



Full wwPDB X-ray Structure Validation Report

Aug 11, 2014 – 06:09 PM EDT

PDB ID : 4OCG
Title : Structure of the Shewanella loihica PV-4 NADH-dependent persulfide reductase F161A Mutant
Authors : Lee, K.-H.; Sazinsky, M.H.; Crane, E.J.
Deposited on : 2014-01-09
Resolution : 2.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

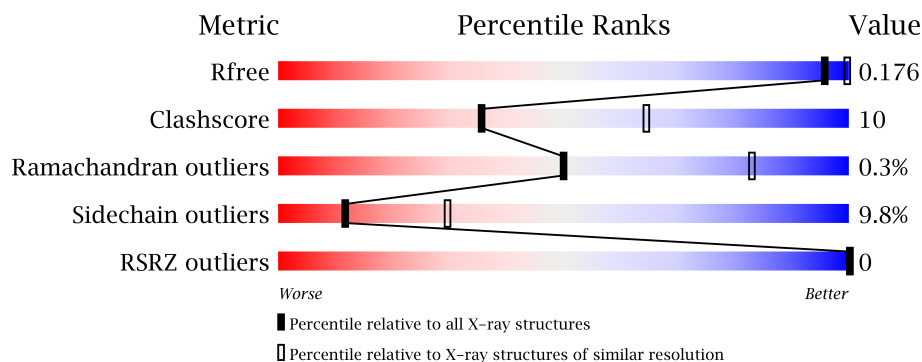
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance



The reported resolution of this entry is 2.75 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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	574	
1	B	574	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8950 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

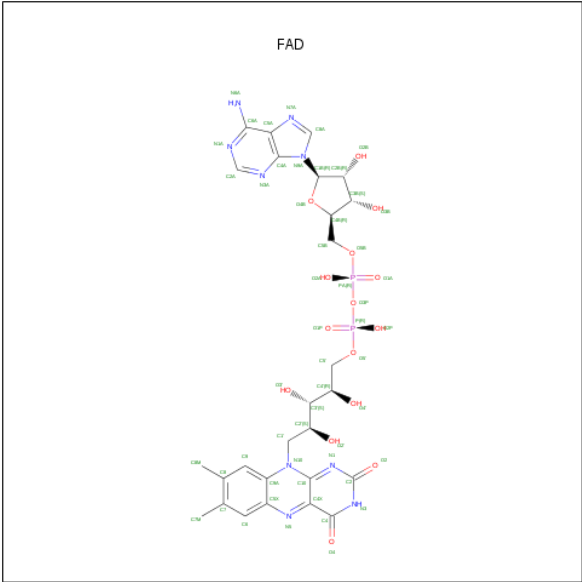
- Molecule 1 is a protein called FAD-dependent pyridine nucleotide-disulphideoxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4292	2690	763	819	20			
1	B	565	Total	C	N	O	S	0	0	0
			4291	2690	762	819	20			

There are 18 discrepancies between the modelled and reference sequences:

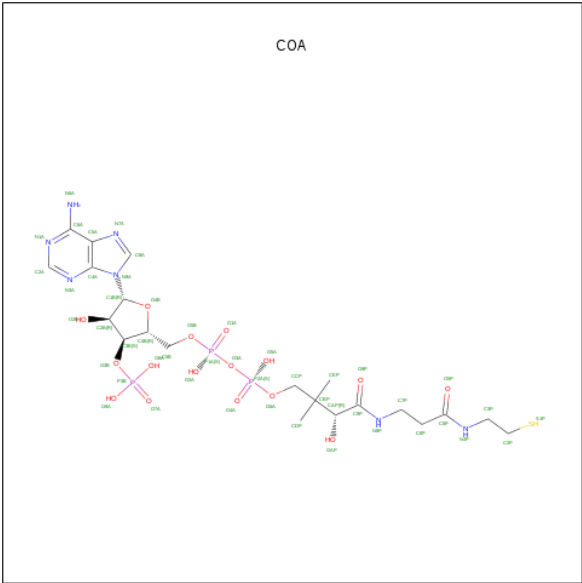
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ALA	PHE	ENGINEERED MUTATION	UNP A3QAV3
A	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
A	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
A	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	574	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	161	ALA	PHE	ENGINEERED MUTATION	UNP A3QAV3
B	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
B	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
B	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	574	HIS	-	EXPRESSION TAG	UNP A3QAV3

- 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 COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total 83	O 83	0	0
4	B	82	Total 82	O 82	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	133.71 Å 133.71 Å 84.32 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.75 35.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.75) 96.3 (35.10-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.73 (at 2.76 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.122 , 0.173 0.127 , 0.176	Depositor DCC
R_{free} test set	2139 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	1.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 4.6	EDS
