Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2016 – 01:19 PM EDT

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PDB ID	:	5JCL
Title	:	Structure and catalytic mechanism of monodehydroascorbate reductase, MD-HAR, from Oryza sativa L. japonica
Authors	:	Park, A.K.; Kim, H.W.
Deposited on	:	2016-04-15
Resolution	:	1.80 Å(reported)

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
Rfree		0.240
Clashscore		3
Ramachandran outliers		0.6%
Sidechain outliers		2.7%
RSRZ outliers		3.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
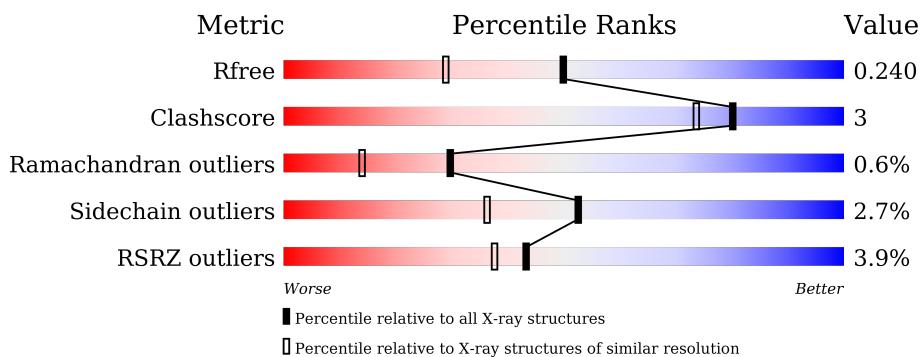
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	451	4% 85% 8% ·· 5%
1	B	451	3% 87% 7% · 5%
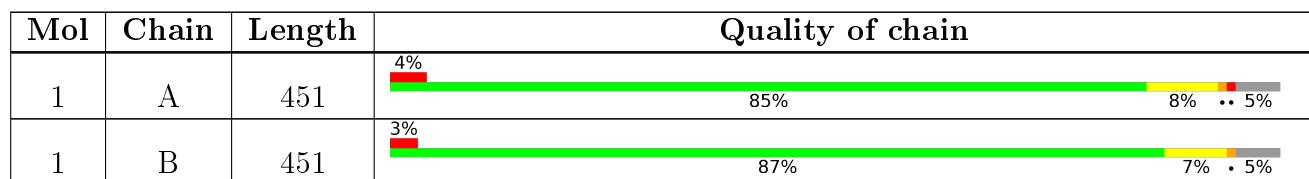
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7575 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 Os09g0567300 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total 3253	C 2097	N 531	O 619	S 6	0	0	0
1	B	428	Total 3240	C 2088	N 531	O 615	S 6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q652L6
A	-14	HIS	-	expression tag	UNP Q652L6
A	-13	HIS	-	expression tag	UNP Q652L6
A	-12	HIS	-	expression tag	UNP Q652L6
A	-11	HIS	-	expression tag	UNP Q652L6
A	-10	HIS	-	expression tag	UNP Q652L6
A	-9	ALA	-	expression tag	UNP Q652L6
A	-8	SER	-	expression tag	UNP Q652L6
A	-7	GLU	-	expression tag	UNP Q652L6
A	-6	ASN	-	expression tag	UNP Q652L6
A	-5	LEU	-	expression tag	UNP Q652L6
A	-4	TYR	-	expression tag	UNP Q652L6
A	-3	PHE	-	expression tag	UNP Q652L6
A	-2	GLN	-	expression tag	UNP Q652L6
A	-1	GLY	-	expression tag	UNP Q652L6
A	0	ALA	-	expression tag	UNP Q652L6
A	1	MET	-	expression tag	UNP Q652L6
A	2	ALA	-	expression tag	UNP Q652L6
A	3	SER	-	expression tag	UNP Q652L6
A	196	ALA	GLU	engineered mutation	UNP Q652L6
B	-15	HIS	-	expression tag	UNP Q652L6
B	-14	HIS	-	expression tag	UNP Q652L6
B	-13	HIS	-	expression tag	UNP Q652L6
B	-12	HIS	-	expression tag	UNP Q652L6
B	-11	HIS	-	expression tag	UNP Q652L6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q652L6
B	-9	ALA	-	expression tag	UNP Q652L6
B	-8	SER	-	expression tag	UNP Q652L6
B	-7	GLU	-	expression tag	UNP Q652L6
B	-6	ASN	-	expression tag	UNP Q652L6
B	-5	LEU	-	expression tag	UNP Q652L6
B	-4	TYR	-	expression tag	UNP Q652L6
B	-3	PHE	-	expression tag	UNP Q652L6
B	-2	GLN	-	expression tag	UNP Q652L6
B	-1	GLY	-	expression tag	UNP Q652L6
B	0	ALA	-	expression tag	UNP Q652L6
B	1	MET	-	expression tag	UNP Q652L6
B	2	ALA	-	expression tag	UNP Q652L6
B	3	SER	-	expression tag	UNP Q652L6
B	196	ALA	GLU	engineered mutation	UNP Q652L6

