



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1QGA  
Title : PEA FNR Y308W MUTANT IN COMPLEX WITH NADP+  
Authors : Deng, Z.; Aliverti, A.; Zanetti, G.; Arakaki, A.K.; Ottado, J.; Orellano, E.G.;  
Calcaterra, N.B.; Ceccarelli, E.A.; Carrillo, N.; Karplus, P.A.  
Deposited on : 1999-04-18  
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 (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

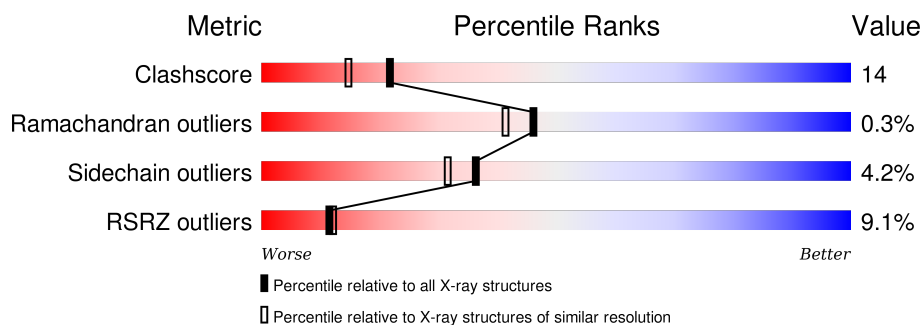
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
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	308	<div> <div>9%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	B	308	<div> <div>9%</div> <div>72%</div> <div>21%</div> <div>.</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5733 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 PROTEIN (FERREDOXIN:NADP+ REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2447	1568	404	459	16			
1	B	295	Total	C	N	O	S	0	0	0
			2349	1506	386	441	16			

There are 2 discrepancies between the modelled and reference sequences:

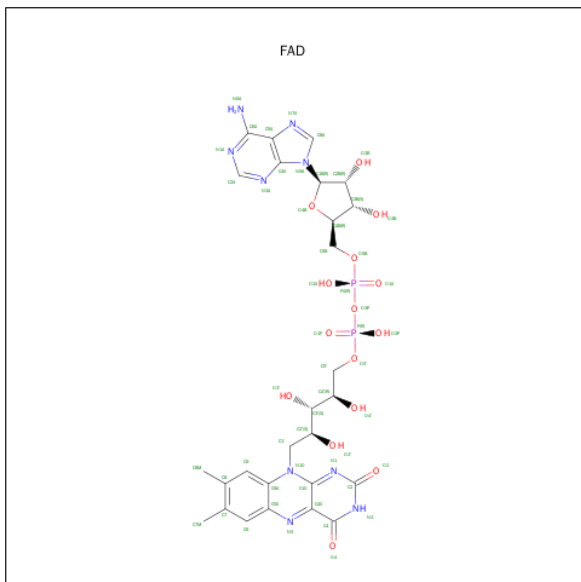
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	TRP	TYR	MUTATION	UNP P10933
B	808	TRP	TYR	MUTATION	UNP P10933

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



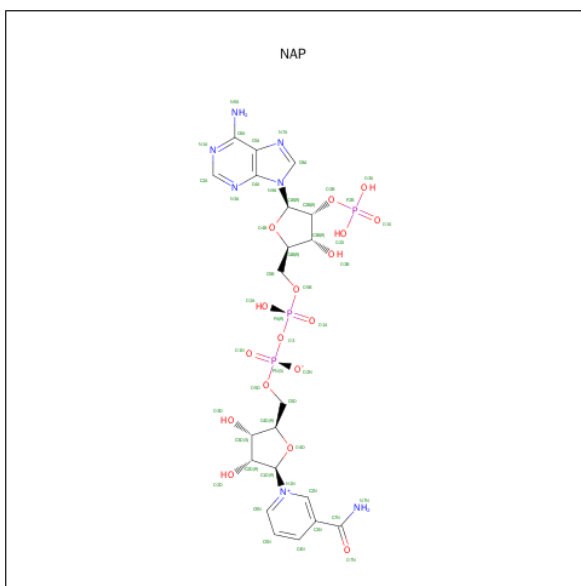
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	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:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

