Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 07:52 PM EST

PDB ID	:	5IQ4
Title	:	Crystal structure of RnTmm mutant Y207S soaking
Authors	:	Zhang, Y.Z.; Li, C.Y.
Deposited on	:	2016-03-10
Resolution	:	1.50 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

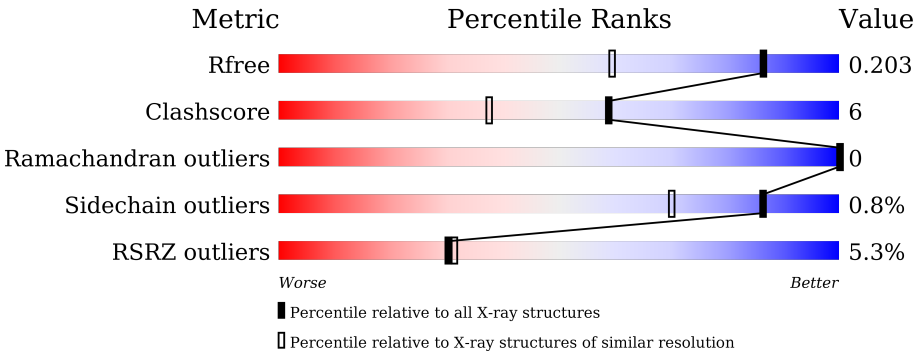
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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 <=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	453	4% 88% 11% ·
1	B	453	6% 87% 11% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8349 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.

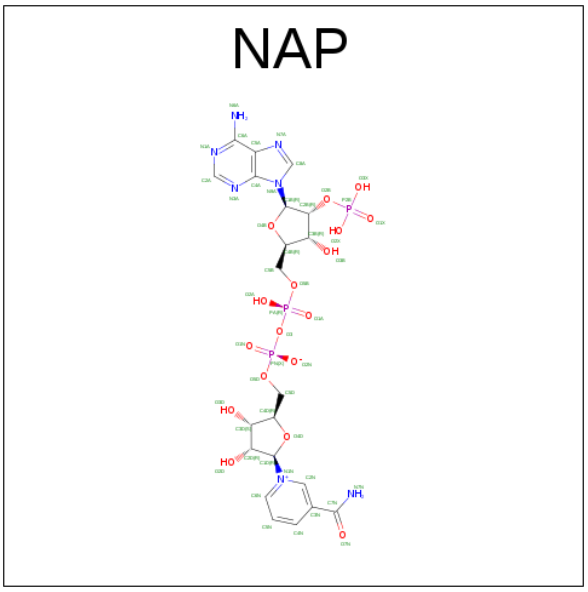
- Molecule 1 is a protein called Flavin-containing monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	3	0
			3597	2295	609	676	17			
1	B	445	Total	C	N	O	S	0	0	0
			3573	2282	605	669	17			

There are 14 discrepancies between the modelled and reference sequences:

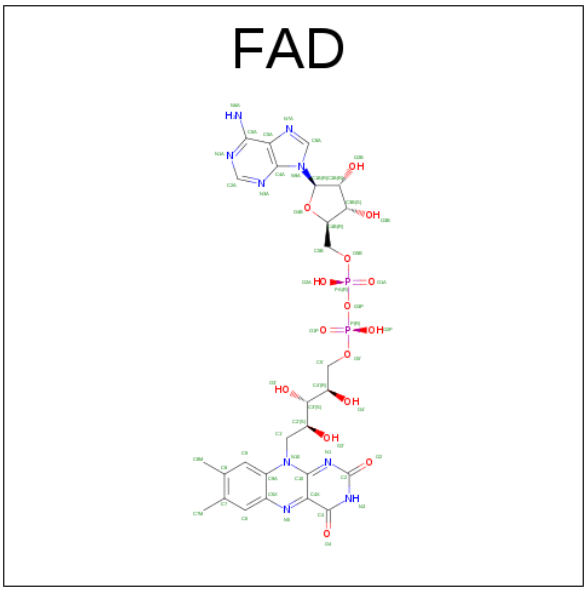
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	TYR	engineered mutation	UNP A3SLM3
A	448	HIS	-	expression tag	UNP A3SLM3
A	449	HIS	-	expression tag	UNP A3SLM3
A	450	HIS	-	expression tag	UNP A3SLM3
A	451	HIS	-	expression tag	UNP A3SLM3
A	452	HIS	-	expression tag	UNP A3SLM3
A	453	HIS	-	expression tag	UNP A3SLM3
B	207	SER	TYR	engineered mutation	UNP A3SLM3
B	448	HIS	-	expression tag	UNP A3SLM3
B	449	HIS	-	expression tag	UNP A3SLM3
B	450	HIS	-	expression tag	UNP A3SLM3
B	451	HIS	-	expression tag	UNP A3SLM3
B	452	HIS	-	expression tag	UNP A3SLM3
B	453	HIS	-	expression tag	UNP A3SLM3