Estimated twinning fraction	0.629 for H, K, L 0.371 for -H, H+K, -L 0.117 for -h,-k,l 0.117 for h,-h-k,-l 0.357 for -k,-h,-l	Xtriage
Reported twinning fraction	0.629 for H, K, L 0.371 for -H, H+K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 42327 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8950	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, 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	1.01	0/4361	0.91	4/5904 (0.1%)
1	B	1.06	3/4360 (0.1%)	0.93	5/5902 (0.1%)
All	All	1.03	3/8721 (0.0%)	0.92	9/11806 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	VAL	CB-CG1	-5.55	1.41	1.52
1	B	558	TYR	CD2-CE2	-5.24	1.31	1.39
1	B	428	VAL	CB-CG2	-5.02	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	244	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	B	550	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	426	MET	CG-SD-CE	-5.27	91.77	100.20
1	B	511	VAL	CB-CA-C	-5.21	101.51	111.40
1	A	290	MET	N-CA-C	5.13	124.86	111.00
1	A	98	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	355	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	89	LYS	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4292	0	4304	94	1
1	B	4291	0	4300	88	0
2	A	53	0	31	5	0
2	B	53	0	31	3	0
3	A	48	0	32	4	0
3	B	48	0	32	7	0
4	A	83	0	0	3	0
4	B	82	0	0	2	0
All	All	8950	0	8730	183	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:ARG:HH11	1:A:341:ARG:HG2	1.19	1.03
1:B:346:GLN:HE21	1:B:430:GLN:HE21	0.96	0.93
1:A:382:THR:OG1	1:A:456:VAL:HG22	1.68	0.92
1:B:43:CYS:HG	3:B:901:COA:HS1	1.02	0.92
1:B:346:GLN:HE21	1:B:430:GLN:NE2	1.70	0.90
1:A:314:GLN:HA	1:A:314:GLN:HE21	1.42	0.82
1:A:290:MET:O	1:A:334:ASN:ND2	2.13	0.81
1:B:243:HIS:CE1	1:B:255:GLU:HG3	2.16	0.80
1:A:425:VAL:HG13	1:B:428:VAL:HG21	1.63	0.79
1:A:531:CYS:SG	1:A:532:GLN:N	2.56	0.79
1:A:376:GLU:HG3	1:A:377:LYS:N	1.99	0.78
1:A:377:LYS:HD3	1:A:476:HIS:CE1	2.18	0.78
1:A:43:CYS:SG	3:A:901:COA:S1P	2.58	0.77
1:B:223:GLN:HE21	1:B:224:THR:N	1.83	0.76
1:B:330:MET:HE1	1:B:342:TYR:HB2	1.69	0.75
1:B:86:ARG:HD2	1:B:295:ASP:OD1	1.87	0.75
1:B:223:GLN:HE21	1:B:224:THR:H	1.33	0.75
1:A:376:GLU:HG3	1:A:377:LYS:H	1.52	0.74
1:B:524:ASP:OD2	1:B:525:LYS:HE3	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:VAL:HG12	1:A:11:ALA:N	2.04	0.73
1:B:346:GLN:NE2	1:B:430:GLN:HE21	1.80	0.72
1:B:2:LYS:HE2	1:B:335:MET:O	1.90	0.72
1:B:288:ASN:HD21	1:B:292:GLN:HG3	1.55	0.71
1:B:431:ARG:O	1:B:431:ARG:HG2	1.91	0.69
1:A:408:ILE:HD12	1:A:434:MET:O	1.93	0.69
