



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:52 AM GMT

PDB ID : 3GD4
Title : Crystal structure of the reduced, NAD-bound form of murine apoptosis inducing factor
Authors : Sevrioukova, I.F.
Deposited on : 2009-02-23
Resolution : 2.24 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

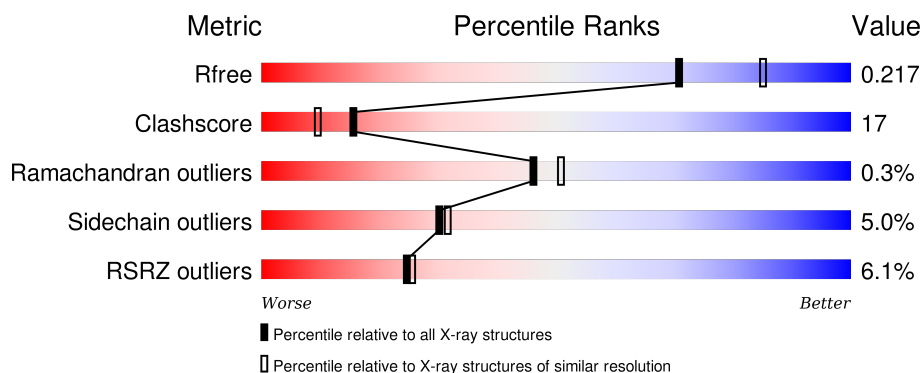
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	511	<div> <div>5%</div> <div>54%</div> <div>32%</div> <div>•</div> <div>13%</div> </div>
1	B	511	<div> <div>5%</div> <div>54%</div> <div>29%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition [i](#)

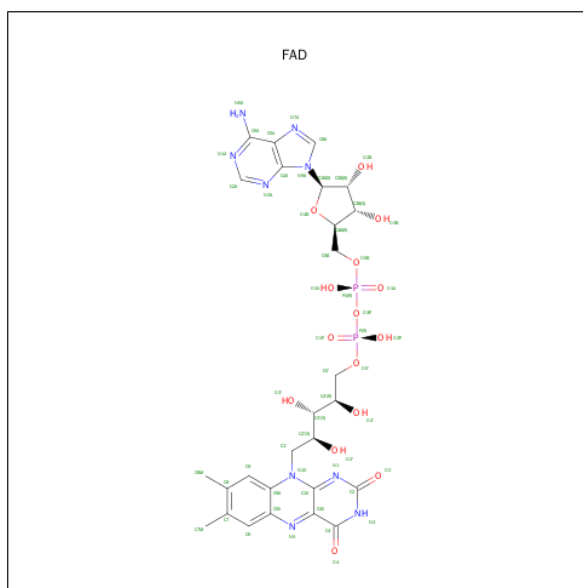
There are 4 unique types of molecules in this entry. The entry contains 7518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Apoptosis-inducing factor 1, mitochondrial.

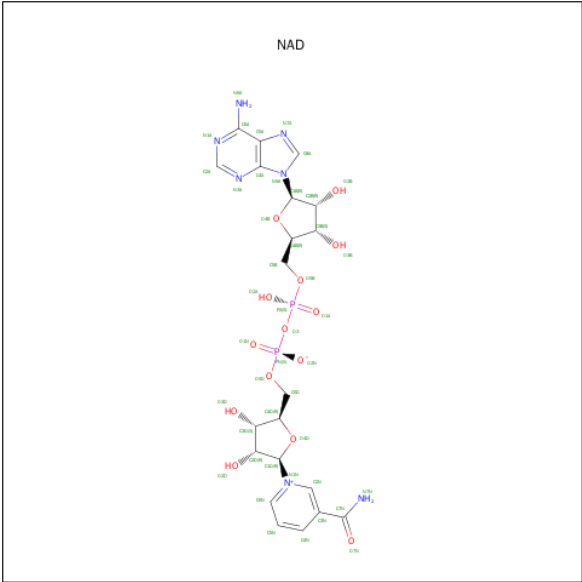
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3437	2187	609	630	11			
1	B	435	Total	C	N	O	S	0	0	0
			3366	2142	599	614	11			

- 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 NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

