WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:29 PM GMT

PDB ID	:	1XT6
Title	:	S35C Flavodoxin Mutant in the semiquinone state
Authors	:	Artali, R.; Marchini, N.; Meneghetti, F.; Cavazzini, D.; Cassetta, A.; Sassone, C.; Bombieri, G.; Rossi, G.L.; Gilardi, G.
Deposited on	:	2004-10-21
Resolution	:	1.80 Å(reported)

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

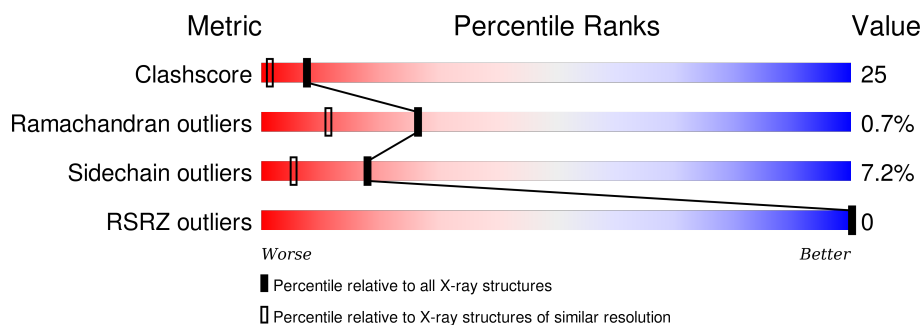|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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 | Percentile Ranks | Value

Clashscore — 25
Ramachandran outliers — 0.7%
Sidechain outliers — 7.2%
RSRZ outliers — 0

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	147	25% 48% 24% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1261 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 Flavodoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1102	684	181	232	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	CONFLICT	UNP P00323
A	35	CYS	SER	ENGINEERED	UNP P00323

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.
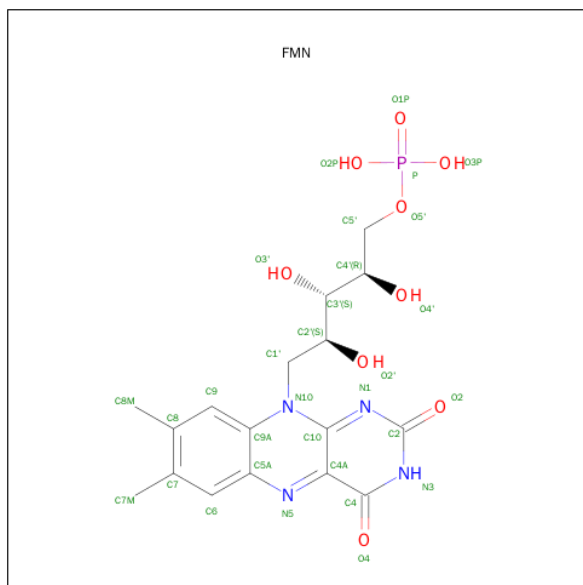
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flavodoxin
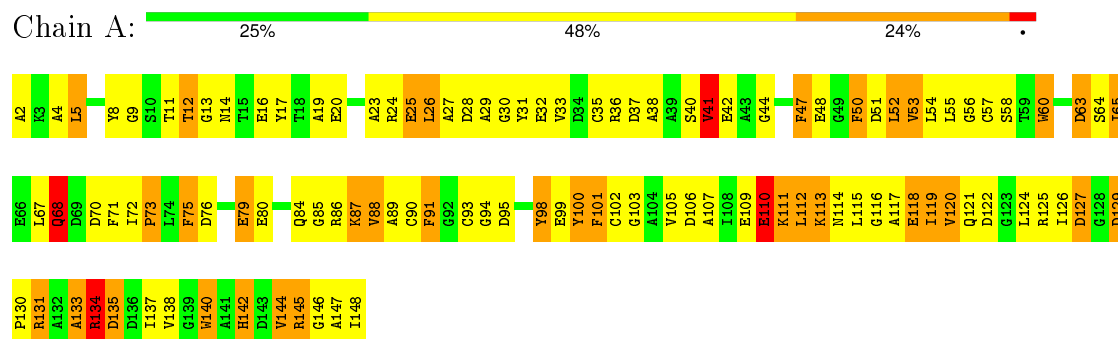
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	51.08Å 51.08Å 138.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.80 19.44 – 1.38	Depositor EDS
% Data completeness (in resolution range)	79.4 (19.99-1.80) 95.7 (19.44-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.89 (at 1.38Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.261 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å²)	21.4	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.43 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Outliers	0 of 36895 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: FMN

