Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:48 AM GMT

PDB ID	:	2OA1
Title	:	Crystal Structure of RebH, a FAD-dependent halogenase from Lechevalieria aerocolonigenes, the L-Tryptophan with FAD complex
Authors	:	Bitto, E.; Bingman, C.A.; Singh, S.; Phillips Jr., G.N.
Deposited on	:	2006-12-14
Resolution	:	2.15 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

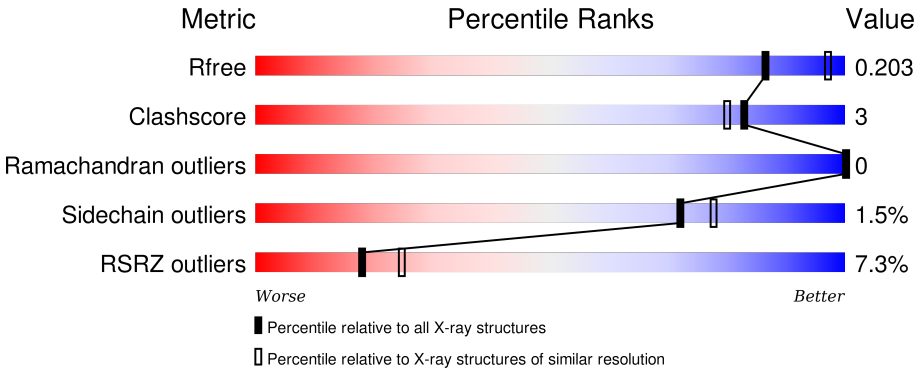
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	550	6% 90% 6% •
1	B	550	8% 87% 8% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	2001	-	-	-	X
4	FAD	A	2004	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9627 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 Tryptophan halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4234	2691	737	787	19			
1	B	527	Total	C	N	O	S	0	0	0
			4234	2691	737	787	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q8KHZ8
A	-18	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
A	-17	SER	-	EXPRESSION TAG	UNP Q8KHZ8
A	-16	SER	-	EXPRESSION TAG	UNP Q8KHZ8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-11	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-10	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
A	-9	SER	-	EXPRESSION TAG	UNP Q8KHZ8
A	-8	SER	-	EXPRESSION TAG	UNP Q8KHZ8
A	-7	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
A	-6	LEU	-	EXPRESSION TAG	UNP Q8KHZ8
A	-5	VAL	-	EXPRESSION TAG	UNP Q8KHZ8
A	-4	PRO	-	EXPRESSION TAG	UNP Q8KHZ8
A	-3	ARG	-	EXPRESSION TAG	UNP Q8KHZ8
A	-2	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
A	-1	SER	-	EXPRESSION TAG	UNP Q8KHZ8
A	0	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-19	MET	-	EXPRESSION TAG	UNP Q8KHZ8
B	-18	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
B	-17	SER	-	EXPRESSION TAG	UNP Q8KHZ8
B	-16	SER	-	EXPRESSION TAG	UNP Q8KHZ8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8KHZ8