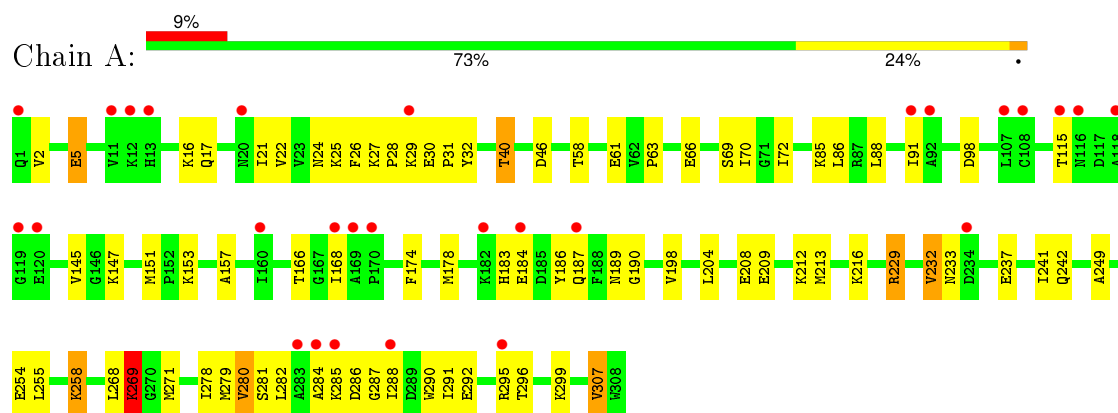
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total	O	0	0
			400	400		
5	B	330	Total	O	0	0
			330	330		

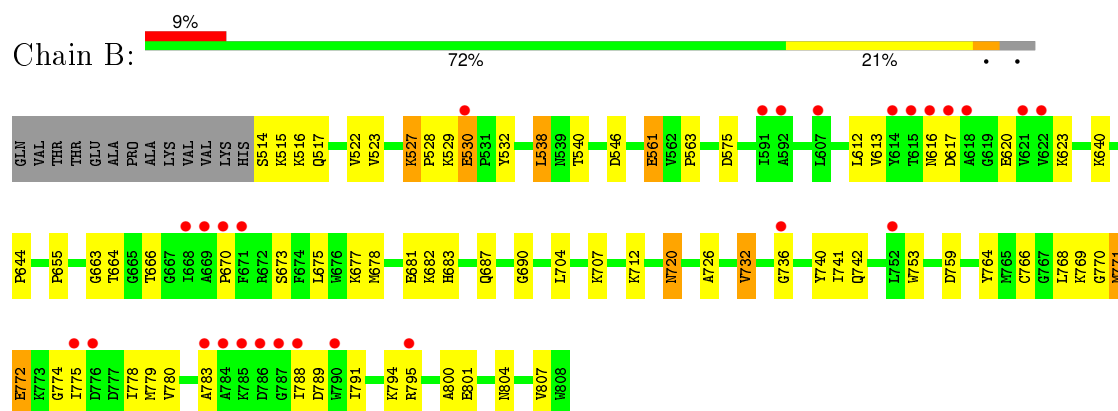
### 3 Residue-property plots [i](#)

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: PROTEIN (FERREDOXIN:NADP+ REDUCTASE)



#### • Molecule 1: PROTEIN (FERREDOXIN:NADP+ REDUCTASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.40 Å 110.30 Å 80.60 Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 27.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (8.00-2.00) 97.3 (27.98-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 1.99 Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.198 , 0.264 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 116.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57733 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.26% 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

### 5.1 Standard geometry

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	0.97	3/2502 (0.1%)	1.00	5/3371 (0.1%)
1	B	0.89	1/2402 (0.0%)	0.95	3/3234 (0.1%)
All	All	0.93	4/4904 (0.1%)	0.98	8/6605 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	LYS	CE-NZ	-10.30	1.23	1.49
1	A	307	VAL	CB-CG2	-9.70	1.32	1.52
1	A	269	LYS	CG-CD	9.16	1.83	1.52
1	B	726	ALA	CA-CB	5.26	1.63	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LYS	CG-CD-CE	10.03	142.00	111.90
1	A	269	LYS	CD-CE-NZ	-9.16	90.64	111.70
1	B	538	LEU	CA-CB-CG	9.07	136.17	115.30
1	A	98	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	720	ASN	N-CA-C	5.57	126.03	111.00
1	B	772	GLU	N-CA-C	5.53	125.94	111.00
1	A	307	VAL	CG1-CB-CG2	-5.08	102.76	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	532	TYR	Sidechain

## 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	2447	0	2451	71	0
1	B	2349	0	2343	66	0
2	A	5	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	48	0	22	3	0
4	B	48	0	21	7	0
5	A	400	0	0	7	0
5	B	330	0	0	7	0
All	All	5733	0	4899	139	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 14.