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	3.22	123/1119 (11.0%)	2.39	53/1514 (3.5%)

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	A	0	2

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLU	CG-CD	17.64	1.78	1.51
1	A	79	GLU	CG-CD	16.62	1.76	1.51
1	A	79	GLU	CD-OE2	12.44	1.39	1.25
1	A	25	GLU	CG-CD	12.20	1.70	1.51
1	A	133	ALA	CA-CB	11.40	1.76	1.52
1	A	35	CYS	CB-SG	11.02	2.00	1.82
1	A	79	GLU	CD-OE1	10.29	1.36	1.25
1	A	110	GLU	CD-OE1	10.19	1.36	1.25
1	A	53	VAL	CB-CG2	9.98	1.73	1.52
1	A	24	ARG	C-O	9.79	1.42	1.23
1	A	100	TYR	CD1-CE1	9.78	1.54	1.39
1	A	95	ASP	CB-CG	9.76	1.72	1.51
1	A	131	ARG	CZ-NH1	9.42	1.45	1.33
1	A	105	VAL	CB-CG1	9.34	1.72	1.52
1	A	40	SER	CB-OG	9.28	1.54	1.42
1	A	120	VAL	CB-CG1	9.21	1.72	1.52
1	A	48	GLU	CD-OE1	9.20	1.35	1.25
1	A	131	ARG	C-O	9.13	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE1	9.02	1.35	1.25
1	A	31	TYR	CE1-CZ	8.83	1.50	1.38
1	A	42	GLU	CD-OE1	8.76	1.35	1.25
1	A	42	GLU	CD-OE2	8.66	1.35	1.25
1	A	71	PHE	CD1-CE1	8.48	1.56	1.39
1	A	94	GLY	CA-C	8.40	1.65	1.51
1	A	113	LYS	CE-NZ	8.34	1.70	1.49
1	A	140	TRP	CE3-CZ3	-8.18	1.24	1.38
1	A	145	ARG	CZ-NH1	8.13	1.43	1.33
1	A	144	VAL	CB-CG2	-8.06	1.35	1.52
1	A	113	LYS	CD-CE	8.00	1.71	1.51
1	A	9	GLY	C-O	7.94	1.36	1.23
1	A	32	GLU	CD-OE2	7.91	1.34	1.25
1	A	109	GLU	CB-CG	7.76	1.66	1.52
1	A	125	ARG	CZ-NH2	7.71	1.43	1.33
1	A	60	TRP	CE3-CZ3	7.56	1.51	1.38
1	A	54	LEU	CA-CB	7.49	1.71	1.53
1	A	58	SER	CB-OG	7.41	1.51	1.42
1	A	91	PHE	CD2-CE2	7.40	1.54	1.39
1	A	38	ALA	CA-CB	7.36	1.68	1.52
1	A	112	LEU	C-O	7.25	1.37	1.23
1	A	42	GLU	CG-CD	7.22	1.62	1.51
1	A	103	GLY	C-O	7.21	1.35	1.23
1	A	2	ALA	N-CA	7.19	1.60	1.46
1	A	47	PHE	CG-CD2	7.19	1.49	1.38
1	A	41	VAL	CB-CG2	-7.03	1.38	1.52
1	A	50	PHE	CG-CD1	7.02	1.49	1.38
1	A	125	ARG	CG-CD	6.97	1.69	1.51
1	A	47	PHE	C-O	-6.97	1.10	1.23
1	A	99	GLU	CD-OE2	6.94	1.33	1.25
1	A	85	GLY	C-O	6.93	1.34	1.23
1	A	27	ALA	N-CA	6.86	1.60	1.46
1	A	113	LYS	CB-CG	-6.85	1.34	1.52
1	A	100	TYR	CB-CG	6.68	1.61	1.51
1	A	131	ARG	CA-CB	-6.61	1.39	1.53
1	A	91	PHE	CB-CG	6.59	1.62	1.51
1	A	121	GLN	CA-CB	6.57	1.68	1.53
1	A	119	ILE	CA-CB	6.54	1.69	1.54
1	A	42	GLU	CB-CG	6.51	1.64	1.52
1	A	118	GLU	CD-OE2	6.50	1.32	1.25
1	A	100	TYR	CZ-OH	6.50	1.49	1.37
1	A	25	GLU	CD-OE1	6.50	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ARG	CZ-NH2	6.49	1.41	1.33
1	A	64	SER	CB-OG	-6.43	1.33	1.42
1	A	75	PHE	C-O	6.37	1.35	1.23