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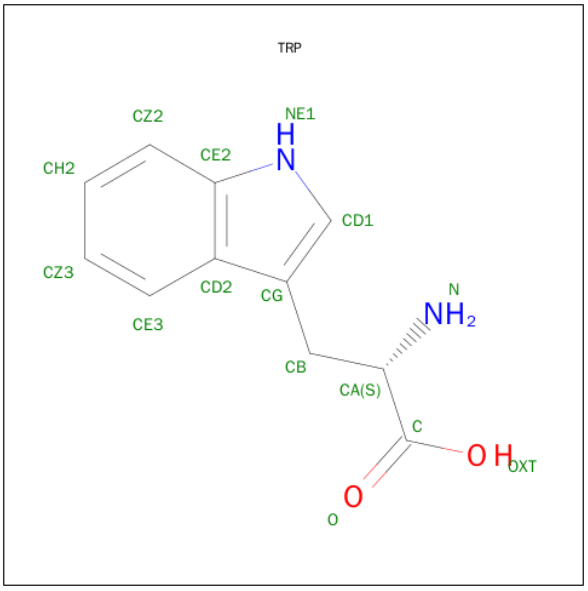
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-11	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-10	HIS	-	EXPRESSION TAG	UNP Q8KHZ8
B	-9	SER	-	EXPRESSION TAG	UNP Q8KHZ8
B	-8	SER	-	EXPRESSION TAG	UNP Q8KHZ8
B	-7	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
B	-6	LEU	-	EXPRESSION TAG	UNP Q8KHZ8
B	-5	VAL	-	EXPRESSION TAG	UNP Q8KHZ8
B	-4	PRO	-	EXPRESSION TAG	UNP Q8KHZ8
B	-3	ARG	-	EXPRESSION TAG	UNP Q8KHZ8
B	-2	GLY	-	EXPRESSION TAG	UNP Q8KHZ8
B	-1	SER	-	EXPRESSION TAG	UNP Q8KHZ8
B	0	HIS	-	EXPRESSION TAG	UNP Q8KHZ8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

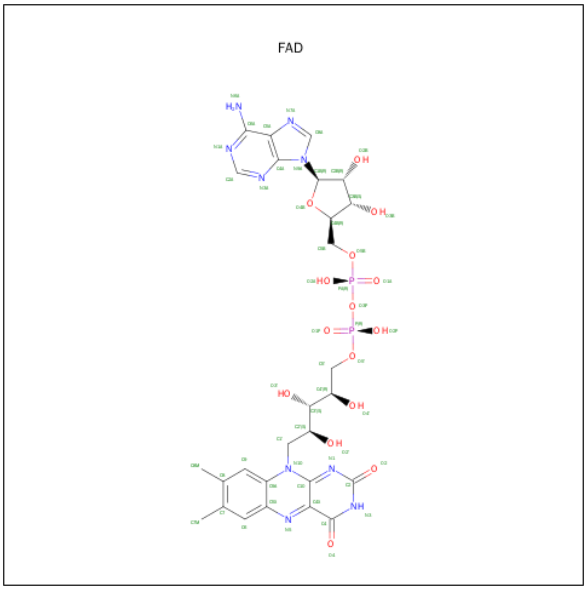
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



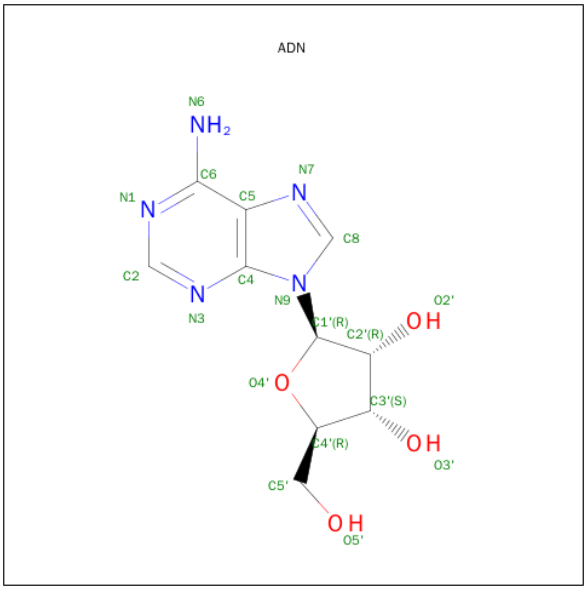
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			30	22	4	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 6 is water.