1:A:290:MET:CE	1:A:339:GLU:HA	2.24	0.68
1:A:341:ARG:HH11	1:A:341:ARG:CG	2.02	0.67
1:B:182:LEU:O	1:B:212:GLY:HA2	1.94	0.67
1:A:397:PHE:CZ	1:A:426:MET:HE1	2.29	0.67
1:B:288:ASN:ND2	1:B:292:GLN:HG3	2.10	0.67
1:A:341:ARG:HG2	1:A:341:ARG:NH1	1.97	0.66
1:A:486:ASP:OD1	1:A:550:ARG:NH2	2.27	0.66
1:B:243:HIS:HE1	1:B:255:GLU:HG3	1.60	0.66
1:A:397:PHE:HZ	1:A:426:MET:HE1	1.60	0.65
1:A:290:MET:HE1	1:A:339:GLU:HA	1.77	0.65
1:A:314:GLN:CA	1:A:314:GLN:HE21	2.09	0.65
1:A:243:HIS:HE1	1:A:255:GLU:OE2	1.79	0.65
1:A:455:ASP:O	1:A:458:ASN:N	2.29	0.63
1:B:43:CYS:SG	3:B:901:COA:S1P	2.72	0.63
1:A:162:ILE:HD12	2:A:900:FAD:C7	2.28	0.62
1:B:494:ASN:HD22	1:B:510:PRO:HB3	1.64	0.62
1:A:422:ARG:NH2	1:A:455:ASP:OD1	2.27	0.62
1:A:442:LEU:HD13	1:B:428:VAL:HG22	1.82	0.62
1:B:531:CYS:SG	1:B:532:GLN:N	2.73	0.62
1:A:56:ARG:NH1	1:A:140:ASP:OD1	2.33	0.61
1:A:90:LEU:HD23	1:A:105:SER:HA	1.80	0.61
1:A:112:SER:N	1:A:113:PRO:HD3	2.16	0.60
1:A:10:VAL:HG12	1:A:11:ALA:H	1.66	0.60
1:B:541:TYR:CZ	1:B:545:VAL:HG21	2.36	0.60
1:A:314:GLN:HA	1:A:314:GLN:NE2	2.15	0.59
1:A:86:ARG:HD2	1:A:295:ASP:OD1	2.02	0.59
1:B:5:LEU:HG	1:B:106:TYR:HB3	1.83	0.59
1:B:21:ARG:HG2	1:B:71:PHE:O	2.01	0.59
1:B:377:LYS:HD2	1:B:379:TYR:CE2	2.38	0.59
1:B:382:THR:HB	1:B:456:VAL:HG22	1.83	0.59
1:A:240:ILE:O	1:A:240:ILE:HG12	2.01	0.59
1:B:43:CYS:HG	3:B:901:COA:C2P	2.15	0.58
1:B:370:GLN:O	1:B:370:GLN:HG2	2.03	0.58
1:B:212:GLY:C	1:B:213:THR:CG2	2.71	0.58
1:B:223:GLN:HE21	1:B:225:HIS:H	1.51	0.57
1:B:431:ARG:CG	1:B:431:ARG:O	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:LEU:HD23	1:A:298:ILE:HD13	1.87	0.57
1:B:223:GLN:NE2	1:B:225:HIS:H	2.03	0.57
1:A:459:GLN:O	1:A:463:VAL:HG23	2.04	0.56
1:B:127:ASN:OD1	1:B:130:THR:HG23	2.05	0.56
1:A:10:VAL:O	1:A:14:ALA:HB3	2.05	0.56
1:B:212:GLY:O	1:B:213:THR:HG22	2.06	0.56
1:B:564:ALA:O	1:B:565:SER:HB3	2.06	0.55
1:A:426:MET:HE1	1:A:457:ILE:HD12	1.88	0.55
1:A:290:MET:N	1:A:291:MET:HA	2.22	0.55
1:B:125:VAL:O	1:B:125:VAL:HG22	2.06	0.55
1:B:188:THR:N	1:B:189:PRO:CD	2.69	0.55
1:B:223:GLN:NE2	1:B:224:THR:H	2.03	0.54
1:A:92:THR:OG1	1:A:103:GLN:NE2	2.37	0.54
1:A:112:SER:N	1:A:113:PRO:CD	2.70	0.53
1:B:9:GLY:O	1:B:38:VAL:HG22	2.09	0.53
1:B:288:ASN:HD21	1:B:292:GLN:HE21	1.56	0.53
1:A:287:VAL:HA	1:A:292:GLN:O	2.09	0.53
1:A:47:TYR:HB3	1:A:53:ILE:HG13	1.90	0.53
1:A:43:CYS:HG	3:A:901:COA:HS1	0.55	0.52
1:A:240:ILE:HG22	4:A:1052:HOH:O	2.09	0.52