1	A	126	ILE	CB-CG2	6.34	1.72	1.52
1	A	33	VAL	CB-CG1	6.34	1.66	1.52
1	A	17	TYR	CD1-CE1	-6.34	1.29	1.39
1	A	73	PRO	CG-CD	6.34	1.71	1.50
1	A	107	ALA	CA-CB	-6.29	1.39	1.52
1	A	25	GLU	CD-OE2	6.29	1.32	1.25
1	A	133	ALA	C-O	-6.28	1.11	1.23
1	A	75	PHE	CD1-CE1	6.26	1.51	1.39
1	A	87	LYS	CA-CB	-6.25	1.40	1.53
1	A	118	GLU	CA-C	6.22	1.69	1.52
1	A	30	GLY	C-O	6.20	1.33	1.23
1	A	68	GLN	CG-CD	6.17	1.65	1.51
1	A	31	TYR	CE2-CZ	-6.10	1.30	1.38
1	A	86	ARG	CZ-NH2	6.06	1.41	1.33
1	A	134	ARG	CZ-NH1	6.03	1.40	1.33
1	A	98	TYR	CG-CD2	6.03	1.47	1.39
1	A	138	VAL	CB-CG1	-6.00	1.40	1.52
1	A	80	GLU	CG-CD	5.96	1.60	1.51
1	A	75	PHE	CE2-CZ	-5.88	1.26	1.37
1	A	19	ALA	CA-C	5.88	1.68	1.52
1	A	102	CYS	CB-SG	-5.87	1.72	1.81
1	A	119	ILE	C-O	5.72	1.34	1.23
1	A	88	VAL	N-CA	5.71	1.57	1.46
1	A	106	ASP	CG-OD2	5.70	1.38	1.25
1	A	20	GLU	N-CA	5.69	1.57	1.46
1	A	50	PHE	CB-CG	5.66	1.60	1.51
1	A	17	TYR	CG-CD2	5.65	1.46	1.39
1	A	131	ARG	N-CA	5.63	1.57	1.46
1	A	8	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	13	GLY	C-O	5.60	1.32	1.23
1	A	93	CYS	CB-SG	5.58	1.91	1.82
1	A	29	ALA	N-CA	-5.55	1.35	1.46
1	A	117	ALA	C-O	5.54	1.33	1.23
1	A	140	TRP	CZ3-CH2	5.53	1.49	1.40
1	A	8	TYR	CG-CD1	5.51	1.46	1.39
1	A	98	TYR	CB-CG	-5.51	1.43	1.51
1	A	101	PHE	C-O	5.46	1.33	1.23
1	A	4	ALA	CA-CB	5.45	1.63	1.52
1	A	135	ASP	CG-OD1	5.44	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	VAL	CB-CG2	5.42	1.64	1.52
1	A	101	PHE	CD2-CE2	5.40	1.50	1.39
1	A	131	ARG	CG-CD	-5.40	1.38	1.51
1	A	17	TYR	CE2-CZ	-5.37	1.31	1.38
1	A	101	PHE	CG-CD1	5.32	1.46	1.38
1	A	23	ALA	CA-CB	5.32	1.63	1.52
1	A	110	GLU	CD-OE2	5.23	1.31	1.25
1	A	71	PHE	CG-CD2	5.20	1.46	1.38
1	A	107	ALA	N-CA	5.18	1.56	1.46
1	A	129	ASP	CA-CB	5.15	1.65	1.53
1	A	121	GLN	C-O	-5.14	1.13	1.23
1	A	8	TYR	CD1-CE1	-5.12	1.31	1.39
1	A	71	PHE	CE2-CZ	5.11	1.47	1.37
1	A	80	GLU	CD-OE1	5.11	1.31	1.25
1	A	16	GLU	N-CA	5.08	1.56	1.46
1	A	101	PHE	CA-CB	-5.04	1.42	1.53
1	A	25	GLU	CB-CG	-5.04	1.42	1.52
1	A	19	ALA	N-CA	5.03	1.56	1.46
1	A	29	ALA	CA-C	5.03	1.66	1.52
1	A	137	ILE	CA-CB	-5.03	1.43	1.54
1	A	122	ASP	CA-C	5.01	1.66	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ASP	CB-CG-OD1	15.80	132.52	118.30
1	A	145	ARG	NE-CZ-NH2	-15.59	112.50	120.30
1	A	127	ASP	CB-CG-OD2	-14.64	105.12	118.30
1	A	135	ASP	CB-CG-OD2	-13.15	106.47	118.30
1	A	51	ASP	CB-CG-OD1	-12.05	107.45	118.30
1	A	91	PHE	CB-CG-CD1	10.67	128.27	120.80