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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		

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

- Molecule 4 is water.

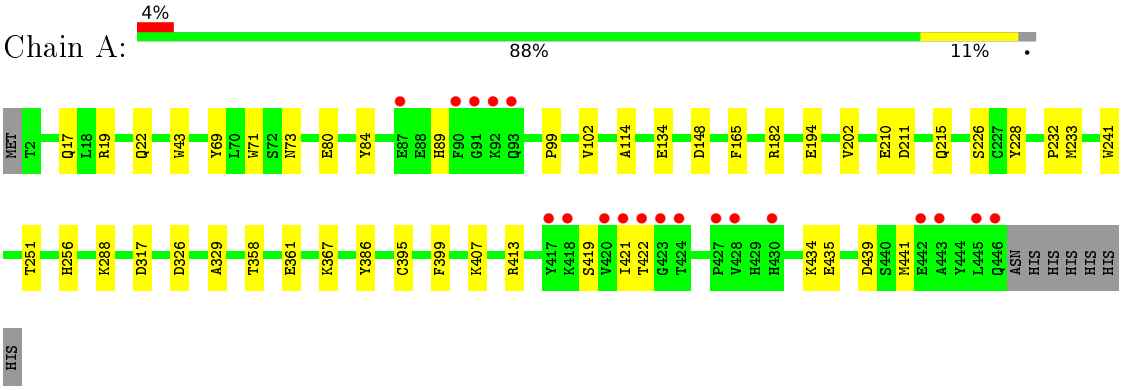
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	513	Total	O	0	0
			513	513		
4	B	464	Total	O	0	0
			464	464		

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.

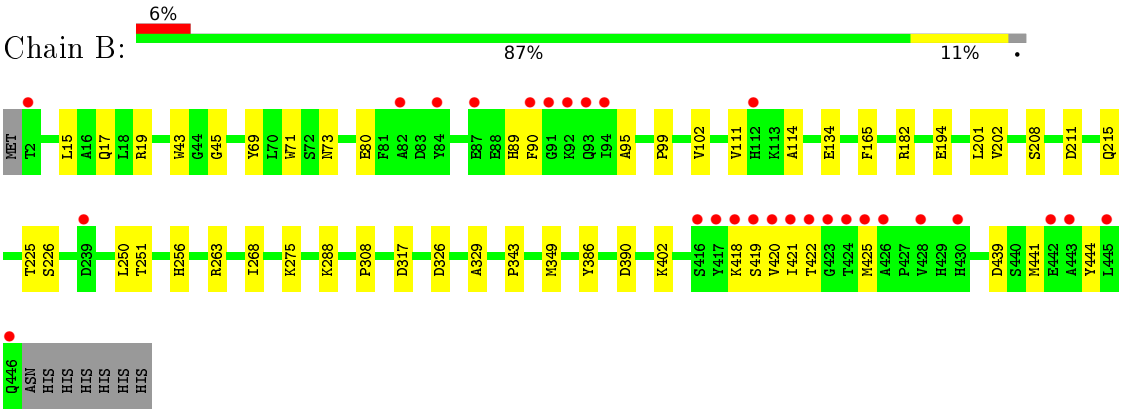
- Molecule 1: Flavin-containing monooxygenase

Chain A:



- Molecule 1: Flavin-containing monooxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.97Å 61.36Å 104.71Å 90.00° 94.04° 90.00°	Depositor
Resolution (Å)	35.72 – 1.50 35.72 – 1.50	Depositor EDS
% Data completeness (in resolution range)	85.8 (35.72-1.50) 88.0 (35.72-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.156 , 0.206 0.152 , 0.203	Depositor DCC
R_{free} test set	6525 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.60$, $< L^2 > = 0.45$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8349	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, 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	0.31	0/3706	0.48	0/5030
1	B	0.30	0/3682	0.47	0/4998
All	All	0.31	0/7388	0.48	0/10028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3597	0	3366	38	0
1	B	3573	0	3350	40	0
2	A	48	0	24	14	0
2	B	48	0	25	8	0
3	A	53	0	31	6	0
3	B	53	0	31	1	0
4	A	513	0	0	9	0
4	B	464	0	0	6	0
All	All	8349	0	6827	83	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 6.

All (83) 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:73:ASN:HD21	2:A:501:NAP:H4N	1.20	1.01
1:B:317:ASP:OD1	2:B:501:NAP:O3D	1.81	0.97
1:A:182:ARG:HD2	1:B:182:ARG:HD2	1.57	0.87
1:A:421:ILE:HG13	1:A:422:THR:HG23	1.57	0.85
1:B:182:ARG:HD3	1:B:194:GLU:OE1	1.81	0.81
1:A:358:THR:HA	4:A:609:HOH:O	1.82	0.80
1:A:361:GLU:HB2	4:A:609:HOH:O	1.80	0.80
1:A:73:ASN:ND2	2:A:501:NAP:H4N	1.98	0.76
1:B:421:ILE:HG13	1:B:422:THR:HG23	1.68	0.74
1:A:182:ARG:HD3	1:A:194:GLU:OE1	1.89	0.72
1:B:208:SER:OG	2:B:501:NAP:H5N	1.91	0.71
1:A:69:TYR:HA	1:A:439:ASP:OD1	1.88	0.71
1:A:80:GLU:HB3	4:A:905:HOH:O	1.96	0.66
1:A:317:ASP:OD1	2:A:501:NAP:O3D	2.11	0.66
1:B:419:SER:OG	1:B:421:ILE:HG12	2.01	0.61
1:A:419:SER:OG	1:A:421:ILE:HG12	2.00	0.61
1:B:69:TYR:HA	1:B:439:ASP:OD1	2.01	0.59
1:B:317:ASP:CG	2:B:501:NAP:HO3N	2.00	0.59
1:B:134:GLU:HB2	4:B:998:HOH:O	2.04	0.57
1:A:317:ASP:OD1	2:A:501:NAP:O2D	2.23	0.56
1:B:251:THR:OG1	1:B:256:HIS:HE1	1.88	0.56
1:B:390:ASP:HB3	1:B:420:VAL:HG22	1.89	0.55
1:A:233:MET:HE1	4:A:623:HOH:O	2.06	0.55
1:A:102:VAL:HG22	1:A:441:MET:HG3	1.90	0.54
1:B:95:ALA:HB3	1:B:444:TYR:OH	2.08	0.53
1:B:73:ASN:CB	2:B:501:NAP:H72N	2.21	0.53
2:A:501:NAP:H5N	3:A:502:FAD:C10	2.39	0.53
1:A:210:GLU:HA	4:A:623:HOH:O	2.09	0.52
1:A:73:ASN:HA	1:A:413:ARG:HH21	1.75	0.52
1:A:251:THR:OG1	1:A:256:HIS:HE1	1.92	0.51
2:A:501:NAP:PA	2:A:501:NAP:H52N	2.51	0.51
1:B:288:LYS:HB2	1:B:288:LYS:NZ	2.26	0.50
2:A:501:NAP:C5N	3:A:502:FAD:N10	2.75	0.50
1:B:208:SER:HG	2:B:501:NAP:H5N	1.78	0.49