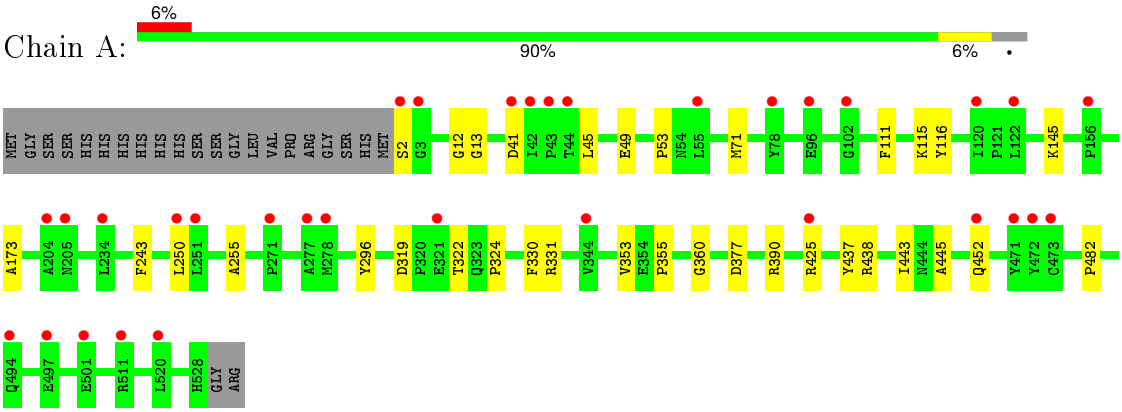
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	513	Total	O	0	0
			513	513		
6	B	543	Total	O	0	0
			543	543		

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.

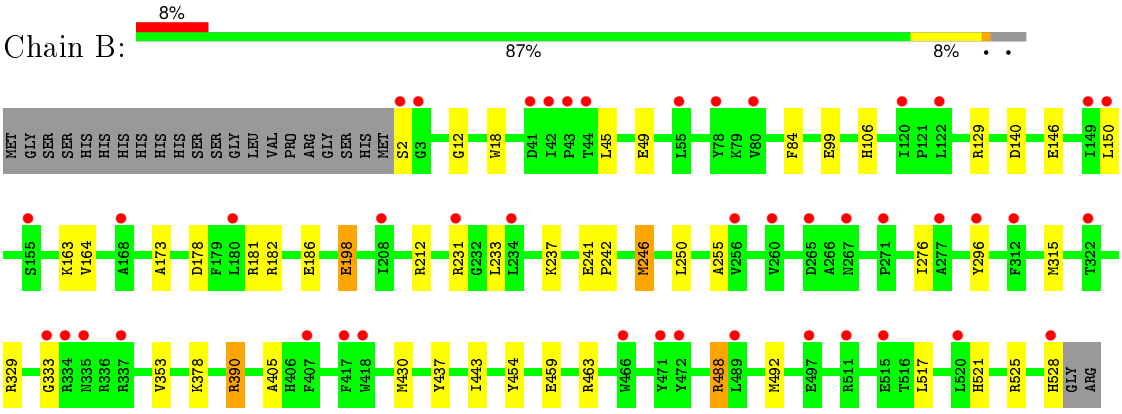
- Molecule 1: Tryptophan halogenase

Chain A:



- Molecule 1: Tryptophan halogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	114.49Å 114.49Å 231.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.95-2.15) 98.8 (19.95-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.152 , 0.194 0.161 , 0.203	Depositor DCC
R_{free} test set	4630 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.8	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 91914 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9627	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 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: ADN, FAD, CL

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	0.71	0/4351	0.69	3/5905 (0.1%)
1	B	0.74	1/4351 (0.0%)	0.71	2/5905 (0.0%)
All	All	0.72	1/8702 (0.0%)	0.70	5/11810 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	GLU	CG-CD	5.27	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	377	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	319	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	330	PHE	CB-CA-C	-5.41	99.59	110.40
1	B	246	MET	CG-SD-CE	5.01	108.22	100.20

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	4234	0	4038	19	0
1	B	4234	0	4038	30	0
2	A	1	0	0	1	0
3	A	30	0	18	1	0
4	A	53	0	31	4	0
5	B	19	0	13	4	0
6	A	513	0	0	7	1
6	B	543	0	0	7	0
All	All	9627	0	8138	51	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 3.