1	A	144	VAL	CG1-CB-CG2	9.92	126.77	110.90
1	A	5	LEU	CB-CG-CD2	-9.05	95.61	111.00
1	A	98	TYR	CZ-CE2-CD2	8.99	127.89	119.80
1	A	106	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	A	36	ARG	NE-CZ-NH1	-8.91	115.84	120.30
1	A	75	PHE	CB-CG-CD1	8.86	127.00	120.80
1	A	63	ASP	CB-CG-OD1	-8.58	110.57	118.30
1	A	99	GLU	OE1-CD-OE2	8.58	133.60	123.30
1	A	145	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	67	LEU	CB-CG-CD1	8.19	124.93	111.00
1	A	95	ASP	OD1-CG-OD2	-7.98	108.14	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	135	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	88	VAL	CG1-CB-CG2	7.36	122.68	110.90
1	A	75	PHE	CB-CG-CD2	-7.29	115.70	120.80
1	A	17	TYR	CG-CD2-CE2	-7.25	115.50	121.30
1	A	111	LYS	CD-CE-NZ	7.12	128.08	111.70
1	A	5	LEU	CB-CG-CD1	6.94	122.80	111.00
1	A	90	CYS	CB-CA-C	-6.79	96.82	110.40
1	A	131	ARG	CD-NE-CZ	-6.63	114.31	123.60
1	A	32	GLU	OE1-CD-OE2	6.58	131.19	123.30
1	A	48	GLU	OE1-CD-OE2	6.48	131.07	123.30
1	A	138	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	A	65	ILE	CB-CG1-CD1	-6.25	96.39	113.90
1	A	25	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	A	71	PHE	CB-CG-CD1	6.06	125.04	120.80
1	A	93	CYS	CA-CB-SG	-5.91	103.36	114.00
1	A	26	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	A	114	ASN	N-CA-CB	5.81	121.06	110.60
1	A	36	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	118	GLU	CB-CA-C	-5.75	98.90	110.40
1	A	124	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	A	71	PHE	CD1-CE1-CZ	-5.67	113.29	120.10
1	A	52	LEU	CB-CG-CD1	5.57	120.47	111.00
1	A	134	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	133	ALA	N-CA-C	-5.47	96.23	111.00
1	A	71	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	A	9	GLY	N-CA-C	-5.37	99.68	113.10
1	A	35	CYS	CA-CB-SG	-5.33	104.40	114.00
1	A	89	ALA	N-CA-CB	5.32	117.54	110.10
1	A	99	GLU	C-N-CA	-5.30	108.44	121.70
1	A	24	ARG	CB-CG-CD	-5.28	97.86	111.60
1	A	87	LYS	CB-CG-CD	-5.23	98.01	111.60
1	A	53	VAL	CA-CB-CG2	-5.19	103.12	110.90
1	A	28	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	57	CYS	CA-CB-SG	-5.15	104.74	114.00
1	A	90	CYS	CA-CB-SG	-5.04	104.93	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	98	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	1102	0	1029	52	1
2	A	31	0	19	3	0
3	A	128	0	0	7	1
All	All	1261	0	1048	55	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 25.