1:B:73:ASN:CG	2:B:501:NAP:H72N	2.17	0.49
1:A:421:ILE:HD11	4:A:971:HOH:O	2.13	0.49
1:A:251:THR:HG22	4:A:762:HOH:O	2.11	0.48
1:B:80:GLU:HB3	4:B:694:HOH:O	2.13	0.48
1:A:434:LYS:HE3	1:A:435:GLU:OE2	2.13	0.48
1:A:73:ASN:HD21	2:A:501:NAP:C4N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PHE:CZ	2:B:501:NAP:O4D	2.67	0.48
1:A:317:ASP:CG	2:A:501:NAP:HO3N	2.13	0.47
1:B:17:GLN:HA	1:B:329:ALA:HB1	1.97	0.47
1:B:71:TRP:HA	1:B:99:PRO:HA	1.96	0.47
1:B:15:LEU:HB3	1:B:111:VAL:HG11	1.96	0.47
1:A:17:GLN:HA	1:A:329:ALA:HB1	1.96	0.46
1:B:211:ASP:O	1:B:215:GLN:HG2	2.15	0.46
1:B:418:LYS:HG2	1:B:425:MET:HG2	1.97	0.46
1:A:165:PHE:CZ	2:A:501:NAP:H1D	2.51	0.46
1:B:250:LEU:HD11	1:B:268:ILE:CD1	2.45	0.46
1:A:71:TRP:HA	1:A:99:PRO:HA	1.97	0.46
1:B:73:ASN:HB3	2:B:501:NAP:H72N	1.80	0.46
1:A:407:LYS:NZ	1:A:407:LYS:HB3	2.31	0.46
1:A:148:ASP:OD2	1:B:288:LYS:HE3	2.17	0.45
1:A:326:ASP:HB3	1:A:386:TYR:CE1	2.51	0.45
1:B:288:LYS:HE2	4:B:996:HOH:O	2.15	0.45
2:A:501:NAP:C4N	3:A:502:FAD:C5X	2.95	0.45
1:A:288:LYS:HD3	4:B:649:HOH:O	2.16	0.44
1:B:402:LYS:HG3	4:B:1041:HOH:O	2.18	0.44
2:A:501:NAP:H5N	3:A:502:FAD:N10	2.32	0.44
1:B:45:GLY:HA2	3:B:502:FAD:O3B	2.17	0.44
2:A:501:NAP:C4N	3:A:502:FAD:C9A	2.95	0.44
1:B:19:ARG:HH11	1:B:114:ALA:HB2	1.83	0.44
1:B:202:VAL:O	1:B:226:SER:HA	2.19	0.43
1:A:228:TYR:CZ	1:A:232:PRO:HG3	2.54	0.43
1:B:201:LEU:HD12	1:B:225:THR:O	2.18	0.43
1:B:343:PRO:HD2	1:B:349:MET:CE	2.49	0.43
1:A:211:ASP:O	1:A:215:GLN:HG2	2.19	0.43
2:A:501:NAP:C5N	3:A:502:FAD:C9A	2.97	0.43
4:A:692:HOH:O	1:B:275:LYS:HE3	2.18	0.42
1:A:367:LYS:NZ	1:A:399:PHE:CG	2.87	0.42
1:A:202:VAL:O	1:A:226:SER:HA	2.20	0.42
1:B:89:HIS:HD2	1:B:90:PHE:CD1	2.38	0.42
1:B:326:ASP:HB3	1:B:386:TYR:CE1	2.55	0.42
1:B:69:TYR:HD1	1:B:439:ASP:OD1	2.04	0.41
1:A:182:ARG:CD	1:A:194:GLU:OE1	2.65	0.41
1:A:84:TYR:CE2	1:A:89:HIS:HB2	2.55	0.41
1:B:102:VAL:HG22	1:B:441:MET:HG3	2.03	0.41
1:A:241:TRP:HZ2	4:A:623:HOH:O	2.03	0.40
1:A:19:ARG:HD2	1:A:22[B]:GLN:NE2	2.37	0.40
1:A:19:ARG:HH11	1:A:114:ALA:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HD2	4:B:618:HOH:O	2.22	0.40
1:B:343:PRO:HD2	1:B:349:MET:HE2	2.03	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	446/453 (98%)	431 (97%)	15 (3%)	0	100	100
1	B	443/453 (98%)	423 (96%)	20 (4%)	0	100	100
All	All	889/906 (98%)	854 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	368/375 (98%)	365 (99%)	3 (1%)	86	70
1	B	365/375 (97%)	362 (99%)	3 (1%)	86	70
All	All	733/750 (98%)	727 (99%)	6 (1%)	86	70