1:A:197:PHE:HB2	1:A:414:VAL:HG11	1.92	0.52
1:B:377:LYS:HD2	1:B:379:TYR:HE2	1.75	0.51
1:A:108:THR:CG2	1:A:297:ALA:O	2.58	0.51
1:A:108:THR:HG23	1:A:297:ALA:O	2.10	0.51
1:B:191:ASP:OD1	1:B:366:LYS:HG3	2.11	0.51
1:A:47:TYR:HB2	1:A:53:ILE:HD12	1.93	0.51
1:B:212:GLY:C	1:B:213:THR:HG22	2.32	0.51
1:B:494:ASN:ND2	1:B:510:PRO:HB3	2.26	0.51
1:A:454:LYS:NZ	3:B:901:COA:O1A	2.44	0.50
1:A:215:LEU:CD1	1:A:246:LEU:HB3	2.42	0.50
1:A:180:LEU:CD2	1:A:210:ARG:HG3	2.42	0.49
1:A:424:ASP:O	1:A:428:VAL:HG12	2.13	0.49
1:B:88:ALA:HB1	1:B:90:LEU:HD22	1.95	0.49
1:A:469:LYS:NZ	4:A:1045:HOH:O	2.46	0.48
1:B:131:HIS:HE1	1:B:145:THR:OG1	1.96	0.48
1:A:151:VAL:HG22	1:A:257:ASP:HB2	1.96	0.48
1:A:380:VAL:HB	1:A:382:THR:HG23	1.95	0.48
1:B:408:ILE:HD12	1:B:434:MET:O	2.13	0.48
1:B:56:ARG:NH2	1:B:140:ASP:OD2	2.45	0.48
1:B:187:MET:C	1:B:189:PRO:HD2	2.34	0.48
1:B:110:LEU:HB2	1:B:335:MET:CE	2.44	0.48
1:A:472:ALA:HA	1:A:541:TYR:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:518:MET:SD	1:A:544:LEU:HD23	2.54	0.48
1:A:10:VAL:CG1	1:A:11:ALA:H	2.24	0.47
1:A:290:MET:HE3	1:A:339:GLU:HA	1.95	0.47
1:B:227:ALA:H	1:B:238:GLN:NE2	2.11	0.47
1:A:178:THR:HG21	1:A:254:LEU:HD11	1.97	0.47
1:A:47:TYR:HB2	1:A:53:ILE:CD1	2.44	0.47
1:B:178:THR:HG21	1:B:254:LEU:HD11	1.97	0.46
1:B:127:ASN:HD21	1:B:130:THR:CG2	2.28	0.46
1:B:112:SER:N	1:B:113:PRO:HD3	2.31	0.46
1:B:42:ASN:HB2	3:B:901:COA:H22	1.98	0.46
1:B:489:LEU:HD23	1:B:506:ALA:HB2	1.97	0.46
1:B:542:ARG:HD2	1:B:542:ARG:HA	1.75	0.46
1:A:180:LEU:HD23	1:A:210:ARG:HG3	1.97	0.46
1:A:440:GLN:NE2	4:A:1045:HOH:O	2.42	0.46
1:B:401:PHE:CZ	1:B:464:ALA:HB1	2.51	0.46
1:B:379:TYR:CE1	1:B:398:LYS:HD2	2.50	0.46
1:A:42:ASN:OD1	3:A:901:COA:H22	2.15	0.46
1:A:162:ILE:CD1	2:A:900:FAD:C7	2.94	0.46
1:A:49:ILE:O	1:A:173:LEU:HD11	2.16	0.45
1:A:34:ARG:O	1:A:78:LYS:HA	2.16	0.45
1:B:130:THR:HG22	1:B:244:LEU:HD11	1.98	0.45
1:B:436:VAL:O	1:B:437:GLU:C	2.53	0.45
1:A:2:LYS:HE2	1:A:335:MET:O	2.16	0.45
1:A:241:LYS:HD2	1:A:241:LYS:HA	1.50	0.45
1:A:198:ALA:O	1:A:202:ILE:HG13	2.16	0.45
1:B:131:HIS:HD2	4:B:1046:HOH:O	1.99	0.45
1:A:178:THR:HA	1:A:208:ASP:O	2.17	0.45
1:B:125:VAL:CG2	1:B:125:VAL:O	2.65	0.45
1:B:191:ASP:O	1:B:192:ARG:C	2.55	0.45
1:B:290:MET:O	1:B:291:MET:HB2	2.17	0.45
1:A:309:ASP:OD1	1:A:363:LYS:HE3	2.18	0.44
1:A:314:GLN:CA	1:A:314:GLN:NE2	2.78	0.44
1:B:185:GLN:HA	1:B:199:HIS:CE1	2.53	0.44
1:B:330:MET:CE	1:B:342:TYR:HB2	2.45	0.44
1:A:397:PHE:CZ	1:A:426:MET:CE	2.99	0.44
