



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2OAL
Title : RebH with bound FAD
Authors : Blasiak, L.C.; Drennan, C.L.
Deposited on : 2006-12-16
Resolution : 2.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

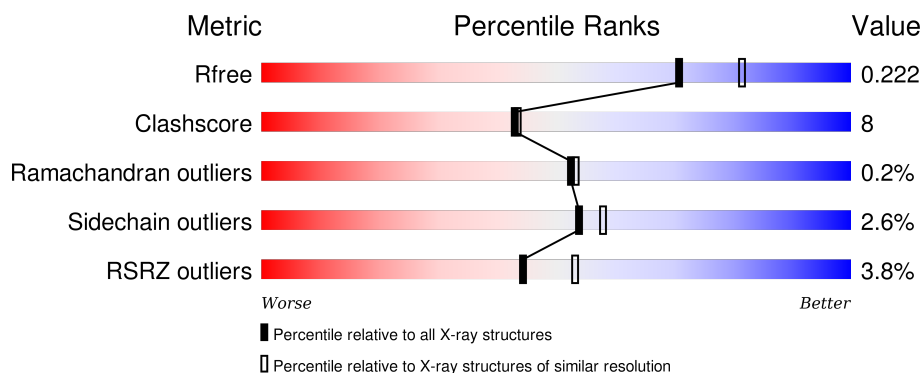
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	550	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9136 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
			4224	2686	734	785	19			
1	B	528	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	-	INITIATING METHIONINE	UNP Q8KHZ8
A	-18	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-17	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-16	SER	-	CLONING ARTIFACT	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	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-8	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-7	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-6	LEU	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-5	VAL	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-4	PRO	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-3	ARG	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-2	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
A	-1	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
A	0	HIS	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-19	MET	-	INITIATING METHIONINE	UNP Q8KHZ8
B	-18	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-17	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-16	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8KHZ8

Continued on next page...

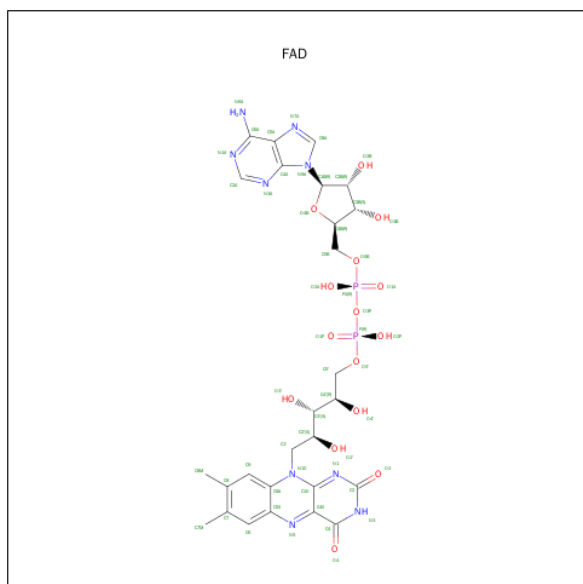
Continued from previous page...

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	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-8	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-7	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-6	LEU	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-5	VAL	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-4	PRO	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-3	ARG	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-2	GLY	-	CLONING ARTIFACT	UNP Q8KHZ8
B	-1	SER	-	CLONING ARTIFACT	UNP Q8KHZ8
B	0	HIS	-	CLONING ARTIFACT	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 FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			52	27	9	14	2		