All (139) 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:269:LYS:CD	1:A:269:LYS:CG	1.83	1.55
1:B:683:HIS:H	1:B:687:GLN:NE2	1.74	0.84
1:B:741:ILE:HG22	4:B:810:NAP:H2A	1.62	0.80
1:B:675:LEU:HD23	1:B:678:MET:CE	2.12	0.80
4:B:810:NAP:H3D	5:B:1723:HOH:O	1.80	0.79
1:A:307:VAL:HG23	5:A:1314:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:H	1:A:187:GLN:NE2	1.81	0.78
1:B:616:ASN:HD21	1:B:620:GLU:HB2	1.50	0.77
1:A:208:GLU:HG2	1:A:212:LYS:HE3	1.69	0.73
1:B:794:LYS:HE3	1:B:795:ARG:HH11	1.55	0.71
1:B:528:PRO:HD2	1:B:529:LYS:HZ3	1.55	0.71
1:A:25:LYS:HD3	1:A:26:PHE:CE1	2.27	0.70
1:A:70:ILE:HG23	1:A:91:ILE:HD11	1.74	0.70
1:B:791:ILE:O	1:B:795:ARG:HD3	1.91	0.70
1:A:281:SER:O	1:A:285:LYS:HG2	1.91	0.69
1:B:527:LYS:HB3	1:B:529:LYS:HZ3	1.58	0.68
1:B:774:GLY:O	1:B:778:ILE:HG13	1.93	0.67
1:A:249:ALA:HB1	1:A:282:LEU:HD21	1.75	0.67
1:A:21:ILE:HD13	1:A:147:LYS:HG2	1.78	0.65
1:B:546:ASP:HB2	5:B:1600:HOH:O	1.97	0.65
1:B:522:VAL:HG11	1:B:563:PRO:HG2	1.79	0.64
1:B:682:LYS:HA	1:B:687:GLN:HE22	1.62	0.64
1:A:69:SER:HB2	1:A:145:VAL:HG13	1.79	0.63
1:B:675:LEU:HD23	1:B:678:MET:HE2	1.79	0.63
1:A:30:GLU:HG3	5:A:1091:HOH:O	1.98	0.63
1:B:753:TRP:CZ2	1:B:783:ALA:HA	2.34	0.62
1:A:29:LYS:HD3	1:A:29:LYS:H	1.64	0.62
1:B:517:GLN:NE2	5:B:1038:HOH:O	2.32	0.61
1:B:683:HIS:H	1:B:687:GLN:HE21	1.48	0.61
3:A:309:FAD:H8A	5:A:1528:HOH:O	2.00	0.61
1:A:21:ILE:CD1	1:A:147:LYS:HG2	2.30	0.61
1:A:183:HIS:H	1:A:187:GLN:HE21	1.48	0.60
1:A:268:LEU:HD23	4:A:310:NAP:H4D	1.81	0.60
1:B:794:LYS:HE3	1:B:795:ARG:NH1	2.17	0.60
1:A:216:LYS:NZ	1:A:216:LYS:HB3	2.17	0.60
1:A:40:THR:HG23	5:A:1302:HOH:O	2.02	0.59
1:B:675:LEU:HD23	1:B:678:MET:HE1	1.83	0.59
1:A:269:LYS:CB	1:A:269:LYS:CD	2.80	0.58
1:B:666:THR:OG1	4:B:810:NAP:H6N	2.04	0.58
1:A:212:LYS:O	1:A:216:LYS:HG3	2.04	0.58
1:A:307:VAL:CG2	5:A:1314:HOH:O	2.45	0.57
1:A:28:PRO:HD2	1:A:29:LYS:HZ2	1.69	0.57
1:A:28:PRO:O	1:A:31:PRO:HD3	2.04	0.57
1:B:783:ALA:HB1	1:B:788:ILE:HB	1.85	0.57
1:B:527:LYS:HB3	1:B:529:LYS:NZ	2.19	0.57
1:A:291:ILE:HD12	1:A:291:ILE:H	1.71	0.56
1:A:29:LYS:HD3	1:A:29:LYS:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:GLU:O	1:B:563:PRO:HD3	2.06	0.56