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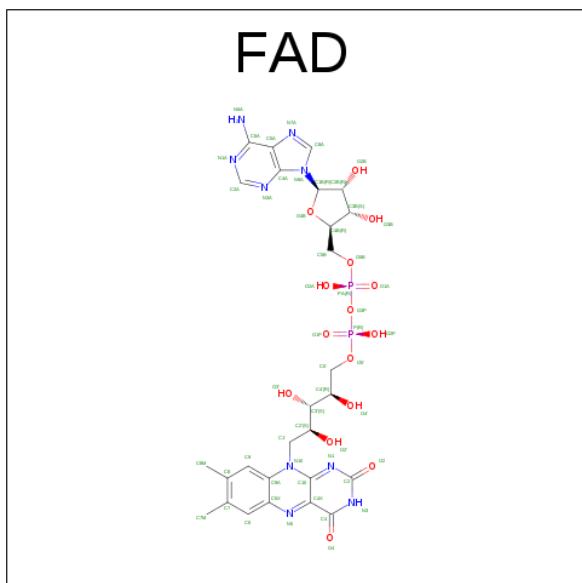
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).
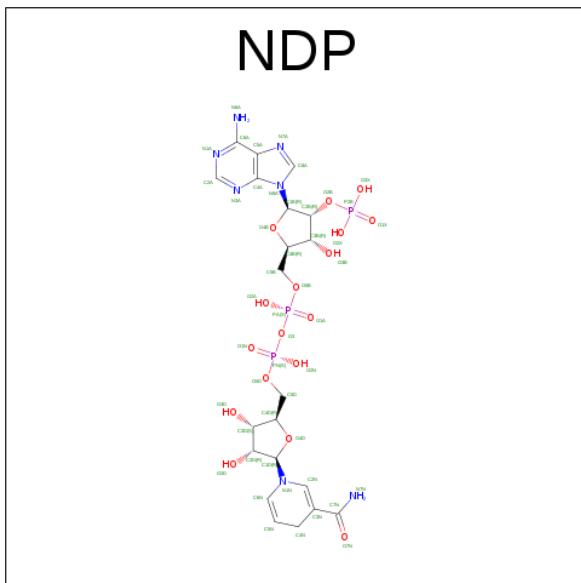
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	435	Total	O	0	0
			435	435		
4	B	445	Total	O	0	0
			445	445		