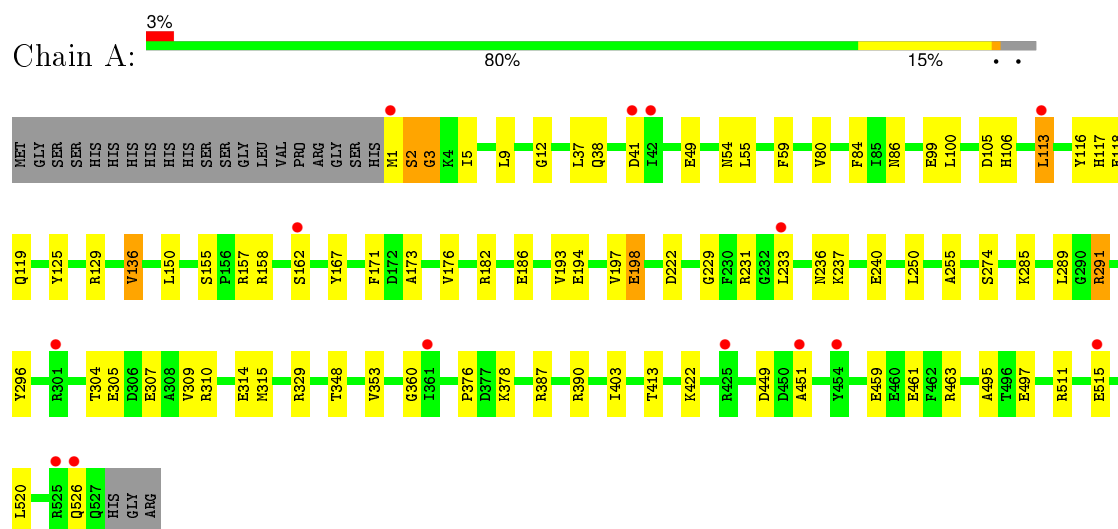
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	308	Total	O	0	0
			308	308		
4	B	264	Total	O	0	0
			264	264		

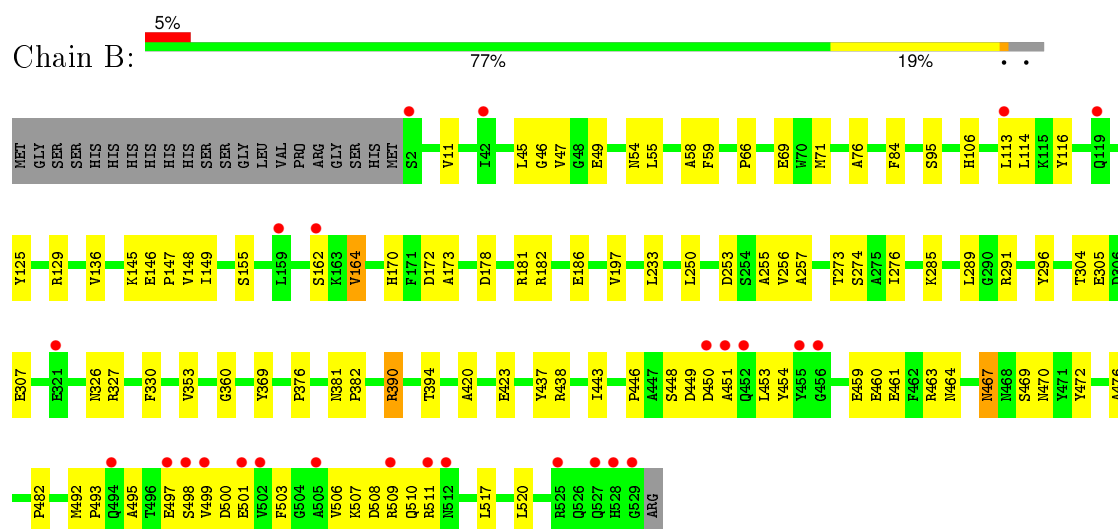
3 Residue-property plots [i](#)

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



• Molecule 1: Tryptophan halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	114.72Å 114.72Å 230.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.90 – 2.10 41.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.90-2.10) 97.9 (41.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.222 0.197 , 0.222	Depositor DCC
R_{free} test set	4874 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	EDS
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 99855 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9136	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 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/4340	0.61	2/5891 (0.0%)
1	B	0.33	0/4351	0.56	0/5905
All	All	0.36	0/8691	0.59	2/11796 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2	SER	N-CA-C	7.85	132.19	111.00
1	A	3	GLY	N-CA-C	-6.33	97.27	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide

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	4224	0	4027	66	0
1	B	4234	0	4035	70	0
2	A	1	0	0	0	0
3	A	53	0	31	3	0
3	B	52	0	31	2	0
4	A	308	0	0	3	0
4	B	264	0	0	2	0
All	All	9136	0	8124	137	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 8.