1:A:296:THR:HA	1:A:299:LYS:HG2	1.87	0.56
1:A:32:TYR:CE1	1:A:61:GLU:HG3	2.42	0.55
1:B:742:GLN:HE22	4:B:810:NAP:C2A	2.20	0.55
1:B:664:THR:OG1	1:B:768:LEU:HG	2.07	0.55
1:B:522:VAL:HG11	1:B:563:PRO:CG	2.37	0.55
1:B:655:PRO:HB2	1:B:687:GLN:O	2.07	0.54
1:B:770:GLY:O	1:B:772:GLU:N	2.40	0.54
1:A:280:VAL:HG23	1:A:290:TRP:HB3	1.90	0.53
1:B:675:LEU:HA	1:B:678:MET:HE2	1.89	0.53
1:B:529:LYS:HB2	1:B:530:GLU:OE1	2.09	0.53
1:A:88:LEU:HD22	1:A:145:VAL:HG11	1.90	0.52
1:B:616:ASN:ND2	1:B:620:GLU:HB2	2.21	0.52
1:A:32:TYR:HE1	1:A:61:GLU:HG3	1.73	0.52
1:B:759:ASP:HB2	5:B:1369:HOH:O	2.10	0.51
1:B:681:GLU:HB3	1:B:683:HIS:CE1	2.46	0.51
1:B:690:GLY:O	1:B:720:ASN:HB2	2.11	0.51
1:B:515:LYS:HG3	1:B:801:GLU:OE1	2.10	0.51
1:A:279:MET:HA	1:A:279:MET:HE3	1.93	0.50
1:B:789:ASP:HA	5:B:1093:HOH:O	2.10	0.50
1:A:198:VAL:HG21	1:A:204:LEU:HD23	1.93	0.49
1:B:740:TYR:HB3	1:B:742:GLN:NE2	2.27	0.49
1:B:527:LYS:HB3	1:B:529:LYS:HE2	1.94	0.49
1:A:174:PHE:O	1:A:178:MET:HG3	2.12	0.49
1:B:529:LYS:HD3	1:B:529:LYS:N	2.28	0.49
1:A:233:ASN:ND2	1:A:237:GLU:OE1	2.37	0.48
1:A:268:LEU:O	1:A:271:MET:HG2	2.13	0.48
1:A:27:LYS:HB3	1:A:29:LYS:NZ	2.29	0.48
1:B:527:LYS:HB3	1:B:529:LYS:CE	2.44	0.47
1:B:741:ILE:CG2	4:B:810:NAP:H2A	2.37	0.47
1:A:27:LYS:CB	1:A:29:LYS:HG2	2.44	0.47
1:A:209:GLU:O	1:A:213:MET:HG3	2.14	0.47
1:A:21:ILE:HG12	1:A:22:VAL:N	2.28	0.47
1:A:166:THR:OG1	4:A:310:NAP:H6N	2.15	0.47
1:A:280:VAL:HA	1:A:290:TRP:HB2	1.95	0.47
1:B:527:LYS:N	1:B:527:LYS:HD3	2.30	0.47
1:A:281:SER:O	1:A:284:ALA:HB3	2.15	0.46
1:A:291:ILE:HD12	1:A:291:ILE:N	2.29	0.46
1:B:712:LYS:HE2	5:B:1218:HOH:O	2.14	0.46
1:B:769:LYS:HA	1:B:807:VAL:HB	1.97	0.46
1:B:523:VAL:HA	1:B:644:PRO:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:CD1	1:A:291:ILE:H	2.28	0.46
1:B:514:SER:N	5:B:1584:HOH:O	2.48	0.46
1:A:2:VAL:HG13	1:A:2:VAL:O	2.16	0.46
1:A:287:GLY:O	1:A:288:ILE:HD13	2.16	0.46
1:A:279:MET:HE3	1:A:282:LEU:HD12	1.98	0.45
1:A:183:HIS:HB2	1:A:186:TYR:O	2.17	0.45
1:A:291:ILE:O	1:A:295:ARG:HG2	2.16	0.45
1:B:517:GLN:HE22	1:B:677:LYS:NZ	2.14	0.45
