1:A:55:ALA:HA	2:A:401:FAD:N5	2.33	0.44
1:B:55:ALA:HA	2:B:401:FAD:N5	2.33	0.44
1:B:7:ILE:HB	1:B:30:LEU:HD23	2.00	0.43
1:C:232:HIS:CE1	2:C:401:FAD:H6	2.53	0.43
1:A:165:ALA:HB2	5:A:512:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:PHE:CZ	1:D:272:LEU:HG	2.54	0.43
1:C:44:LYS:HE3	1:C:45:ARG:O	2.18	0.43
1:A:323:LEU:HD23	1:A:327:LEU:HG	1.99	0.43
1:B:133:ARG:NH1	1:B:295:LEU:O	2.49	0.43
1:C:160:ALA:HB3	1:C:161:PRO:HD3	2.01	0.43
1:D:110:SER:HB2	4:D:403:FMT:H	2.01	0.43
1:D:197:GLN:CB	5:D:510:HOH:O	2.67	0.42
1:C:270:PHE:CZ	1:C:272:LEU:HG	2.54	0.42
1:A:72:TRP:HB3	1:A:78:VAL:HG13	2.00	0.42
1:C:279:ALA:HB1	2:C:401:FAD:HM83	2.00	0.42
1:A:279:ALA:HB1	2:A:401:FAD:HM83	2.00	0.42
1:D:213:LEU:HA	1:D:230:VAL:O	2.19	0.42
2:B:401:FAD:C9A	3:B:402:NAI:H4N	2.50	0.42
1:C:258:ALA:HB2	1:C:265:MET:CE	2.50	0.42
1:A:188:VAL:HA	1:A:272:LEU:O	2.19	0.41
1:B:263:CYS:O	1:D:251:GLU:OE2	2.38	0.41
1:A:73:GLN:HG3	1:A:78:VAL:CG2	2.50	0.41
1:D:160:ALA:O	1:D:164:THR:HG23	2.20	0.41
1:A:323:LEU:HD23	1:A:323:LEU:C	2.40	0.41
1:C:159:PRO:HD3	2:C:401:FAD:H51A	2.03	0.41
1:C:55:ALA:HA	2:C:401:FAD:C5X	2.51	0.41
1:C:217:ARG:HB2	5:C:588:HOH:O	2.21	0.40
1:C:133:ARG:HB3	1:C:138:TRP:CD2	2.56	0.40
1:C:193:GLU:HB2	1:C:269:VAL:HG11	2.02	0.40
1:B:232:HIS:CE1	2:B:401:FAD:H6	2.56	0.40
1:C:280:ARG:HB3	3:C:402:NAI:H5N	2.03	0.40
1:A:291:SER:HB2	1:A:298:TYR:CD2	2.56	0.40
1:D:279:ALA:CB	2:D:401:FAD:HM83	2.51	0.40
1:B:211:ASP:HB3	1:B:234:THR:HG22	2.02	0.40

All (1) 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)
1:C:318:GLU:OE2	1:D:225:THR:OG1[2_553]	1.97	0.23

## 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	316/336 (94%)	310 (98%)	5 (2%)	1 (0%)	46	41
1	B	315/336 (94%)	310 (98%)	5 (2%)	0	100	100
1	C	317/336 (94%)	314 (99%)	3 (1%)	0	100	100
1	D	326/336 (97%)	323 (99%)	3 (1%)	0	100	100
All	All	1274/1344 (95%)	1257 (99%)	16 (1%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	LEU

### 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	252/266 (95%)	252 (100%)	0	100	100
1	B	251/266 (94%)	250 (100%)	1 (0%)	93	95
1	C	255/266 (96%)	251 (98%)	4 (2%)	70	73
1	D	258/266 (97%)	257 (100%)	1 (0%)	93	95
All	All	1016/1064 (96%)	1010 (99%)	6 (1%)	90	93

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

Mol	Chain	Res	Type
1	B	12	ILE
1	C	44	LYS
1	C	46	SER
1	C	147	ASN
1	C	217	ARG
1	D	173	LEU