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: Os09g0567300 protein
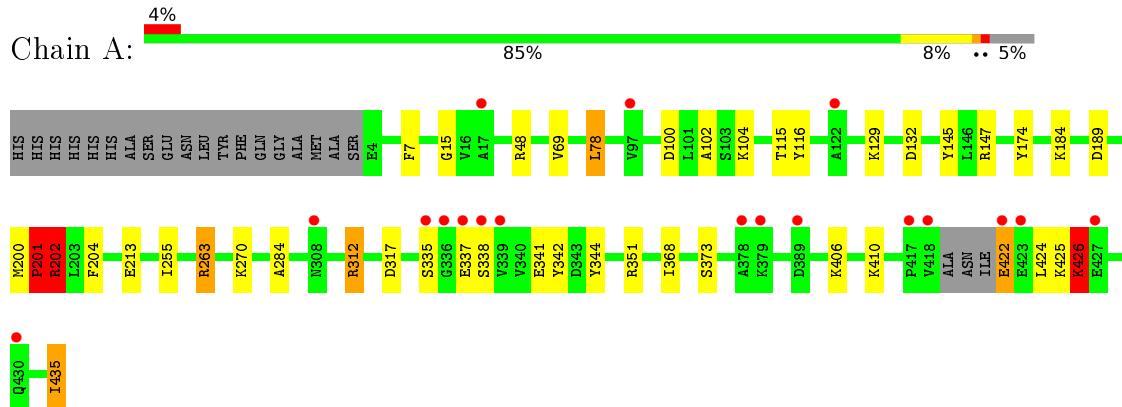
- Molecule 1: Os09g0567300 protein
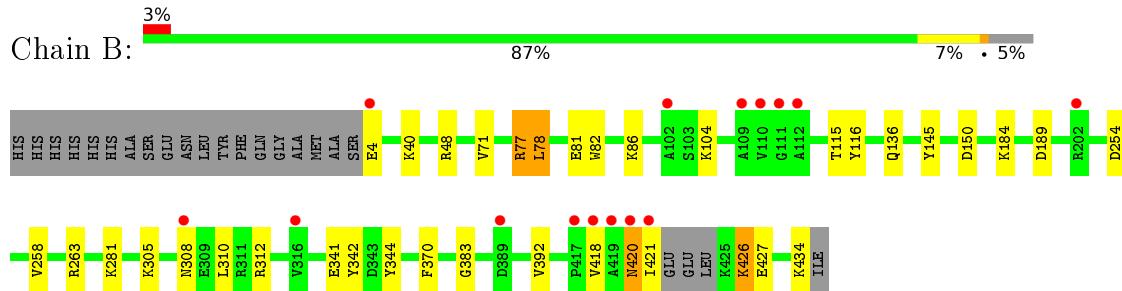
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.25Å 85.52Å 131.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 30.64 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.80) 99.2 (30.64-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.42 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.234 0.192 , 0.240	Depositor DCC
R_{free} test set	4089 reflections (5.26%)	DCC
Wilson B-factor (Å²)	30.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 45.9	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NDP, 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	0.93	1/3322 (0.0%)	1.02	13/4494 (0.3%)
1	B	0.90	0/3309	0.96	9/4477 (0.2%)
All	All	0.91	1/6631 (0.0%)	0.99	22/8971 (0.2%)

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLU	CD-OE1	5.31	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	A	312	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	48	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	312	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	189	ASP	CB-CG-OD1	7.91	125.42	118.30
1	B	77	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	B	150	ASP	CB-CG-OD1	7.52	125.07	118.30
1	B	189	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	201	PRO	N-CA-C	6.72	129.59	112.10
1	B	48	ARG	NE-CZ-NH1	6.40	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	A	202	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	312	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	132	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	189	ASP	CB-CG-OD1	5.52	123.26	118.30
1	A	317	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	201	PRO	CA-C-N	5.37	129.02	117.20
1	A	351	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	201	PRO	C-N-CA	5.24	134.80	121.70
1	B	78	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	147	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	254	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	254	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	PRO	Peptide
1	A	422	GLU	Peptide
1	A	425	LYS	Peptide
1	A	426	LYS	Peptide

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	3253	0	3256	24	0
1	B	3240	0	3244	18	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	48	0	26	1	0
3	B	48	0	26	3	0
4	A	435	0	0	6	0
4	B	445	0	0	6	0
All	All	7575	0	6614	45	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 3.