All (137) 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:113:LEU:CD1	1:A:451:ALA:HB2	1.29	1.53
1:A:113:LEU:CD1	1:A:451:ALA:CB	2.24	1.15
1:A:113:LEU:H	1:A:113:LEU:HD22	1.11	1.13
1:A:113:LEU:CD2	1:A:113:LEU:H	1.66	1.06
1:A:113:LEU:HD11	1:A:451:ALA:HB2	1.12	1.06
1:A:113:LEU:HD12	1:A:451:ALA:HB2	1.08	1.05
1:A:113:LEU:HD12	1:A:451:ALA:CB	1.88	1.02
1:A:113:LEU:HD11	1:A:451:ALA:CB	1.92	0.97
1:A:113:LEU:HD22	1:A:113:LEU:N	1.82	0.93
1:A:49:GLU:HG3	1:A:173:ALA:HB2	1.52	0.92
1:B:113:LEU:HD21	1:B:451:ALA:HB2	1.50	0.92
1:B:45:LEU:H	1:B:326:ASN:HD21	1.25	0.84
1:B:49:GLU:HG3	1:B:173:ALA:HB2	1.62	0.82
1:B:467:ASN:HD22	1:B:469:SER:H	1.37	0.73
1:B:467:ASN:H	1:B:470:ASN:HD22	1.36	0.72
1:A:387:ARG:HH12	1:A:390:ARG:NH1	1.90	0.70
1:A:116:TYR:HD1	1:A:449:ASP:HB3	1.57	0.70
1:B:148:VAL:HG21	1:B:510:GLN:HB2	1.74	0.69
1:B:304:THR:OG1	1:B:307:GLU:HG3	1.94	0.68
1:A:511:ARG:O	1:A:515:GLU:HG3	1.93	0.68
1:B:45:LEU:N	1:B:326:ASN:HD21	1.92	0.67
3:B:601:FAD:PA	3:B:601:FAD:P	2.93	0.66
1:B:148:VAL:CG2	1:B:510:GLN:HB2	2.25	0.66
1:A:12:GLY:HA2	3:A:600:FAD:H1B	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD21	1:B:451:ALA:CB	2.25	0.65
1:A:233:LEU:HD12	1:A:237:LYS:HD3	1.78	0.64
1:B:507:LYS:O	1:B:511:ARG:HG3	1.97	0.64
1:A:310:ARG:O	1:A:314:GLU:HG3	1.97	0.64
1:A:129:ARG:HD3	4:A:1178:HOH:O	1.96	0.63
1:B:498:SER:O	1:B:501:GLU:HG2	1.99	0.63
1:A:387:ARG:NH1	1:A:390:ARG:HD2	2.14	0.62
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.79	0.62
1:B:113:LEU:CD2	1:B:451:ALA:HB2	2.26	0.61
1:B:467:ASN:H	1:B:470:ASN:ND2	1.98	0.61
1:A:113:LEU:HD12	1:A:451:ALA:CA	2.31	0.60
1:A:197:VAL:HB	1:A:233:LEU:HD21	1.83	0.60
1:A:459:GLU:O	1:A:463:ARG:HD3	2.00	0.60
1:A:49:GLU:CG	1:A:173:ALA:HB2	2.29	0.60
1:B:450:ASP:OD1	1:B:453:LEU:HG	2.02	0.59
1:A:80:VAL:HB	1:A:150:LEU:HD21	1.83	0.59
1:B:503:PHE:O	1:B:506:VAL:HG22	2.03	0.59
1:B:459:GLU:O	1:B:463:ARG:HG3	2.03	0.58
1:B:369:TYR:OH	1:B:459:GLU:HG2	2.03	0.58
1:B:164:VAL:HG11	1:B:517:LEU:HD21	1.87	0.56
1:B:467:ASN:HD22	1:B:469:SER:N	2.03	0.56
1:A:158:ARG:HD2	1:A:162:SER:OG	2.06	0.56