All (55) 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:133:ALA:CB	1:A:133:ALA:CA	1.76	1.56
1:A:113:LYS:CE	1:A:113:LYS:NZ	1.69	1.55
1:A:79:GLU:CG	1:A:79:GLU:CD	1.76	1.53
1:A:110:GLU:CD	1:A:110:GLU:CG	1.78	1.52
2:A:149:FMN:C4'	2:A:149:FMN:O4'	1.65	1.39
1:A:68:GLN:HE22	1:A:70:ASP:HB2	1.31	0.92
1:A:25:GLU:HB3	3:A:157:HOH:O	1.69	0.91
1:A:120:VAL:HB	1:A:147:ALA:CB	2.09	0.82
1:A:120:VAL:HB	1:A:147:ALA:HB1	1.64	0.76
1:A:25:GLU:OE1	3:A:182:HOH:O	2.07	0.73
1:A:110:GLU:OE1	1:A:113:LYS:NZ	2.19	0.72
1:A:146:GLY:O	1:A:148:ILE:N	2.24	0.70
1:A:118:GLU:OE2	3:A:241:HOH:O	2.11	0.68
1:A:142:HIS:CD2	1:A:142:HIS:C	2.66	0.68
1:A:53:VAL:HB	1:A:88:VAL:HG12	1.75	0.67
2:A:149:FMN:O4'	2:A:149:FMN:C3'	2.44	0.66
1:A:133:ALA:CB	1:A:133:ALA:N	2.54	0.66
1:A:52:LEU:HD13	1:A:148:ILE:HD11	1.78	0.65
1:A:87:LYS:NZ	1:A:118:GLU:OE2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HB	1:A:147:ALA:HB3	1.80	0.63
1:A:76:ASP:OD2	3:A:190:HOH:O	2.16	0.61
1:A:129:ASP:OD1	1:A:131:ARG:NH1	2.34	0.60
1:A:146:GLY:C	1:A:148:ILE:H	2.05	0.59
1:A:26:LEU:HD23	1:A:145:ARG:HD3	1.85	0.59
1:A:65:ILE:HA	3:A:223:HOH:O	2.01	0.58
1:A:146:GLY:C	1:A:148:ILE:N	2.57	0.58
1:A:140:TRP:O	1:A:144:VAL:HG13	2.04	0.57
1:A:84:GLN:NE2	1:A:116:GLY:HA3	2.20	0.57
1:A:56:GLY:HA2	1:A:91:PHE:O	2.06	0.56
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.88	0.56
1:A:84:GLN:HE22	1:A:116:GLY:HA3	1.71	0.55
1:A:11:THR:HG22	1:A:12:THR:HG22	1.89	0.55
1:A:68:GLN:HE22	1:A:70:ASP:CB	2.11	0.54
2:A:149:FMN:C4'	2:A:149:FMN:HO4'	2.09	0.51
1:A:129:ASP:OD1	1:A:130:PRO:HD2	2.10	0.51
1:A:47:PHE:N	1:A:47:PHE:CD1	2.75	0.51
1:A:101:PHE:CZ	1:A:127:ASP:HB2	2.46	0.51
1:A:84:GLN:NE2	1:A:115:LEU:O	2.45	0.50
1:A:84:GLN:HB3	3:A:270:HOH:O	2.12	0.47
1:A:5:LEU:HB2	1:A:50:PHE:CE1	2.49	0.47
1:A:14:ASN:HB3	1:A:130:PRO:HG3	1.97	0.47
1:A:111:LYS:HG3	1:A:111:LYS:O	2.14	0.47
1:A:65:ILE:HG21	1:A:65:ILE:HD13	1.55	0.47
1:A:5:LEU:HB2	1:A:50:PHE:CD1	2.51	0.46
1:A:37:ASP:O	1:A:41:VAL:HG13	2.17	0.45
1:A:11:THR:HB	1:A:60:TRP:CZ2	2.53	0.44
1:A:146:GLY:O	1:A:147:ALA:C	2.55	0.42
1:A:55:LEU:HD12	1:A:112:LEU:HD11	2.02	0.42
1:A:134:ARG:HG2	1:A:135:ASP:N	2.25	0.41
1:A:68:GLN:NE2	1:A:70:ASP:HB2	2.15	0.41
1:A:120:VAL:HG11	1:A:148:ILE:HD13	2.03	0.41
1:A:120:VAL:O	1:A:147:ALA:CB	2.69	0.41
1:A:110:GLU:CD	1:A:110:GLU:HA	2.40	0.40
1:A:84:GLN:CB	3:A:270:HOH:O	2.69	0.40
1:A:113:LYS:HE3	1:A:113:LYS:HB2	1.78	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:A:100:TYR:OH	3:A:169:HOH:O[6_455]	2.11	0.09