1:A:26:PHE:CE2	1:A:32:TYR:HB2	2.52	0.45
1:A:22:VAL:HG11	1:A:63:PRO:CG	2.47	0.45
1:B:764:TYR:CD2	1:B:804:ASN:HB2	2.52	0.45
1:A:29:LYS:CD	1:A:29:LYS:H	2.22	0.44
1:A:72:ILE:O	1:A:86:LEU:HA	2.17	0.44
1:B:682:LYS:HA	1:B:687:GLN:NE2	2.31	0.44
1:A:24:ASN:HA	5:A:1310:HOH:O	2.17	0.44
1:A:258:LYS:HE3	5:A:1573:HOH:O	2.18	0.44
1:B:740:TYR:CB	1:B:742:GLN:HE21	2.30	0.44
1:A:168:ILE:O	1:A:168:ILE:HG13	2.18	0.44
1:A:58:THR:O	1:A:61:GLU:HG2	2.18	0.44
1:B:612:LEU:HD21	3:B:809:FAD:C8A	2.47	0.43
1:A:85:LYS:HD3	1:A:85:LYS:HA	1.86	0.43
1:A:16:LYS:O	1:A:153:LYS:HE3	2.18	0.43
1:A:157:ALA:O	1:A:190:GLY:HA3	2.19	0.43
1:A:66:GLU:H	1:A:66:GLU:CD	2.22	0.43
1:B:768:LEU:HD23	4:B:810:NAP:C4D	2.50	0.42
1:A:27:LYS:HB2	1:A:29:LYS:HG2	2.01	0.42
1:B:768:LEU:HD23	4:B:810:NAP:H4D	2.01	0.42
1:B:800:ALA:O	1:B:801:GLU:HB2	2.19	0.42
1:A:242:GLN:H	1:A:242:GLN:CD	2.22	0.42
1:B:522:VAL:CG1	1:B:563:PRO:HG2	2.47	0.42
1:A:232:VAL:HA	1:A:237:GLU:O	2.20	0.42
1:A:255:LEU:HA	1:A:258:LYS:HD3	2.00	0.42
1:B:768:LEU:O	1:B:771:MET:HG2	2.19	0.42
1:A:17:GLN:HG3	1:A:151:MET:O	2.20	0.42
1:A:187:GLN:NE2	1:A:187:GLN:HA	2.34	0.42
1:B:670:PRO:O	1:B:673:SER:HB3	2.19	0.42
1:A:241:ILE:HG22	4:A:310:NAP:H2A	2.02	0.41
1:B:663:GLY:HA2	1:B:766:CYS:O	2.20	0.41
1:B:732:VAL:HG13	1:B:736:GLY:HA2	2.02	0.41
1:A:5:GLU:HG3	1:A:5:GLU:O	2.21	0.41
1:B:775:ILE:O	1:B:779:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:HD13	1:B:707:LYS:HD2	2.02	0.41
1:B:794:LYS:CE	1:B:795:ARG:NH1	2.83	0.41
1:A:254:GLU:O	1:A:258:LYS:HD2	2.21	0.41
1:A:279:MET:CE	1:A:282:LEU:HD12	2.51	0.41
1:B:740:TYR:HB3	1:B:742:GLN:HE21	1.86	0.41
1:B:681:GLU:OE1	1:B:683:HIS:HE1	2.04	0.40
1:B:783:ALA:HB1	1:B:788:ILE:CB	2.51	0.40
1:B:613:VAL:HG22	1:B:623:LYS:HD2	2.03	0.40
1:A:27:LYS:HB3	1:A:29:LYS:HG2	2.04	0.40
1:B:575:ASP:OD1	1:B:640:LYS:NZ	2.48	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	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	293/308 (95%)	279 (95%)	12 (4%)	2 (1%)	26	19
All	All	599/616 (97%)	575 (96%)	22 (4%)	2 (0%)	46	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	771	MET
1	B	780	VAL