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.80	0.44
1:A:397:PHE:HZ	1:A:426:MET:CE	2.30	0.43
1:B:221:GLN:HB3	1:B:221:GLN:HE21	1.69	0.43
1:B:529:ILE:HD11	1:B:544:LEU:HD12	1.99	0.43
1:B:314:GLN:OE1	1:B:314:GLN:HA	2.18	0.43
1:A:345:THR:HG22	1:A:347:GLY:H	1.83	0.43
1:A:455:ASP:OD2	1:A:456:VAL:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:11:ALA:HB3	2:B:900:FAD:O5'	2.18	0.43
1:B:122:ILE:O	1:B:125:VAL:HG12	2.18	0.43
1:B:215:LEU:CD1	1:B:246:LEU:HB3	2.49	0.43
1:A:234:ASP:C	1:A:234:ASP:OD1	2.57	0.43
1:A:162:ILE:HD12	2:A:900:FAD:C7M	2.49	0.43
3:B:901:COA:H131	3:B:901:COA:O9P	2.18	0.43
1:A:426:MET:CE	1:A:457:ILE:HD12	2.48	0.43
1:B:455:ASP:HB2	4:B:1058:HOH:O	2.19	0.43
1:A:421:LYS:O	1:A:425:VAL:HG23	2.19	0.43
1:B:377:LYS:HZ2	1:B:476:HIS:CG	2.37	0.43
1:A:188:THR:N	1:A:189:PRO:CD	2.81	0.43
1:A:450:TYR:OH	1:B:352:LYS:HG3	2.20	0.42
1:B:211:LEU:O	1:B:213:THR:HG23	2.19	0.42
1:A:529:ILE:HG13	1:A:552:ARG:O	2.19	0.42
1:B:127:ASN:ND2	1:B:130:THR:HG23	2.34	0.42
1:B:171:HIS:CE1	1:B:205:GLN:HE21	2.38	0.42
1:A:279:ILE:HG22	1:A:280:GLY:O	2.20	0.42
2:A:900:FAD:H9	2:A:900:FAD:H1'1	1.83	0.41
1:A:227:ALA:H	1:A:238:GLN:NE2	2.18	0.41
1:A:518:MET:HE1	1:A:547:ASN:OD1	2.19	0.41
1:B:215:LEU:HD11	1:B:246:LEU:HB3	2.01	0.41
1:B:376:GLU:HG3	1:B:377:LYS:H	1.85	0.41
1:B:425:VAL:HG11	1:B:457:ILE:HD12	2.01	0.41
2:B:900:FAD:H1'1	2:B:900:FAD:H9	1.82	0.41
1:A:434:MET:HB3	1:A:434:MET:HE2	1.95	0.41
1:B:386:ALA:HB1	1:B:388:TYR:CE2	2.55	0.41
1:A:455:ASP:O	1:A:456:VAL:C	2.59	0.41
1:A:499:GLN:NE2	1:A:499:GLN:H	2.18	0.41
1:A:40:PHE:O	3:A:901:COA:H62	2.21	0.41
1:A:430:GLN:O	1:A:430:GLN:HG2	2.20	0.41
1:A:188:THR:N	1:A:189:PRO:HD2	2.36	0.41
1:B:112:SER:O	2:B:900:FAD:H52A	2.20	0.41
1:A:162:ILE:H	1:A:162:ILE:HG12	1.72	0.40
1:B:267:PRO:HB3	1:B:304:ALA:HA	2.03	0.40
1:B:198:ALA:O	1:B:202:ILE:HG13	2.22	0.40
1:B:521:LEU:HA	1:B:522:PRO:HD2	1.86	0.40
1:A:112:SER:O	2:A:900:FAD:H52A	2.21	0.40
3:B:901:COA:HO2A	3:B:901:COA:P3B	2.44	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	Distance(Å)	Clash(Å)
1:A:225:HIS:ND1	1:A:512:ASP:OD2[2_555]	2.16	0.04

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	563/574 (98%)	541 (96%)	21 (4%)	1 (0%)	56	87
1	B	563/574 (98%)	537 (95%)	24 (4%)	2 (0%)	43	79
All	All	1126/1148 (98%)	1078 (96%)	45 (4%)	3 (0%)	50	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	B	10	VAL
1	B	263	ILE