1:B:467:ASN:HD21	1:B:469:SER:HB2	1.71	0.56
1:A:413:THR:HG22	1:A:422:LYS:HE3	1.88	0.56
1:B:71:MET:HB2	1:B:76:ALA:HB3	1.88	0.55
1:A:5:ILE:HG23	1:A:222:ASP:HB2	1.87	0.55
1:A:182:ARG:O	1:A:186:GLU:HB2	2.06	0.54
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.89	0.54
1:A:125:TYR:O	1:A:129:ARG:HG3	2.08	0.54
1:B:467:ASN:ND2	1:B:469:SER:H	2.05	0.53
1:A:38:GLN:O	1:A:194:GLU:HA	2.09	0.53
1:A:305:GLU:O	1:A:309:VAL:HG23	2.09	0.52
1:B:467:ASN:N	1:B:470:ASN:HD22	2.05	0.52
1:A:116:TYR:CD1	1:A:449:ASP:HB3	2.42	0.51
1:A:37:LEU:HD23	1:A:193:VAL:HB	1.92	0.51
1:A:231:ARG:HG2	4:A:1306:HOH:O	2.11	0.51
1:B:420:ALA:HA	1:B:423:GLU:OE2	2.11	0.50
1:A:387:ARG:HH12	1:A:390:ARG:HD2	1.76	0.50
1:B:509:ARG:HD2	4:B:789:HOH:O	2.11	0.50
1:A:250:LEU:HD13	1:A:353:VAL:HG23	1.93	0.50
1:B:256:VAL:O	1:B:256:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLU:HG3	1:A:463:ARG:HH11	1.78	0.49
1:B:305:GLU:OE2	1:B:327:ARG:HD3	2.13	0.49
1:B:182:ARG:O	1:B:186:GLU:HB2	2.12	0.49
1:A:387:ARG:HH12	1:A:390:ARG:HH11	1.59	0.49
1:B:66:PRO:HG2	1:B:69:GLU:HB2	1.95	0.49
1:B:492:MET:HB3	1:B:495:ALA:HB3	1.94	0.49
1:A:84:PHE:O	1:A:106:HIS:HA	2.13	0.48
1:B:113:LEU:HD11	1:B:451:ALA:HB2	1.95	0.48
1:B:508:ASP:OD1	1:B:511:ARG:NH2	2.46	0.48
1:B:113:LEU:HD11	1:B:451:ALA:CB	2.45	0.47
1:B:155:SER:HB2	1:B:520:LEU:HA	1.96	0.47
1:B:116:TYR:CD2	1:B:449:ASP:HB3	2.49	0.47
1:A:12:GLY:HA2	3:A:600:FAD:C1B	2.44	0.47
1:A:3:GLY:O	1:A:378:LYS:HG3	2.15	0.47
1:B:145:LYS:HD3	1:B:509:ARG:HG2	1.96	0.47
1:A:353:VAL:HG21	1:A:403:ILE:HD12	1.96	0.46
1:B:197:VAL:HG11	1:B:233:LEU:HD21	1.96	0.46
1:B:55:LEU:O	1:B:59:PHE:HB3	2.15	0.46
1:A:233:LEU:O	1:A:237:LYS:HB3	2.15	0.46
1:A:117:HIS:HB3	1:A:125:TYR:CE2	2.51	0.46
1:A:229:GLY:HA2	1:A:348:THR:OG1	2.16	0.46
1:B:438:ARG:HA	1:B:482:PRO:HA	1.98	0.46
1:A:54:ASN:ND2	1:A:461:GLU:OE1	2.41	0.46
1:A:171:PHE:CE1	1:A:176:VAL:HG21	2.51	0.45
1:A:54:ASN:HD22	1:A:461:GLU:CD	2.17	0.45
1:A:9:LEU:HD11	1:A:37:LEU:HG	1.98	0.45
1:B:113:LEU:HD21	1:B:451:ALA:CA	2.46	0.45
1:B:360:GLY:HA3	3:B:601:FAD:N1	2.32	0.44
1:B:289:LEU:HD12	1:B:289:LEU:N	2.33	0.44