### 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	267/267 (100%)	253 (95%)	14 (5%)	29	23
1	B	256/267 (96%)	248 (97%)	8 (3%)	47	46
All	All	523/534 (98%)	501 (96%)	22 (4%)	36	31

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	40	THR
1	A	46	ASP
1	A	115	THR
1	A	184	GLU
1	A	189	ASN
1	A	229	ARG
1	A	232	VAL
1	A	258	LYS
1	A	269	LYS
1	A	278	ILE
1	A	280	VAL
1	A	286	ASP
1	A	292	GLU
1	B	516	LYS
1	B	527	LYS
1	B	530	GLU
1	B	538	LEU
1	B	540	THR
1	B	561	GLU
1	B	617	ASP
1	B	732	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	17	GLN
1	A	156	ASN
1	A	187	GLN
1	A	247	GLN

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Mol	Chain	Res	Type
1	B	517	GLN
1	B	683	HIS
1	B	687	GLN
1	B	742	GLN
1	B	747	GLN

### 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](#)

5 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	$\# Z  > 2$
3	FAD	A	309	-	48,58,58	1.63	13 (27%)	54,89,89	1.63	6 (11%)
4	NAP	A	310	1	42,52,52	1.44	6 (14%)	54,80,80	1.98	8 (14%)
2	SO4	A	311	-	4,4,4	0.45	0	6,6,6	0.64	0
3	FAD	B	809	-	48,58,58	1.39	7 (14%)	54,89,89	1.53	5 (9%)
4	NAP	B	810	1	42,52,52	1.27	4 (9%)	54,80,80	1.91	9 (16%)

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
3	FAD	A	309	-	-	0/30/50/50	0/6/6/6
4	NAP	A	310	1	-	0/27/67/67	0/5/5/5
2	SO4	A	311	-	-	0/0/0/0	0/0/0/0
3	FAD	B	809	-	-	0/30/50/50	0/6/6/6
4	NAP	B	810	1	-	0/27/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	309	FAD	P-O2P	-3.37	1.40	1.54
4	A	310	NAP	C5A-C4A	-3.20	1.33	1.40
4	A	310	NAP	P2B-O3X	-2.94	1.44	1.54
3	A	309	FAD	C6-C5X	-2.78	1.37	1.41
3	A	309	FAD	PA-O2A	-2.53	1.44	1.54
3	A	309	FAD	P-O1P	-2.52	1.42	1.51
4	A	310	NAP	PN-O2N	-2.48	1.44	1.54
4	B	810	NAP	C5A-C4A	-2.40	1.35	1.40
3	A	309	FAD	C8A-N7A	-2.28	1.30	1.34
3	B	809	FAD	C4'-C3'	-2.20	1.49	1.53
3	A	309	FAD	PA-O5B	-2.19	1.49	1.59
4	B	810	NAP	P2B-O3X	-2.04	1.47	1.54
4	A	310	NAP	P2B-O2X	-2.02	1.47	1.54
3	B	809	FAD	P-O2P	-2.02	1.46	1.54
3	A	309	FAD	O4B-C1B	2.06	1.43	1.41
3	A	309	FAD	C2A-N1A	2.08	1.37	1.33
3	B	809	FAD	C5'-C4'	2.28	1.55	1.51
3	A	309	FAD	C10-N1	2.36	1.39	1.35
4	B	810	NAP	O4B-C1B	2.37	1.44	1.41
3	B	809	FAD	O5'-C5'	2.41	1.54	1.44
3	A	309	FAD	C2A-N3A	2.43	1.36	1.32
3	A	309	FAD	C5'-C4'	2.47	1.55	1.51
3	B	809	FAD	C4X-N5	2.77	1.37	1.33
4	A	310	NAP	C4N-C3N	2.88	1.44	1.39
3	A	309	FAD	C4X-N5	3.02	1.38	1.33
3	B	809	FAD	C4-N3	3.54	1.39	1.33
3	B	809	FAD	O4B-C1B	3.89	1.46	1.41
3	A	309	FAD	C4-N3	3.93	1.40	1.33
4	B	810	NAP	O4D-C1D	3.97	1.46	1.41
4	A	310	NAP	O4D-C1D	4.12	1.46	1.41