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	153	HIS
1	A	326	HIS
1	B	153	HIS
1	C	153	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	401	-	51,58,58	1.24	5 (9%)	50,89,89	1.99	5 (10%)
3	NAI	A	402	-	41,48,48	0.98	2 (4%)	46,73,73	1.82	6 (13%)
4	FMT	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FAD	B	401	-	51,58,58	1.33	7 (13%)	50,89,89	2.04	6 (12%)
3	NAI	B	402	-	41,48,48	0.94	1 (2%)	46,73,73	1.74	9 (19%)
4	FMT	B	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FAD	C	401	-	51,58,58	1.36	7 (13%)	50,89,89	2.24	6 (12%)
3	NAI	C	402	-	41,48,48	1.15	5 (12%)	46,73,73	1.72	6 (13%)
4	FMT	C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FAD	D	401	-	51,58,58	1.45	11 (21%)	50,89,89	2.46	7 (14%)
3	NAI	D	402	-	41,48,48	1.17	4 (9%)	46,73,73	2.18	8 (17%)
4	FMT	D	403	-	0,2,2	0.00	-	0,1,1	0.00	-

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	401	-	-	0/30/50/50	0/6/6/6
3	NAI	A	402	-	-	0/25/72/72	0/5/5/5
4	FMT	A	403	-	-	0/0/0/0	0/0/0/0
2	FAD	B	401	-	-	0/30/50/50	0/6/6/6
3	NAI	B	402	-	-	0/25/72/72	0/5/5/5
4	FMT	B	403	-	-	0/0/0/0	0/0/0/0
2	FAD	C	401	-	-	0/30/50/50	0/6/6/6
3	NAI	C	402	-	-	0/25/72/72	0/5/5/5
4	FMT	C	403	-	-	0/0/0/0	0/0/0/0
2	FAD	D	401	-	-	0/30/50/50	0/6/6/6
3	NAI	D	402	-	-	0/25/72/72	0/5/5/5
4	FMT	D	403	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NAI	C2N-N1N	-2.89	1.32	1.37
3	C	402	NAI	C2N-N1N	-2.29	1.33	1.37
2	D	401	FAD	C4'-C3'	-2.18	1.49	1.53
3	C	402	NAI	C2B-C1B	-2.08	1.50	1.53
2	D	401	FAD	C1'-N10	-2.04	1.46	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C2A-N3A	2.03	1.35	1.32
3	C	402	NAI	O4B-C1B	2.04	1.44	1.41
2	D	401	FAD	C4X-N5	2.09	1.36	1.33
2	B	401	FAD	C5'-C4'	2.19	1.55	1.51
2	A	401	FAD	C5A-C4A	2.32	1.45	1.40
2	D	401	FAD	C5'-C4'	2.37	1.55	1.51
2	C	401	FAD	C5A-C4A	2.37	1.45	1.40
2	A	401	FAD	C8-C7	2.38	1.47	1.41
2	D	401	FAD	C9A-N10	2.41	1.42	1.38
2	D	401	FAD	C8-C7	2.43	1.47	1.41
2	C	401	FAD	C8-C7	2.47	1.47	1.41
2	C	401	FAD	C9A-N10	2.48	1.42	1.38
3	D	402	NAI	O4B-C1B	2.48	1.44	1.41
2	B	401	FAD	C8-C7	2.52	1.47	1.41
3	A	402	NAI	C5A-C4A	2.60	1.46	1.40
2	A	401	FAD	C4-C4X	2.87	1.46	1.40
2	D	401	FAD	C5A-C4A	2.96	1.47	1.40
3	B	402	NAI	C6N-C5N	2.99	1.38	1.33
2	C	401	FAD	O4B-C1B	2.99	1.45	1.41
3	C	402	NAI	C5A-C4A	3.04	1.47	1.40
3	D	402	NAI	C5A-C4A	3.14	1.47	1.40
2	B	401	FAD	C2A-N3A	3.17	1.37	1.32
2	B	401	FAD	C5A-C4A	3.19	1.47	1.40
2	B	401	FAD	C4X-C10	3.22	1.46	1.40