1:A:360:GLY:HA3	3:A:600:FAD:H1'2	1.99	0.44
1:B:95:SER:HA	1:B:276:ILE:HD13	1.99	0.44
1:A:237:LYS:HD3	4:A:1213:HOH:O	2.18	0.44
1:B:170:HIS:NE2	1:B:273:THR:OG1	2.44	0.44
1:B:472:TYR:O	1:B:476:ALA:HB3	2.18	0.44
1:B:255:ALA:HA	1:B:296:TYR:O	2.18	0.43
1:A:157:ARG:NH1	1:A:167:TYR:OH	2.51	0.43
1:B:47:VAL:HG11	1:B:257:ALA:CB	2.48	0.43
1:B:250:LEU:CD1	1:B:353:VAL:HG23	2.48	0.43
1:B:54:ASN:HB3	1:B:461:GLU:OE1	2.19	0.43
1:B:11:VAL:HG11	1:B:233:LEU:HD23	2.00	0.43
1:B:253:ASP:HA	1:B:330:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD23	1:A:113:LEU:H	1.70	0.43
1:B:113:LEU:CG	1:B:451:ALA:HB2	2.48	0.43
1:A:289:LEU:O	1:A:291:ARG:HD2	2.19	0.43
1:A:304:THR:OG1	1:A:307:GLU:HG3	2.19	0.42
1:A:387:ARG:HH12	1:A:390:ARG:CZ	2.32	0.42
1:A:86:ASN:HA	1:A:105:ASP:OD2	2.20	0.42
1:B:148:VAL:HG23	1:B:149:ILE:N	2.35	0.42
1:A:459:GLU:HG3	1:A:463:ARG:NH1	2.33	0.42
1:B:46:GLY:HA3	1:B:172:ASP:OD2	2.19	0.42
1:A:117:HIS:HE1	1:A:495:ALA:O	2.02	0.42
1:A:274:SER:HB2	1:A:285:LYS:HB3	2.00	0.42
1:A:255:ALA:HA	1:A:296:TYR:O	2.19	0.42
1:A:236:ASN:O	1:A:240:GLU:HA	2.19	0.42
1:B:136:VAL:O	1:B:136:VAL:HG12	2.20	0.42
1:A:155:SER:HB2	1:A:520:LEU:HA	2.01	0.42
1:A:136:VAL:O	1:A:136:VAL:HG13	2.20	0.42
1:B:181:ARG:HH11	1:B:181:ARG:HG2	1.85	0.42
1:B:250:LEU:HD13	1:B:353:VAL:HG23	2.02	0.41
1:B:493:PRO:O	1:B:497:GLU:HB2	2.20	0.41
1:B:125:TYR:CG	1:B:499:VAL:HG21	2.55	0.41
1:B:84:PHE:O	1:B:106:HIS:HA	2.20	0.41
1:A:55:LEU:O	1:A:59:PHE:HB3	2.20	0.41
1:B:162:SER:HA	4:B:675:HOH:O	2.20	0.41
1:B:446:PRO:HB2	1:B:448:SER:O	2.21	0.41
1:B:54:ASN:O	1:B:58:ALA:HB3	2.20	0.41
1:B:390:ARG:O	1:B:394:THR:HG23	2.21	0.40
1:A:198:GLU:O	1:A:198:GLU:HG3	2.21	0.40
1:B:467:ASN:HD22	1:B:467:ASN:C	2.25	0.40
1:A:118:GLU:O	1:A:119:GLN:HB2	2.21	0.40
1:B:146:GLU:HB2	1:B:147:PRO:HD3	2.04	0.40
1:B:381:ASN:HA	1:B:382:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	511 (97%)	13 (2%)	1 (0%)	52	53
1	B	526/550 (96%)	504 (96%)	21 (4%)	1 (0%)	52	53
All	All	1051/1100 (96%)	1015 (97%)	34 (3%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	B	454	TYR