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	449/458 (98%)	407 (91%)	42 (9%)	13	32
1	B	448/458 (98%)	402 (90%)	46 (10%)	10	27
All	All	897/916 (98%)	809 (90%)	88 (10%)	12	30

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	34	ARG
1	A	42	ASN
1	A	56	ARG
1	A	57	SER
1	A	67	PHE
1	A	111	LEU
1	A	119	VAL
1	A	129	LEU
1	A	132	SER
1	A	143	LEU
1	A	200	GLN
1	A	208	ASP
1	A	209	LEU
1	A	210	ARG
1	A	229	ASP
1	A	240	ILE
1	A	241	LYS
1	A	254	LEU
1	A	259	LEU
1	A	266	ARG
1	A	267	PRO
1	A	269	THR
1	A	282	LEU
1	A	291	MET
1	A	307	GLU
1	A	314	GLN
1	A	341	ARG
1	A	356	LEU
1	A	370	GLN
1	A	377	LYS
1	A	378	VAL
1	A	407	THR
1	A	428	VAL
1	A	445	SER
1	A	483	LEU
1	A	486	ASP
1	A	490	LEU
1	A	523	LYS
1	A	525	LYS
1	A	531	CYS
1	B	24	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	34	ARG
1	B	38	VAL
1	B	42	ASN
1	B	52	GLU
1	B	67	PHE
1	B	90	LEU
1	B	97	LEU
1	B	103	GLN
1	B	119	VAL
1	B	130	THR
1	B	144	GLN
1	B	176	LYS
1	B	181	GLU
1	B	182	LEU
1	B	208	ASP
1	B	209	LEU
1	B	213	THR
1	B	219	SER
1	B	221	GLN
1	B	241	LYS
1	B	254	LEU
1	B	255	GLU
1	B	258	LEU
1	B	273	ARG
1	B	279	ILE
1	B	281	GLU
1	B	292	GLN
1	B	307	GLU
1	B	308	GLN
1	B	341	ARG
1	B	356	LEU
1	B	378	VAL
1	B	380	VAL
1	B	385	HIS
1	B	407	THR
1	B	436	VAL
1	B	437	GLU
1	B	483	LEU
1	B	485	GLU
1	B	488	LEU
1	B	498	LEU
1	B	511	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	525	LYS
1	B	531	CYS
1	B	533	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	238	GLN
1	A	243	HIS
1	A	292	GLN
1	A	314	GLN
1	A	385	HIS
1	A	440	GLN
1	A	441	HIS
1	A	499	GLN
1	A	543	GLN
1	A	546	ASN
1	B	62	GLN
1	B	131	HIS
1	B	200	GLN
1	B	205	GLN
1	B	221	GLN
1	B	223	GLN
1	B	238	GLN
1	B	243	HIS
1	B	292	GLN
1	B	308	GLN
1	B	370	GLN
1	B	430	GLN
1	B	440	GLN
1	B	482	ASN
1	B	494	ASN
1	B	543	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	900	-	58,58,58	1.20	4 (6%)	85,89,89	2.30	28 (32%)
3	COA	A	901	-	50,50,50	1.66	5 (10%)	75,75,75	1.97	17 (22%)
2	FAD	B	900	-	58,58,58	1.14	4 (6%)	85,89,89	2.04	21 (24%)
3	COA	B	901	-	50,50,50	1.53	4 (8%)	75,75,75	1.97	19 (25%)

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	900	-	-	0/34/50/50	0/6/6/6
3	COA	A	901	-	-	0/48/64/64	0/3/3/3
2	FAD	B	900	-	-	0/34/50/50	0/6/6/6
3	COA	B	901	-	-	0/48/64/64	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	COA	O9P-C9P	8.87	1.41	1.23
3	B	901	COA	O9P-C9P	7.99	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	FAD	C2A-N3A	4.33	1.39	1.32
2	A	900	FAD	C4X-N5	4.07	1.40	1.33
3	B	901	COA	C2A-N3A	3.50	1.38	1.32