All (45) 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:136:GLN:HG2	4:B:866:HOH:O	1.55	1.03
1:B:71:VAL:CG1	1:B:77:ARG:HG2	2.12	0.79
3:B:501:NDP:O2B	4:B:601:HOH:O	2.08	0.71
1:A:100:ASP:OD1	4:A:601:HOH:O	2.14	0.64
1:B:71:VAL:HG11	1:B:77:ARG:HD3	1.79	0.63
1:A:200:MET:SD	1:A:202:ARG:NH2	2.73	0.62
3:B:501:NDP:P2B	4:B:601:HOH:O	2.59	0.59
1:A:312:ARG:O	4:A:602:HOH:O	2.16	0.59
1:A:102:ALA:N	4:A:609:HOH:O	2.37	0.57
1:A:263:ARG:NE	4:A:606:HOH:O	2.35	0.56
1:A:7:PHE:O	1:A:116:TYR:HA	2.07	0.54
1:A:200:MET:HB2	1:A:204:PHE:CD2	2.43	0.53
1:B:71:VAL:HG13	1:B:77:ARG:HG2	1.92	0.51
1:B:421:ILE:O	1:B:426:LYS:HG3	2.11	0.50
1:A:201:PRO:N	1:A:202:ARG:HB2	2.26	0.50
1:A:69:VAL:HG23	1:A:78:LEU:HD22	1.93	0.50
1:A:104:LYS:O	1:A:115:THR:HG23	2.12	0.49
1:A:200:MET:C	1:A:202:ARG:HB2	2.33	0.49
3:B:501:NDP:O1X	4:B:602:HOH:O	2.20	0.48
1:A:284:ALA:HB1	1:A:341:GLU:HB2	1.96	0.47
1:B:71:VAL:HG12	1:B:77:ARG:HG2	1.96	0.47
1:B:420:ASN:O	1:B:421:ILE:HG23	2.15	0.47
1:B:145:TYR:CE1	1:B:258:VAL:HB	2.49	0.47
1:B:421:ILE:O	1:B:421:ILE:HD12	2.15	0.47
1:B:392:VAL:HG23	1:B:418:VAL:CG2	2.44	0.46
1:B:104:LYS:HA	1:B:116:TYR:CZ	2.51	0.46
1:B:370:PHE:CZ	1:B:383:GLY:HA3	2.51	0.45
1:A:422:GLU:N	4:A:628:HOH:O	2.50	0.45
1:B:281:LYS:HE3	1:B:310:LEU:HD11	1.99	0.45
1:A:424:LEU:C	1:A:426:LYS:HB2	2.38	0.44
4:A:654:HOH:O	1:B:263:ARG:HG3	2.17	0.44
1:B:71:VAL:HG11	1:B:77:ARG:CD	2.48	0.43
1:A:200:MET:N	1:A:201:PRO:CD	2.81	0.43
1:A:342:TYR:CE2	1:A:344:TYR:HB2	2.55	0.42
1:B:82:TRP:CZ2	1:B:86:LYS:HD2	2.54	0.42
1:A:368:ILE:HD13	1:A:368:ILE:HA	1.84	0.42
1:A:435:ILE:HA	1:A:435:ILE:HD13	1.85	0.42
1:A:410:LYS:HD3	1:A:435:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD13	1:A:255:ILE:HG21	1.85	0.41
1:A:174:TYR:HB3	3:A:501:NDP:H42N	2.02	0.41
1:A:129:LYS:HA	1:A:145:TYR:CE1	2.55	0.41
1:A:406:LYS:HE3	4:B:992:HOH:O	2.21	0.41
1:A:15:GLY:HA3	2:A:500:FAD:O5B	2.20	0.41
1:B:342:TYR:CE2	1:B:344:TYR:HB2	2.56	0.41
1:B:4:GLU:N	4:B:625:HOH:O	2.53	0.41

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	425/451 (94%)	404 (95%)	18 (4%)	3 (1%)	26	11
1	B	424/451 (94%)	406 (96%)	16 (4%)	2 (0%)	34	17
All	All	849/902 (94%)	810 (95%)	34 (4%)	5 (1%)	30	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	420	ASN
1	A	202	ARG
1	B	427	GLU
1	A	426	LYS
1	A	337	GLU

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	335/352 (95%)	327 (98%)	8 (2%)	57	41
1	B	333/352 (95%)	323 (97%)	10 (3%)	48	31
All	All	668/704 (95%)	650 (97%)	18 (3%)	52	36

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	184	LYS
1	A	202	ARG
1	A	270	LYS
1	A	335	SER
1	A	338	SER
1	A	373	SER
1	A	435	ILE
1	B	40	LYS
1	B	78	LEU
1	B	81	GLU
1	B	115	THR
1	B	184	LYS
1	B	305	LYS
1	B	308	ASN
1	B	341	GLU
1	B	426	LYS
1	B	434	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN

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	FAD	A	500	-	52,58,58	1.57	11 (21%)	52,89,89	3.34	22 (42%)
3	NDP	A	501	-	44,52,52	1.20	4 (9%)	55,80,80	1.87	10 (18%)
3	NDP	B	501	-	44,52,52	1.26	6 (13%)	55,80,80	2.00	10 (18%)
2	FAD	B	502	-	52,58,58	1.30	8 (15%)	52,89,89	2.98	18 (34%)