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	441/463 (95%)	429 (97%)	12 (3%)	52	56
1	B	443/463 (96%)	432 (98%)	11 (2%)	55	59
All	All	884/926 (96%)	861 (97%)	23 (3%)	54	58

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	99	GLU
1	A	100	LEU
1	A	113	LEU
1	A	136	VAL
1	A	198	GLU
1	A	291	ARG
1	A	315	MET
1	A	329	ARG
1	A	376	PRO
1	A	497	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	526	GLN
1	B	114	LEU
1	B	129	ARG
1	B	164	VAL
1	B	178	ASP
1	B	291	ARG
1	B	376	PRO
1	B	390	ARG
1	B	460	GLU
1	B	464	ASN
1	B	467	ASN
1	B	500	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	205	ASN
1	A	207	ASN
1	A	252	ASN
1	A	259	GLN
1	A	464	ASN
1	A	494	GLN
1	A	510	GLN
1	A	526	GLN
1	B	119	GLN
1	B	124	HIS
1	B	153	ASN
1	B	205	ASN
1	B	207	ASN
1	B	252	ASN
1	B	267	ASN
1	B	326	ASN
1	B	457	ASN
1	B	467	ASN
1	B	470	ASN
1	B	494	GLN
1	B	510	GLN
1	B	527	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	FAD	A	600	-	48,58,58	2.06	10 (20%)	54,89,89	2.56	8 (14%)
3	FAD	B	601	-	40,56,58	2.16	9 (22%)	43,82,89	2.75	7 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	FAD	B	601	-	-	0/18/42/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C5'-C4'	2.67	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C1'-N10	3.23	1.51	1.48
3	B	601	FAD	C2A-N1A	3.26	1.40	1.33
3	A	600	FAD	C2A-N1A	3.37	1.40	1.33
3	B	601	FAD	C10-N10	3.46	1.43	1.39
3	A	600	FAD	C4-N3	3.73	1.40	1.33
3	A	600	FAD	C10-N10	3.74	1.43	1.39
3	B	601	FAD	C4-N3	3.76	1.40	1.33
3	A	600	FAD	C5X-N5	3.82	1.41	1.35
3	B	601	FAD	C5X-N5	3.92	1.41	1.35
3	B	601	FAD	C9A-N10	3.99	1.44	1.38
3	B	601	FAD	C10-N1	4.01	1.42	1.35
3	A	600	FAD	C10-N1	4.04	1.42	1.35
3	A	600	FAD	C9A-N10	4.27	1.44	1.38
3	A	600	FAD	C2A-N3A	4.49	1.40	1.32
3	A	600	FAD	C1'-N10	4.56	1.53	1.48
3	B	601	FAD	C2A-N3A	4.88	1.40	1.32
3	A	600	FAD	C4X-N5	5.69	1.42	1.33
3	B	601	FAD	C4X-N5	5.84	1.42	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	N3A-C2A-N1A	-12.47	119.35	128.89
3	B	601	FAD	N3A-C2A-N1A	-12.11	119.62	128.89
3	A	600	FAD	C1B-N9A-C4A	-5.27	119.00	126.94
3	B	601	FAD	C4X-C4-N3	-4.47	117.47	123.59
3	B	601	FAD	C1B-N9A-C4A	-4.38	120.33	126.94
3	A	600	FAD	C4X-C4-N3	-4.36	117.62	123.59
3	A	600	FAD	O2'-C2'-C1'	2.00	114.87	109.94
3	B	601	FAD	O2'-C2'-C1'	2.20	115.36	109.94
3	A	600	FAD	O3P-P-O5'	2.24	108.87	102.94
3	B	601	FAD	O4'-C4'-C3'	2.70	115.80	109.02
3	A	600	FAD	O4'-C4'-C3'	2.72	115.85	109.02
3	B	601	FAD	C4X-N5-C5X	4.00	121.36	116.76
3	A	600	FAD	C4X-N5-C5X	4.08	121.45	116.76
3	A	600	FAD	C4-N3-C2	8.93	122.97	115.25
3	B	601	FAD	C4-N3-C2	8.96	123.00	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	3	0
3	B	601	FAD	2	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, 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	527/550 (95%)	-0.04	14 (2%) 58 65	19, 33, 55, 74	0
1	B	528/550 (96%)	0.10	26 (4%) 33 42	20, 37, 66, 83	0
All	All	1055/1100 (95%)	0.03	40 (3%) 44 53	19, 35, 62, 83	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ALA	5.1
1	B	501	GLU	4.1
1	B	2	SER	4.1
1	B	505	ALA	4.1
1	B	452	GLN	4.0
1	B	113	LEU	3.7
1	B	499	VAL	3.7
1	A	451	ALA	3.3
1	B	450	ASP	3.1
1	B	528	HIS	3.1
1	A	1	MET	2.9
1	B	455	TYR	2.7
1	B	162	SER	2.7
1	B	529	GLY	2.7
1	B	509	ARG	2.6
1	A	361	ILE	2.6
1	B	498	SER	2.5
1	B	525	ARG	2.5
1	B	497	GLU	2.5
1	A	301	ARG	2.5
1	B	456	GLY	2.5
1	A	113	LEU	2.4
1	B	494	GLN	2.4
1	B	511	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	2.4
1	B	159	LEU	2.4
1	A	162	SER	2.4
1	B	42	ILE	2.4
1	B	502	VAL	2.3
1	A	233	LEU	2.3
1	A	425	ARG	2.3
1	A	515	GLU	2.3
1	B	321	GLU	2.3
1	B	527	GLN	2.2
1	A	525	ARG	2.1
1	A	526	GLN	2.1
1	A	42	ILE	2.1
1	B	119	GLN	2.1
1	A	454	TYR	2.0
1	B	512	ASN	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
3	FAD	A	600	53/53	0.83	0.20	1.30	57,68,75,77	0
3	FAD	B	601	52/53	0.89	0.14	0.42	42,54,62,63	0
2	CL	A	1000	1/1	0.83	0.08	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.