2	A	900	FAD	C5X-N5	3.42	1.40	1.35
2	B	900	FAD	C2A-N1A	3.37	1.40	1.33
2	A	900	FAD	C2A-N3A	3.28	1.37	1.32
3	A	901	COA	CBP-CAP	-3.18	1.53	1.55
3	A	901	COA	C2A-N3A	3.07	1.37	1.32
3	B	901	COA	CBP-CAP	-2.87	1.53	1.55
3	A	901	COA	C2A-N1A	2.80	1.39	1.33
2	A	900	FAD	O2-C2	2.71	1.25	1.21
3	B	901	COA	C2A-N1A	2.62	1.39	1.33
2	B	900	FAD	C4X-N5	2.58	1.37	1.33
3	A	901	COA	P2A-O3A	2.56	1.64	1.59
2	B	900	FAD	O4B-C1B	2.40	1.44	1.41

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FAD	N3A-C2A-N1A	-11.68	118.61	128.89
3	A	901	COA	N3A-C2A-N1A	-10.28	119.85	128.89
3	B	901	COA	N3A-C2A-N1A	-8.01	121.84	128.89
2	A	900	FAD	C2-N1-C10	7.86	122.51	114.95
2	B	900	FAD	C5A-C4A-N3A	-6.90	119.26	125.98
2	B	900	FAD	N3A-C2A-N1A	-6.72	122.98	128.89
3	B	901	COA	C5A-C4A-N3A	-6.28	119.86	125.98
2	B	900	FAD	N3A-C4A-N9A	5.46	134.75	125.39
2	B	900	FAD	C2-N1-C10	5.00	119.76	114.95
2	A	900	FAD	C4B-O4B-C1B	-4.82	104.42	109.72
3	A	901	COA	C5A-C4A-N3A	-4.79	121.31	125.98
2	B	900	FAD	C5X-C9A-N10	4.62	121.04	117.63
3	B	901	COA	C3P-N4P-C5P	4.51	131.98	122.81
2	A	900	FAD	C5A-C4A-N3A	-4.39	121.70	125.98
2	B	900	FAD	C6A-C5A-C4A	4.19	122.25	117.55
3	B	901	COA	OAP-CAP-C9P	3.72	118.81	110.41
2	A	900	FAD	C5X-C9A-N10	3.72	120.37	117.63
3	A	901	COA	O9A-P3B-O8A	3.71	121.30	107.38
2	B	900	FAD	C4X-N5-C5X	3.70	121.00	116.68
2	B	900	FAD	O3P-PA-O5B	3.63	112.52	102.91
2	A	900	FAD	C2'-C1'-N10	3.60	117.53	112.60
2	A	900	FAD	C10-C4X-N5	-3.53	118.78	122.57
2	A	900	FAD	C4X-N5-C5X	3.41	120.66	116.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	COA	N3A-C4A-N9A	3.36	131.15	125.39
2	B	900	FAD	O4B-C1B-C2B	-3.21	102.02	106.69
2	A	900	FAD	N3A-C4A-N9A	3.15	130.79	125.39
2	B	900	FAD	C9A-N10-C10	-3.08	118.73	121.77
3	B	901	COA	O4B-C1B-C2B	-3.07	102.22	106.69
2	A	900	FAD	O2'-C2'-C1'	-3.04	102.62	109.88
3	A	901	COA	CCP-CBP-CAP	-3.03	102.70	108.97
3	B	901	COA	C6A-C5A-C4A	3.02	120.94	117.55
3	B	901	COA	P2A-O3A-P1A	-3.01	123.59	131.93
3	A	901	COA	C6A-C5A-C4A	2.98	120.89	117.55
3	B	901	COA	O9P-C9P-CAP	-2.93	115.99	120.05
3	B	901	COA	C8A-N9A-C4A	-2.91	104.59	106.96
2	A	900	FAD	C5'-C4'-C3'	-2.89	106.61	112.06
2	B	900	FAD	C4X-C10-N1	-2.88	118.94	123.00
3	A	901	COA	N3A-C4A-N9A	2.86	130.30	125.39
2	B	900	FAD	C4-C4X-C10	2.83	121.90	117.18
3	B	901	COA	CAP-C9P-N8P	2.83	122.67	116.48
3	B	901	COA	O9A-P3B-O3B	-2.80	99.03	107.09
3	A	901	COA	O5A-P2A-O3A	2.80	118.41	105.14