All (28) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	310	NAP	N3A-C2A-N1A	-10.01	121.23	128.89
4	B	810	NAP	N3A-C2A-N1A	-9.58	121.56	128.89
3	B	809	FAD	C4X-C4-N3	-4.60	117.29	123.59
3	A	309	FAD	C4X-C4-N3	-4.25	117.78	123.59
4	B	810	NAP	PN-O3-PA	-3.83	121.97	132.73
3	B	809	FAD	C2B-C1B-N9A	-3.81	108.47	114.29
4	A	310	NAP	C1B-N9A-C4A	-3.24	122.05	126.94
3	A	309	FAD	C4-C4X-C10	-3.07	117.98	119.94
4	B	810	NAP	O3-PN-O5D	-3.00	94.97	102.94
3	A	309	FAD	C4X-C10-N10	-2.93	118.79	120.52
4	B	810	NAP	C1B-N9A-C4A	-2.92	122.54	126.94
4	A	310	NAP	C4B-O4B-C1B	-2.91	106.52	109.72
3	A	309	FAD	C4A-C5A-N7A	-2.76	106.94	109.48
3	A	309	FAD	C2B-C1B-N9A	-2.39	110.64	114.29
4	A	310	NAP	O5B-PA-O1A	-2.30	100.69	109.62
4	B	810	NAP	C4B-O4B-C1B	-2.20	107.30	109.72
3	B	809	FAD	C4-C4X-C10	-2.17	118.56	119.94
4	A	310	NAP	O3-PN-O5D	2.05	108.37	102.94
4	A	310	NAP	O4B-C1B-C2B	2.08	110.37	106.60
4	B	810	NAP	O4D-C1D-N1N	2.20	110.54	108.13
3	B	809	FAD	C1'-N10-C9A	2.28	121.43	118.86
4	B	810	NAP	O4B-C4B-C5B	2.85	119.53	109.32
4	B	810	NAP	O3-PA-O5B	3.32	111.73	102.94
4	B	810	NAP	O2N-PN-O3	3.55	121.18	105.09
4	A	310	NAP	O4D-C1D-N1N	4.12	112.65	108.13
4	A	310	NAP	O3-PA-O5B	4.33	114.42	102.94
3	B	809	FAD	C4-N3-C2	7.53	121.75	115.25
3	A	309	FAD	C4-N3-C2	8.36	122.47	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	309	FAD	1	0
4	A	310	NAP	3	0
3	B	809	FAD	1	0
4	B	810	NAP	7	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	308/308 (100%)	0.30	28 (9%)	11 12	17, 34, 69, 81	1 (0%)
1	B	295/308 (95%)	0.34	27 (9%)	11 12	22, 37, 75, 88	1 (0%)
All	All	603/616 (97%)	0.32	55 (9%)	11 12	17, 36, 72, 88	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	HIS	6.3
1	B	783	ALA	6.1
1	A	11	VAL	5.2
1	B	788	ILE	5.1
1	B	785	LYS	5.0
1	A	12	LYS	4.9
1	A	118	ALA	4.5
1	A	288	ILE	4.0
1	A	234	ASP	3.8
1	B	615	THR	3.6
1	A	119	GLY	3.5
1	B	617	ASP	3.5
1	B	795	ARG	3.4
1	A	168	ILE	3.3
1	A	283	ALA	3.3
1	B	618	ALA	3.2
1	B	591	ILE	3.2
1	A	295	ARG	3.2
1	B	790	TRP	3.1
1	B	669	ALA	3.1
1	B	787	GLY	3.1
1	B	592	ALA	3.0
1	B	776	ASP	3.0
1	B	784	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	607	LEU	2.9
1	B	621	VAL	2.9
1	B	616	ASN	2.9
1	B	668	ILE	2.8
1	B	786	ASP	2.8
1	B	530	GLU	2.7
1	A	187	GLN	2.7
1	A	116	ASN	2.6
1	B	775	ILE	2.6
1	A	1	GLN	2.6
1	B	670	PRO	2.5
1	A	169	ALA	2.4
1	A	107	LEU	2.4
1	A	91	ILE	2.3
1	A	92	ALA	2.3
1	A	182	LYS	2.3
1	A	120	GLU	2.3
1	B	622	VAL	2.3
1	A	108	CYS	2.3
1	A	285	LYS	2.2
1	B	671	PHE	2.2
1	A	170	PRO	2.2
1	A	284	ALA	2.2
1	B	752	LEU	2.2
1	A	29	LYS	2.1
1	A	115	THR	2.1
1	A	184	GLU	2.1
1	A	20	ASN	2.0
1	B	614	TYR	2.0
1	A	160	ILE	2.0
1	B	736	GLY	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 [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
4	NAP	B	810	48/48	0.90	0.16	0.65	25,64,80,86	18
4	NAP	A	310	48/48	0.94	0.12	-0.22	14,37,56,59	18
3	FAD	B	809	53/53	0.92	0.12	-0.32	17,28,81,83	0
3	FAD	A	309	53/53	0.94	0.11	-0.42	17,23,59,60	0
2	SO4	A	311	5/5	0.96	0.11	-	44,54,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.