All (51) 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:231:ARG:HH12	5:B:2005:ADN:H8	1.16	1.06
1:A:71:MET:HE3	6:A:2385:HOH:O	1.60	1.01
1:B:231:ARG:NH1	5:B:2005:ADN:H8	1.80	0.95
1:A:49:GLU:HG3	1:A:173:ALA:HB2	1.53	0.90
1:B:12:GLY:HA2	5:B:2005:ADN:H1'	1.58	0.85
1:B:49:GLU:HG3	1:B:173:ALA:HB2	1.59	0.84
1:B:231:ARG:NH1	5:B:2005:ADN:C8	2.52	0.72
1:A:13:GLY:O	6:A:2358:HOH:O	2.11	0.68
1:A:437:TYR:HB2	1:A:443:ILE:HD11	1.79	0.65
1:B:390:ARG:HD2	6:B:2274:HOH:O	1.96	0.64
1:A:12:GLY:HA2	4:A:2004:FAD:H1B	1.83	0.60
1:A:250:LEU:HD13	1:A:353:VAL:HG23	1.84	0.59
1:A:390:ARG:NH1	6:A:2468:HOH:O	2.36	0.59
3:A:2003:TRP:N	1:B:454:TYR:HH	2.00	0.59
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.83	0.58
1:B:198:GLU:OE1	1:B:212:ARG:NH2	2.37	0.58
4:A:2004:FAD:H5'1	6:A:2116:HOH:O	2.05	0.56
1:B:492:MET:HE2	6:B:2331:HOH:O	2.06	0.55
1:A:243:PHE:CE2	1:A:331:ARG:HG2	2.41	0.55
1:B:255:ALA:HA	1:B:296:TYR:O	2.09	0.53
1:B:378:LYS:NZ	6:B:2066:HOH:O	2.41	0.53
1:B:528:HIS:C	6:B:2324:HOH:O	2.47	0.53
1:A:45:LEU:HD11	1:A:324:PRO:HB2	1.90	0.52
1:A:360:GLY:HA3	4:A:2004:FAD:H1'2	1.92	0.52
1:A:425:ARG:HD3	6:A:2307:HOH:O	2.10	0.51
1:B:129:ARG:HD2	6:B:2299:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:CZ	1:A:331:ARG:HG2	2.49	0.48
1:B:84:PHE:O	1:B:106:HIS:HA	2.14	0.47
1:B:18:TRP:CZ2	1:B:181:ARG:HG3	2.50	0.47
1:B:488:ARG:O	1:B:492:MET:HE3	2.13	0.47
1:A:71:MET:HG2	6:A:2385:HOH:O	2.14	0.47
4:A:2004:FAD:H51A	6:A:2481:HOH:O	2.15	0.46
1:A:49:GLU:CG	1:A:173:ALA:HB2	2.37	0.46
1:B:45:LEU:HD23	6:B:2514:HOH:O	2.14	0.46
1:A:255:ALA:HA	1:A:296:TYR:O	2.16	0.46
1:B:146:GLU:O	1:B:150:LEU:HG	2.16	0.46
1:B:250:LEU:HD13	1:B:353:VAL:HG23	1.99	0.45
1:B:521:HIS:NE2	1:B:525:ARG:HD2	2.32	0.44
1:A:438:ARG:HA	1:A:482:PRO:HA	2.00	0.44
1:A:355:PRO:HA	2:A:2001:CL:CL	2.56	0.43
1:B:178:ASP:OD2	1:B:182:ARG:NH1	2.52	0.43
1:B:163:LYS:HE3	6:B:2258:HOH:O	2.19	0.42
1:B:241:GLU:HA	1:B:242:PRO:HD3	1.94	0.42
1:B:276:ILE:HG21	1:B:315:MET:HE3	2.02	0.42
1:B:164:VAL:HG21	1:B:517:LEU:HD11	2.00	0.42
1:B:459:GLU:O	1:B:463:ARG:HG3	2.20	0.42
1:B:246:MET:HG3	1:B:333:GLY:HA2	2.02	0.41
1:A:116:TYR:OH	1:A:445:ALA:HB1	2.20	0.41
1:B:405:ALA:HB2	1:B:430:MET:CE	2.50	0.41
1:B:182:ARG:O	1:B:186:GLU:HB2	2.21	0.41
1:A:53:PRO:HD3	1:A:111:PHE:CE1	2.55	0.41