3	A	901	COA	O3A-P2A-O6A	-2.71	95.72	102.91
3	A	901	COA	O2A-P1A-O3A	2.71	117.98	105.14
3	A	901	COA	O9A-P3B-O3B	-2.67	99.41	107.09
3	B	901	COA	O8A-P3B-O3B	2.63	114.67	107.09
2	A	900	FAD	C4-N3-C2	-2.62	120.01	125.39
2	A	900	FAD	O2A-PA-O3P	2.60	117.46	105.14
3	B	901	COA	O5A-P2A-O3A	2.56	117.27	105.14
2	B	900	FAD	C2'-C1'-N10	2.55	116.09	112.60
2	A	900	FAD	C1B-N9A-C4A	-2.49	122.33	126.64
2	B	900	FAD	C4-N3-C2	-2.46	120.34	125.39
3	A	901	COA	C6P-C5P-N4P	-2.42	112.10	116.48
2	A	900	FAD	C9A-C5X-N5	-2.40	118.84	122.39
2	B	900	FAD	C9A-C5X-N5	-2.40	118.84	122.39
3	B	901	COA	O2B-C2B-C3B	-2.40	104.16	111.20
3	A	901	COA	O6A-CCP-CBP	2.30	114.24	110.55
3	A	901	COA	O5B-C5B-C4B	-2.28	100.59	108.96
2	A	900	FAD	O4B-C4B-C3B	2.26	109.76	105.16
2	B	900	FAD	C1B-N9A-C4A	2.24	130.50	126.64
2	A	900	FAD	C4X-C10-N1	-2.23	119.85	123.00
3	B	901	COA	C4A-C5A-N7A	-2.23	107.25	109.41
2	A	900	FAD	C9A-N10-C10	-2.22	119.58	121.77
2	A	900	FAD	C2A-N3A-C4A	2.22	119.66	113.27
3	A	901	COA	CEP-CBP-CCP	2.21	111.77	108.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	FAD	C1'-N10-C9A	2.21	120.99	118.67
3	B	901	COA	O2A-P1A-O3A	2.21	115.61	105.14
2	A	900	FAD	O4B-C1B-N9A	2.18	112.83	108.10
2	B	900	FAD	C5A-C6A-N6A	-2.17	115.81	120.72
3	B	901	COA	C2P-C3P-N4P	-2.16	107.64	112.45
2	B	900	FAD	C1'-N10-C10	2.13	121.14	118.82
2	A	900	FAD	N7A-C8A-N9A	-2.13	107.36	112.20
2	B	900	FAD	C6-C5X-C9A	2.13	121.85	119.02
2	A	900	FAD	C2A-N1A-C6A	2.12	122.54	118.76
3	A	901	COA	CDP-CBP-CAP	2.11	112.49	108.82
2	B	900	FAD	C10-C4X-N5	-2.11	120.30	122.57
2	A	900	FAD	C2B-C1B-N9A	-2.09	107.65	113.35
3	B	901	COA	C2A-N3A-C4A	2.08	119.27	113.27
2	A	900	FAD	C4'-C3'-C2'	-2.08	108.61	113.52
2	A	900	FAD	C8A-N9A-C4A	2.05	108.62	106.96
3	A	901	COA	P2A-O3A-P1A	-2.05	126.25	131.93
2	A	900	FAD	C4A-C5A-N7A	-2.04	107.44	109.41
2	A	900	FAD	C4X-C10-N10	2.02	121.76	120.53
3	A	901	COA	C4A-C5A-N7A	-2.02	107.46	109.41
2	B	900	FAD	C5'-C4'-C3'	-2.02	108.25	112.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	565/574 (98%)	-0.46	0 100 100	26, 36, 54, 72	0
1	B	565/574 (98%)	-0.43	0 100 100	24, 35, 53, 76	0
All	All	1130/1148 (98%)	-0.45	0 100 100	24, 35, 54, 76	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	A	900	53/53	0.14	0.16	23,30,33,35	0
2	FAD	B	900	53/53	0.14	-0.00	18,27,31,32	0
3	COA	B	901	48/48	0.14	-0.17	24,32,41,46	0
3	COA	A	901	48/48	0.13	-0.41	20,30,35,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.