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	500	-	-	0/30/50/50	0/6/6/6
3	NDP	A	501	-	-	0/30/77/77	0/5/5/5
3	NDP	B	501	-	-	0/30/77/77	0/5/5/5
2	FAD	B	502	-	-	0/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C10-N1	-3.78	1.29	1.35
2	B	502	FAD	C2-N3	-2.60	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FAD	C10-N10	-2.46	1.36	1.39
2	A	500	FAD	C1'-N10	-2.40	1.45	1.48
2	A	500	FAD	O2B-C2B	-2.37	1.37	1.43
2	A	500	FAD	P-O2P	-2.21	1.45	1.55
3	B	501	NDP	C4N-C5N	-2.19	1.44	1.49
3	A	501	NDP	C2N-N1N	-2.07	1.33	1.37
2	A	500	FAD	C6-C5X	-2.05	1.38	1.41
3	B	501	NDP	C2A-N1A	2.01	1.37	1.33
3	B	501	NDP	C3B-C2B	2.01	1.57	1.53
2	B	502	FAD	C4-C4X	2.08	1.45	1.41
2	B	502	FAD	C8-C7	2.09	1.46	1.41
3	B	501	NDP	C2N-C3N	2.30	1.41	1.34
2	A	500	FAD	C5A-C4A	2.37	1.45	1.40
2	B	502	FAD	C9A-C5X	2.39	1.47	1.42
2	B	502	FAD	C4X-C10	2.44	1.45	1.40
2	A	500	FAD	C2A-N3A	2.64	1.36	1.32
3	B	501	NDP	C5A-C4A	2.67	1.46	1.40
2	A	500	FAD	C4X-C10	2.69	1.45	1.40
3	A	501	NDP	C2N-C3N	2.75	1.42	1.34
3	A	501	NDP	O4B-C1B	2.76	1.45	1.41
2	A	500	FAD	O4B-C4B	2.81	1.51	1.45
2	A	500	FAD	C10-N10	2.85	1.42	1.39
2	B	502	FAD	C2A-N3A	2.86	1.37	1.32
3	A	501	NDP	C6N-C5N	3.09	1.38	1.33
2	A	500	FAD	C4-C4X	3.16	1.47	1.41
3	B	501	NDP	C6N-C5N	3.17	1.39	1.33
2	B	502	FAD	C4X-N5	3.21	1.38	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NDP	N3A-C2A-N1A	-10.51	120.62	128.87
2	A	500	FAD	N3A-C2A-N1A	-9.95	121.05	128.87
2	B	502	FAD	N3A-C2A-N1A	-8.68	122.05	128.87
2	B	502	FAD	C4-C4X-C10	-8.56	114.46	119.94
3	A	501	NDP	N3A-C2A-N1A	-7.15	123.25	128.87
2	A	500	FAD	C4B-O4B-C1B	-6.23	103.04	109.64
2	A	500	FAD	C1B-N9A-C4A	-6.15	119.94	126.81
2	B	502	FAD	C1B-N9A-C4A	-5.86	120.27	126.81
2	A	500	FAD	C4-C4X-C10	-5.75	116.26	119.94
3	A	501	NDP	C4B-O4B-C1B	-5.73	103.56	109.64
2	A	500	FAD	C4X-C4-N3	-5.33	116.55	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	NDP	C1B-N9A-C4A	-5.09	121.13	126.81
2	A	500	FAD	C4X-C10-N10	-4.75	117.06	120.52
2	B	502	FAD	N3-C2-N1	-4.23	120.57	127.69
3	B	501	NDP	C1B-N9A-C4A	-4.18	122.14	126.81
3	B	501	NDP	C4B-O4B-C1B	-3.70	105.72	109.64
2	A	500	FAD	N3-C2-N1	-3.98	120.99	127.69
3	B	501	NDP	C4B-O4B-C1B	-3.70	105.72	109.64
2	A	500	FAD	O4B-C1B-N9A	-3.62	101.27	108.11
2	B	502	FAD	C4X-C10-N10	-3.53	117.95	120.52
3	A	501	NDP	O3X-P2B-O2B	-3.47	96.23	106.62
2	B	502	FAD	C4X-C4-N3	-3.23	119.31	123.52
2	B	502	FAD	C4B-O4B-C1B	-2.85	106.63	109.64
3	B	501	NDP	C1D-N1N-C2N	-2.69	116.17	120.85
2	A	500	FAD	C9A-C5X-N5	-2.53	118.06	122.18
2	A	500	FAD	O2A-PA-O5B	-2.39	96.87	108.24
2	B	502	FAD	C9A-C5X-N5	-2.38	118.30	122.18
2	B	502	FAD	C8M-C8-C7	-2.29	115.79	120.73
3	B	501	NDP	C3B-C2B-C1B	-2.29	98.25	102.63
3	A	501	NDP	C3B-C2B-C1B	-2.24	98.35	102.63