2	D	401	FAD	C4X-C10	3.22	1.46	1.40
2	B	401	FAD	C9A-C5X	3.26	1.49	1.42
2	B	401	FAD	C4-C4X	3.36	1.47	1.40
2	C	401	FAD	C4X-C10	3.42	1.47	1.40
2	C	401	FAD	C9A-C5X	3.42	1.49	1.42
3	A	402	NAI	C6N-C5N	3.46	1.39	1.33
2	A	401	FAD	C9A-C5X	3.50	1.50	1.42
3	C	402	NAI	C6N-C5N	3.56	1.39	1.33
3	D	402	NAI	C6N-C5N	3.61	1.39	1.33
2	C	401	FAD	C4-C4X	3.69	1.48	1.40
2	D	401	FAD	C4-C4X	3.85	1.48	1.40
2	D	401	FAD	C9A-C5X	4.01	1.51	1.42
2	A	401	FAD	C4X-C10	4.17	1.48	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	N3A-C2A-N1A	-8.63	122.09	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FAD	N3A-C2A-N1A	-8.23	122.41	128.87
3	A	402	NAI	N3A-C2A-N1A	-8.09	122.52	128.87
3	C	402	NAI	N3A-C2A-N1A	-7.29	123.15	128.87
3	D	402	NAI	N3A-C2A-N1A	-7.27	123.16	128.87
2	A	401	FAD	N3A-C2A-N1A	-7.15	123.26	128.87
3	B	402	NAI	N3A-C2A-N1A	-7.03	123.35	128.87
2	B	401	FAD	N3A-C2A-N1A	-6.91	123.44	128.87
3	D	402	NAI	C1D-N1N-C2N	-6.26	109.98	120.85
3	D	402	NAI	C4D-O4D-C1D	-5.35	97.73	109.52
3	A	402	NAI	C1D-N1N-C2N	-4.22	113.52	120.85
3	C	402	NAI	C1D-N1N-C2N	-4.13	113.68	120.85
2	A	401	FAD	C1B-N9A-C4A	-3.44	122.97	126.81
3	A	402	NAI	C4D-O4D-C1D	-3.20	102.47	109.52
3	B	402	NAI	C1D-N1N-C2N	-3.10	115.47	120.85
3	C	402	NAI	C4D-O4D-C1D	-3.05	102.80	109.52
3	A	402	NAI	C3D-C2D-C1D	-3.03	95.34	101.44
2	D	401	FAD	O2'-C2'-C1'	-2.72	103.21	109.93
3	D	402	NAI	C2D-C3D-C4D	-2.68	97.14	102.64
2	B	401	FAD	C4B-O4B-C1B	-2.50	106.99	109.64
2	D	401	FAD	C1'-C2'-C3'	-2.47	102.75	109.82
3	B	402	NAI	C1B-N9A-C4A	-2.47	124.05	126.81
3	D	402	NAI	C5B-C4B-C3B	-2.41	105.86	115.20
2	C	401	FAD	C4X-C10-N10	-2.39	118.78	120.52
3	B	402	NAI	C3D-C2D-C1D	-2.32	96.76	101.44
2	B	401	FAD	C1B-N9A-C4A	-2.32	124.22	126.81
3	B	402	NAI	C3N-C2N-N1N	-2.22	119.98	123.24
3	B	402	NAI	O2B-C2B-C1B	-2.13	104.96	111.61
2	D	401	FAD	C1B-N9A-C4A	-2.07	124.50	126.81
3	C	402	NAI	O2A-PA-O1A	2.07	123.34	112.56
3	C	402	NAI	C4N-C3N-C7N	2.12	123.94	118.19
2	C	401	FAD	O2P-P-O1P	2.15	123.75	112.56
2	B	401	FAD	C4X-N5-C5X	2.45	119.61	116.72
3	B	402	NAI	C4B-O4B-C1B	2.46	112.25	109.64
3	B	402	NAI	C6N-N1N-C2N	2.47	124.88	118.52
3	A	402	NAI	N6A-C6A-N1A	2.51	122.73	118.52
3	A	402	NAI	C6N-N1N-C2N	2.56	125.11	118.52
2	D	401	FAD	C4X-N5-C5X	2.91	120.15	116.72
3	D	402	NAI	C1D-N1N-C6N	2.99	127.48	120.80
3	D	402	NAI	C4N-C3N-C7N	3.08	126.55	118.19
3	C	402	NAI	O4D-C1D-N1N	3.20	114.20	108.09
2	B	401	FAD	C1'-N10-C9A	3.53	122.92	118.83