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	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	26	11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLY

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	111/111 (100%)	103 (93%)	8 (7%)	18	5

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	41	VAL
1	A	63	ASP
1	A	68	GLN
1	A	110	GLU

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Mol	Chain	Res	Type
1	A	119	ILE
1	A	134	ARG
1	A	142	HIS

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	68	GLN
1	A	84	GLN
1	A	121	GLN
1	A	142	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)

1 ligand is 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	FMN	A	149	-	32,33,33	4.40	19 (59%)	34,50,50	4.46	20 (58%)

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	FMN	A	149	-	-	0/18/18/18	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C10-N10	-10.51	1.26	1.39
2	A	149	FMN	P-O5'	-3.92	1.48	1.59
2	A	149	FMN	C6-C7	-2.50	1.30	1.37
2	A	149	FMN	C10-N1	2.02	1.39	1.35
2	A	149	FMN	C2'-C3'	2.10	1.57	1.53
2	A	149	FMN	C4'-C3'	3.66	1.60	1.53
2	A	149	FMN	C2-N3	3.86	1.46	1.38
2	A	149	FMN	O4-C4	3.96	1.34	1.24
2	A	149	FMN	P-O1P	3.98	1.63	1.50
2	A	149	FMN	C8-C7	4.11	1.52	1.41
2	A	149	FMN	C1'-N10	4.44	1.53	1.48
2	A	149	FMN	C9A-C5A	5.47	1.54	1.42
2	A	149	FMN	C4-N3	5.62	1.43	1.33
2	A	149	FMN	C5'-C4'	5.68	1.60	1.51
2	A	149	FMN	C9A-N10	5.83	1.47	1.38
2	A	149	FMN	C8M-C8	6.16	1.63	1.51
2	A	149	FMN	C6-C5A	6.37	1.51	1.41
2	A	149	FMN	C4A-C10	8.26	1.56	1.40
2	A	149	FMN	O4'-C4'	9.89	1.65	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C4A-C10-N10	-10.77	112.69	120.52
2	A	149	FMN	C4-C4A-C10	-9.52	113.85	119.94
2	A	149	FMN	C5A-C9A-N10	-6.91	112.40	117.58
2	A	149	FMN	N3-C2-N1	-6.57	116.63	127.69
2	A	149	FMN	O4'-C4'-C3'	-4.62	97.08	108.96
2	A	149	FMN	C7M-C7-C8	-3.90	112.33	120.73
2	A	149	FMN	O3P-P-O1P	-3.54	99.06	110.63
2	A	149	FMN	C6-C5A-C9A	-2.98	115.82	119.11
2	A	149	FMN	C1'-N10-C9A	-2.95	115.41	118.83
2	A	149	FMN	O3'-C3'-C2'	-2.82	101.41	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	FMN	C4A-C4-N3	-2.79	119.87	123.52
2	A	149	FMN	C9A-C5A-N5	-2.66	117.85	122.18
2	A	149	FMN	O3P-P-O5'	-2.53	99.35	106.72
2	A	149	FMN	O2'-C2'-C3'	-2.51	102.49	108.96
2	A	149	FMN	O5'-P-O1P	3.07	114.79	107.08
2	A	149	FMN	C4-C4A-N5	4.17	123.77	118.70
2	A	149	FMN	O2P-P-O1P	4.88	126.55	110.63
2	A	149	FMN	C6-C5A-N5	5.91	126.28	118.92
2	A	149	FMN	C4A-N5-C5A	6.13	123.94	116.72
2	A	149	FMN	C4-N3-C2	11.73	124.95	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	149	FMN	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	147/147 (100%)	-0.08	0	100	100	14, 26, 40, 47	0

There are no RSRZ outliers to report.

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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FMN	A	149	31/31	0.96	0.09	0.26	12,19,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.