3	A	501	NDP	C1D-N1N-C2N	-2.15	117.11	120.85
3	B	501	NDP	O4B-C1B-C2B	-2.14	102.74	106.60
2	B	502	FAD	O5B-PA-O1A	-2.09	100.64	109.21
3	A	501	NDP	C3N-C2N-N1N	-2.09	120.17	123.24
3	B	501	NDP	C4D-O4D-C1D	-2.09	104.92	109.52
2	A	500	FAD	O2P-P-O3P	2.06	114.10	105.27
3	B	501	NDP	N6A-C6A-N1A	2.06	121.98	118.52
3	A	501	NDP	O3X-P2B-O2X	2.06	115.02	107.44
2	A	500	FAD	O2A-PA-O3P	2.09	114.21	105.27
3	A	501	NDP	O3X-P2B-O1X	2.17	117.72	110.63
2	A	500	FAD	O3B-C3B-C2B	2.27	119.19	111.86
2	A	500	FAD	O2P-P-O1P	2.36	124.84	112.56
2	B	502	FAD	C2A-N1A-C6A	2.36	122.98	118.77
3	B	501	NDP	O4D-C1D-C2D	2.48	112.21	106.61
3	B	501	NDP	C2A-N1A-C6A	2.53	123.28	118.77
2	A	500	FAD	C4-C4X-N5	2.69	121.97	118.70
2	A	500	FAD	C6-C5X-N5	2.83	122.45	118.92
2	B	502	FAD	N6A-C6A-N1A	2.93	123.44	118.52
2	B	502	FAD	C5X-C9A-N10	3.10	119.90	117.58
3	A	501	NDP	N6A-C6A-N1A	3.11	123.74	118.52
2	A	500	FAD	N6A-C6A-N1A	3.26	123.99	118.52
2	A	500	FAD	C2A-N1A-C6A	3.38	124.79	118.77
2	B	502	FAD	C4X-N5-C5X	3.51	120.86	116.72
2	B	502	FAD	O2'-C2'-C1'	3.53	118.66	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C5X-C9A-N10	3.65	120.31	117.58
2	B	502	FAD	C4-C4X-N5	3.93	123.47	118.70
2	B	502	FAD	C1'-N10-C9A	5.11	124.75	118.83
2	A	500	FAD	C4X-N5-C5X	5.17	122.82	116.72
2	A	500	FAD	C1'-N10-C9A	5.94	125.72	118.83
2	B	502	FAD	C4-N3-C2	9.73	123.27	115.16
2	A	500	FAD	C4-N3-C2	11.17	124.48	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	1	0
3	A	501	NDP	1	0
3	B	501	NDP	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	429/451 (95%)	0.09	18 (4%)	40	34	20, 34, 59, 103	0
1	B	428/451 (94%)	0.02	15 (3%)	48	42	22, 34, 60, 88	0
All	All	857/902 (95%)	0.06	33 (3%)	43	37	20, 34, 60, 103	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	VAL	4.5
1	A	335	SER	4.1
1	A	418	VAL	3.8
1	A	308	ASN	3.7
1	A	337	GLU	3.5
1	B	418	VAL	3.4
1	B	109	ALA	3.2
1	B	419	ALA	3.1
1	B	308	ASN	3.1
1	A	427	GLU	3.0
1	B	420	ASN	2.9
1	B	111	GLY	2.9
1	B	417	PRO	2.9
1	A	423	GLU	2.7
1	A	338	SER	2.6
1	A	339	VAL	2.6
1	B	421	ILE	2.4
1	B	112	ALA	2.4
1	A	17	ALA	2.3
1	B	316	VAL	2.3
1	A	417	PRO	2.3
1	A	122	ALA	2.2
1	A	379	LYS	2.2
1	B	202	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	2.2
1	A	97	VAL	2.2
1	A	336	GLY	2.2
1	B	102	ALA	2.1
1	B	389	ASP	2.1
1	A	430	GLN	2.1
1	A	389	ASP	2.1
1	A	422	GLU	2.0
1	A	378	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, 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	FAD	B	502	53/53	0.96	0.15	0.51	20,25,36,40	0
2	FAD	A	500	53/53	0.97	0.14	-0.01	20,24,32,39	0
3	NDP	B	501	48/48	0.94	0.11	-0.12	20,25,51,61	0
3	NDP	A	501	48/48	0.96	0.08	-0.80	19,28,51,60	0

6.5 Other polymers (i)

There are no such residues in this entry.