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)
6:A:2207:HOH:O	6:A:2207:HOH:O[4_565]	2.03	0.17

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	525/550 (96%)	514 (98%)	11 (2%)	0	100	100
1	B	525/550 (96%)	513 (98%)	12 (2%)	0	100	100
All	All	1050/1100 (96%)	1027 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/463 (96%)	438 (99%)	6 (1%)	74	80
1	B	444/463 (96%)	437 (98%)	7 (2%)	70	76
All	All	888/926 (96%)	875 (98%)	13 (2%)	72	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	41	ASP
1	A	115	LYS
1	A	145	LYS
1	A	322	THR
1	A	452	GLN
1	B	2	SER
1	B	198	GLU
1	B	233	LEU
1	B	237	LYS
1	B	329	ARG
1	B	390	ARG
1	B	488	ARG

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	267	ASN
1	A	452	GLN
1	A	494	GLN
1	B	29	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	TRP	A	2002	-	12,16,16	1.32	2 (16%)	7,22,22	1.08	0
3	TRP	A	2003	-	12,16,16	1.22	2 (16%)	7,22,22	1.02	0
4	FAD	A	2004	-	48,58,58	1.44	6 (12%)	54,89,89	2.47	12 (22%)
5	ADN	B	2005	-	16,21,21	1.17	2 (12%)	16,31,31	2.89	7 (43%)