3	B	402	NAI	N6A-C6A-N1A	3.55	124.47	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	C4X-N5-C5X	3.60	120.97	116.72
2	A	401	FAD	C5X-C9A-N10	3.67	120.33	117.58
3	D	402	NAI	O4D-C1D-N1N	4.44	116.56	108.09
2	A	401	FAD	C1'-N10-C9A	4.74	124.32	118.83
2	C	401	FAD	C1'-N10-C9A	4.94	124.56	118.83
2	D	401	FAD	C1'-N10-C9A	6.31	126.14	118.83
2	A	401	FAD	C2-N1-C10	8.02	120.23	113.39
2	C	401	FAD	C2-N1-C10	9.34	121.36	113.39
2	B	401	FAD	C2-N1-C10	10.30	122.18	113.39
2	D	401	FAD	C2-N1-C10	11.37	123.09	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FAD	3	0
3	A	402	NAI	2	0
2	B	401	FAD	3	0
3	B	402	NAI	3	0
2	C	401	FAD	5	0
3	C	402	NAI	2	0
2	D	401	FAD	3	0
4	D	403	FMT	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<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	320/336 (95%)	-0.08	8 (2%) 61 61	16, 26, 59, 111	0
1	B	319/336 (94%)	-0.12	4 (1%) 79 80	16, 25, 58, 104	0
1	C	321/336 (95%)	0.04	15 (4%) 35 37	16, 30, 70, 114	0
1	D	328/336 (97%)	-0.07	4 (1%) 81 81	17, 29, 65, 88	0
All	All	1288/1344 (95%)	-0.06	31 (2%) 62 63	16, 27, 67, 114	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLN	5.8
1	A	89	HIS	4.7
1	C	192	PHE	3.8
1	C	45	ARG	3.8
1	C	262	ASP	3.6
1	C	269	VAL	3.1
1	B	89	HIS	3.1
1	C	89	HIS	3.1
1	A	51	LEU	3.1
1	A	90	GLY	3.0
1	D	226	LEU	3.0
1	D	261	ILE	2.9
1	C	220	PRO	2.8
1	B	224	ASP	2.8
1	A	327	LEU	2.8
1	C	221	GLY	2.7
1	C	90	GLY	2.7
1	B	223	ASP	2.6
1	B	327	LEU	2.5
1	D	136	GLN	2.4
1	D	193	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	224	ASP	2.3
1	C	217	ARG	2.2
1	C	50	SER	2.2
1	C	92	ARG	2.2
1	C	3	VAL	2.2
1	C	270	PHE	2.1
1	A	99	GLU	2.1
1	C	272	LEU	2.1
1	A	92	ARG	2.0
1	C	198	THR	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(Å <sup>2</sup> )	Q<0.9
3	NAI	C	402	44/44	0.95	0.14	1.41	24,44,104,118	0
3	NAI	D	402	44/44	0.93	0.14	1.24	26,45,85,112	0
3	NAI	B	402	44/44	0.94	0.14	1.19	18,50,77,102	0
3	NAI	A	402	44/44	0.92	0.14	0.97	22,49,71,93	0
2	FAD	B	401	53/53	0.97	0.11	0.79	10,19,26,31	0
2	FAD	A	401	53/53	0.98	0.10	0.25	9,19,31,40	0
2	FAD	C	401	53/53	0.97	0.09	0.22	14,22,35,37	0
4	FMT	D	403	3/3	0.96	0.09	0.20	32,37,39,47	0
2	FAD	D	401	53/53	0.98	0.09	-0.06	13,20,31,41	0
4	FMT	C	403	3/3	0.97	0.07	-1.01	28,34,38,45	0
4	FMT	A	403	3/3	0.97	0.07	-1.04	23,23,25,28	0
4	FMT	B	403	3/3	0.99	0.06	-1.18	20,21,28,34	0

## 6.5 Other polymers

There are no such residues in this entry.