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

Mol	Chain	Res	Type
1	A	43	TRP
1	A	134	GLU
1	A	395	CYS
1	B	43	TRP
1	B	263	ARG
1	B	308	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	73	ASN
1	A	256	HIS
1	B	48	ASN
1	B	256	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)

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	NAP	A	501	-	45,52,52	1.07	3 (6%)	55,80,80	2.23	10 (18%)
3	FAD	A	502	-	52,58,58	1.17	6 (11%)	52,89,89	2.37	13 (25%)
2	NAP	B	501	-	45,52,52	0.85	1 (2%)	55,80,80	1.42	6 (10%)
3	FAD	B	502	-	52,58,58	1.18	5 (9%)	52,89,89	2.23	10 (19%)

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	NAP	A	501	-	-	0/27/67/67	0/5/5/5
3	FAD	A	502	-	-	0/30/50/50	0/6/6/6
2	NAP	B	501	-	-	0/27/67/67	0/5/5/5
3	FAD	B	502	-	-	0/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	O2D-C2D	-2.88	1.36	1.43
2	A	501	NAP	C2D-C1D	-2.58	1.49	1.53
3	A	502	FAD	C2-N3	-2.07	1.33	1.38
3	A	502	FAD	C5A-C4A	2.29	1.45	1.40
3	B	502	FAD	C5A-C4A	2.42	1.46	1.40
3	A	502	FAD	C8-C7	2.45	1.47	1.41
3	B	502	FAD	C8-C7	2.54	1.47	1.41
2	B	501	NAP	C5A-C4A	2.61	1.46	1.40
2	A	501	NAP	C5A-C4A	2.67	1.46	1.40
3	A	502	FAD	C9A-C5X	2.89	1.48	1.42
3	B	502	FAD	C9A-C5X	3.03	1.49	1.42
3	A	502	FAD	C4-C4X	3.14	1.47	1.41
3	B	502	FAD	C4-C4X	3.22	1.47	1.41
3	B	502	FAD	C4X-C10	3.41	1.47	1.40
3	A	502	FAD	C4X-C10	3.41	1.47	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	N3A-C2A-N1A	-6.83	123.51	128.87
3	A	502	FAD	N3A-C2A-N1A	-6.68	123.62	128.87
2	B	501	NAP	N3A-C2A-N1A	-6.67	123.63	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	FAD	C4-C4X-C10	-6.58	115.73	119.94
3	A	502	FAD	C4-C4X-C10	-6.53	115.76	119.94
2	A	501	NAP	O2D-C2D-C1D	-6.43	91.48	111.61
3	B	502	FAD	N3A-C2A-N1A	-5.06	124.90	128.87
2	A	501	NAP	C2D-C1D-N1N	-4.71	104.29	113.53
3	A	502	FAD	C4X-C4-N3	-3.89	118.43	123.52
3	B	502	FAD	C4X-C4-N3	-3.84	118.51	123.52
2	A	501	NAP	C4D-O4D-C1D	-3.83	105.58	109.64
3	B	502	FAD	N3-C2-N1	-3.62	121.60	127.69
3	A	502	FAD	N3-C2-N1	-3.41	121.94	127.69
3	A	502	FAD	C1B-N9A-C4A	-3.24	123.19	126.81
2	A	501	NAP	C1B-N9A-C4A	-2.69	123.80	126.81
2	B	501	NAP	C5N-C4N-C3N	-2.43	117.45	120.35
3	B	502	FAD	C1B-N9A-C4A	-2.42	124.11	126.81
3	A	502	FAD	C4B-O4B-C1B	-2.32	107.18	109.64
3	A	502	FAD	O2'-C2'-C1'	-2.31	104.21	109.93
2	A	501	NAP	O4D-C4D-C5D	-2.31	101.01	109.29
2	B	501	NAP	C2A-N1A-C6A	2.01	122.36	118.77