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	TRP	A	2002	-	-	0/3/8/8	0/2/2/2
3	TRP	A	2003	-	-	0/3/8/8	0/2/2/2
4	FAD	A	2004	-	-	0/30/50/50	0/6/6/6
5	ADN	B	2005	-	-	0/2/22/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	TRP	CB-CG	2.03	1.57	1.51
5	B	2005	ADN	O4'-C1'	2.07	1.43	1.41
3	A	2003	TRP	CH2-CZ3	2.17	1.43	1.38
3	A	2002	TRP	CB-CG	2.32	1.58	1.51
4	A	2004	FAD	C10-N1	2.41	1.39	1.35
4	A	2004	FAD	C2A-N1A	2.54	1.38	1.33
3	A	2002	TRP	CZ3-CE3	2.99	1.43	1.36
5	B	2005	ADN	C5-C4	3.25	1.47	1.40
4	A	2004	FAD	C4-N3	3.36	1.39	1.33
4	A	2004	FAD	C1'-N10	3.43	1.52	1.48
4	A	2004	FAD	C2A-N3A	3.69	1.38	1.32
4	A	2004	FAD	C4X-N5	4.78	1.40	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2004	FAD	N3A-C2A-N1A	-12.15	119.59	128.89
5	B	2005	ADN	C2'-C1'-N9	-6.97	103.65	114.29
5	B	2005	ADN	N3-C2-N1	-6.47	123.94	128.89
4	A	2004	FAD	C4X-C4-N3	-3.63	118.62	123.59
4	A	2004	FAD	C1B-N9A-C4A	-3.15	122.19	126.94
5	B	2005	ADN	O3'-C3'-C2'	-2.92	102.34	111.83
4	A	2004	FAD	C4A-C5A-N7A	-2.82	106.88	109.48
5	B	2005	ADN	C4-C5-N7	-2.59	107.09	109.48
4	A	2004	FAD	C2B-C1B-N9A	-2.49	110.48	114.29
4	A	2004	FAD	O3'-C3'-C2'	2.04	113.90	108.75
4	A	2004	FAD	O3P-PA-O5B	2.15	108.64	102.94
5	B	2005	ADN	C2-N1-C6	2.18	122.67	118.77
5	B	2005	ADN	C4'-O4'-C1'	2.27	112.21	109.72
4	A	2004	FAD	O4B-C1B-N9A	2.37	113.06	108.10
4	A	2004	FAD	C4-C4X-N5	2.50	121.75	118.72
4	A	2004	FAD	C5X-C9A-N10	2.96	119.86	117.62
4	A	2004	FAD	C4X-N5-C5X	3.66	120.97	116.76
5	B	2005	ADN	O4'-C1'-N9	3.69	115.82	108.10
4	A	2004	FAD	C4-N3-C2	8.96	122.99	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	TRP	1	0
4	A	2004	FAD	4	0
5	B	2005	ADN	4	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	527/550 (95%)	0.39	33 (6%)	23	32	30, 36, 44, 58	0
1	B	527/550 (95%)	0.42	44 (8%)	14	20	30, 36, 44, 57	0
All	All	1054/1100 (95%)	0.40	77 (7%)	18	25	30, 36, 44, 58	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	7.6
1	A	2	SER	5.7
1	B	42	ILE	5.5
1	A	102	GLY	4.6
1	B	122	LEU	4.6
1	B	2	SER	4.5
1	B	520	LEU	4.4
1	A	44	THR	4.3
1	B	41	ASP	3.9
1	A	43	PRO	3.8
1	B	120	ILE	3.5
1	A	78	TYR	3.4
1	B	335	ASN	3.4
1	A	3	GLY	3.3
1	B	296	TYR	3.3
1	B	322	THR	3.3
1	A	321	GLU	3.2
1	A	204	ALA	3.1
1	A	452	GLN	3.1
1	B	472	TYR	3.1
1	B	312	PHE	3.0
1	B	334	ARG	3.0
1	A	494	GLN	3.0
1	A	41	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	MET	2.8
1	A	501	GLU	2.7
1	B	43	PRO	2.7
1	B	417	PHE	2.7
1	B	256	VAL	2.7
1	B	44	THR	2.7
1	A	425	ARG	2.6
1	B	515	GLU	2.6
1	A	471	TYR	2.6
1	B	418	TRP	2.6
1	A	205	ASN	2.6
1	A	520	LEU	2.5
1	A	120	ILE	2.5
1	B	231	ARG	2.5
1	A	472	TYR	2.5
1	B	511	ARG	2.5
1	B	497	GLU	2.4
1	A	55	LEU	2.4
1	A	251	LEU	2.4
1	B	407	PHE	2.4
1	A	497	GLU	2.4
1	B	337	ARG	2.4
1	A	122	LEU	2.4
1	B	234	LEU	2.4
1	B	149	ILE	2.3
1	B	55	LEU	2.3
1	A	511	ARG	2.3
1	B	155	SER	2.3
1	B	150	LEU	2.3
1	B	333	GLY	2.3
1	A	277	ALA	2.3
1	B	180	LEU	2.3
1	B	277	ALA	2.2
1	B	466	TRP	2.2
1	A	250	LEU	2.2
1	B	208	ILE	2.2
1	B	168	ALA	2.2
1	A	271	PRO	2.2
1	B	267	ASN	2.2
1	A	156	PRO	2.2
1	A	96	GLU	2.2
1	A	344	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLY	2.1
1	B	489	LEU	2.1
1	B	78	TYR	2.1
1	B	471	TYR	2.1
1	B	260	VAL	2.1
1	B	528	HIS	2.1
1	A	234	LEU	2.1
1	A	473	CYS	2.1
1	B	265	ASP	2.0
1	B	271	PRO	2.0
1	B	80	VAL	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
2	CL	A	2001	1/1	0.97	0.28	7.78	48,48,48,48	0
4	FAD	A	2004	53/53	0.88	0.22	2.04	30,45,55,56	53
5	ADN	B	2005	19/19	0.74	0.27	1.43	48,50,54,56	19
3	TRP	A	2002	15/15	0.93	0.18	1.26	37,40,43,43	0
3	TRP	A	2003	15/15	0.93	0.18	0.99	29,31,32,34	0

6.5 Other polymers (i)

There are no such residues in this entry.