2	B	501	NAP	O3X-P2B-O2X	2.22	115.58	107.44
2	A	501	NAP	O3X-P2B-O2X	2.23	115.63	107.44
2	A	501	NAP	N6A-C6A-N1A	2.33	122.42	118.52
2	A	501	NAP	O3D-C3D-C2D	2.34	119.43	111.86
3	A	502	FAD	C5X-C9A-N10	2.57	119.51	117.58
3	A	502	FAD	N6A-C6A-N1A	2.65	122.97	118.52
3	B	502	FAD	C5X-C9A-N10	2.72	119.62	117.58
2	B	501	NAP	C2N-C3N-C4N	2.81	121.45	118.27
3	A	502	FAD	C4-C4X-N5	2.93	122.26	118.70
3	B	502	FAD	C4X-N5-C5X	3.09	120.36	116.72
3	A	502	FAD	C4X-N5-C5X	3.09	120.37	116.72
2	B	501	NAP	O4D-C1D-N1N	3.30	111.66	108.10
3	B	502	FAD	C4-C4X-N5	3.34	122.76	118.70
3	A	502	FAD	C1'-N10-C9A	4.01	123.47	118.83
3	B	502	FAD	C1'-N10-C9A	4.02	123.49	118.83
3	B	502	FAD	C4-N3-C2	9.31	122.92	115.16
3	A	502	FAD	C4-N3-C2	9.47	123.06	115.16
2	A	501	NAP	O4D-C1D-N1N	9.64	118.51	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	14	0
3	A	502	FAD	6	0
2	B	501	NAP	8	0
3	B	502	FAD	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^{th} 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	445/453 (98%)	-0.06	19 (4%)	39	41	7, 19, 44, 65	0
1	B	445/453 (98%)	0.11	28 (6%)	23	24	7, 20, 57, 76	0
All	All	890/906 (98%)	0.03	47 (5%)	30	31	7, 20, 48, 76	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ILE	10.6
1	A	421	ILE	7.4
1	B	91	GLY	7.3
1	B	420	VAL	6.7
1	B	424	THR	6.4
1	B	423	GLY	6.0
1	B	422	THR	5.8
1	B	428	VAL	5.4
1	B	90	PHE	5.0
1	B	446	GLN	5.0
1	B	445	LEU	4.9
1	A	445	LEU	4.7
1	A	91	GLY	4.7
1	B	425	MET	4.6
1	A	424	THR	4.2
1	A	428	VAL	4.1
1	B	418	LYS	3.9
1	A	422	THR	3.9
1	B	87	GLU	3.8
1	B	417	TYR	3.8
1	B	426	ALA	3.7
1	A	423	GLY	3.6
1	B	92	LYS	3.5
1	B	443	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	82	ALA	3.4
1	A	446	GLN	3.4
1	B	94	ILE	3.4
1	B	93	GLN	3.0
1	A	90	PHE	3.0
1	B	84	TYR	3.0
1	A	87	GLU	3.0
1	B	419	SER	2.9
1	A	417	TYR	2.8
1	A	418	LYS	2.8
1	B	430	HIS	2.6
1	A	430	HIS	2.6
1	B	239	ASP	2.6
1	B	442	GLU	2.5
1	A	427	PRO	2.4
1	A	92	LYS	2.4
1	A	420	VAL	2.4
1	A	93	GLN	2.3
1	A	442	GLU	2.3
1	B	416	SER	2.3
1	B	112	HIS	2.3
1	B	2	THR	2.1
1	A	443	ALA	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^{th} 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^2)	Q<0.9
3	FAD	A	502	53/53	0.98	0.10	0.62	6,10,17,18	0
3	FAD	B	502	53/53	0.98	0.09	0.08	6,11,19,22	0
2	NAP	B	501	48/48	0.97	0.08	0.02	14,18,56,58	0
2	NAP	A	501	48/48	0.97	0.07	-0.18	13,17,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.