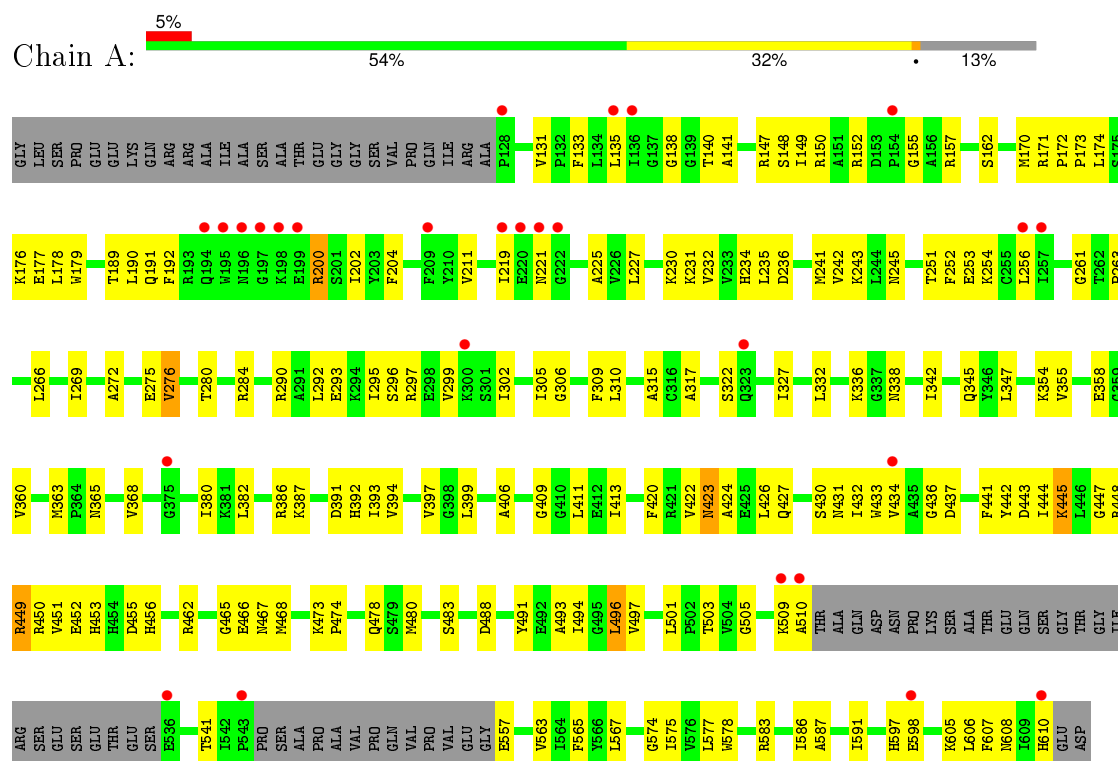
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	257	Total	O	0	0
			257	257		
4	B	264	Total	O	0	0
			264	264		

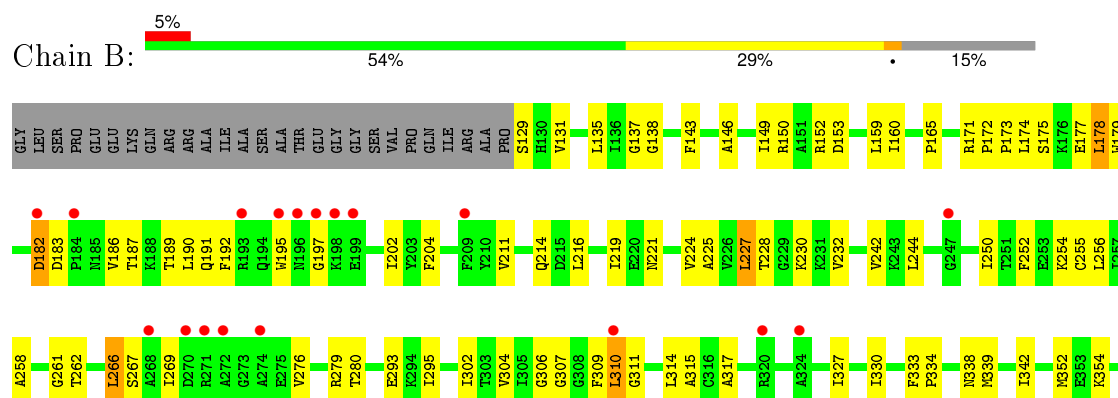
3 Residue-property plots

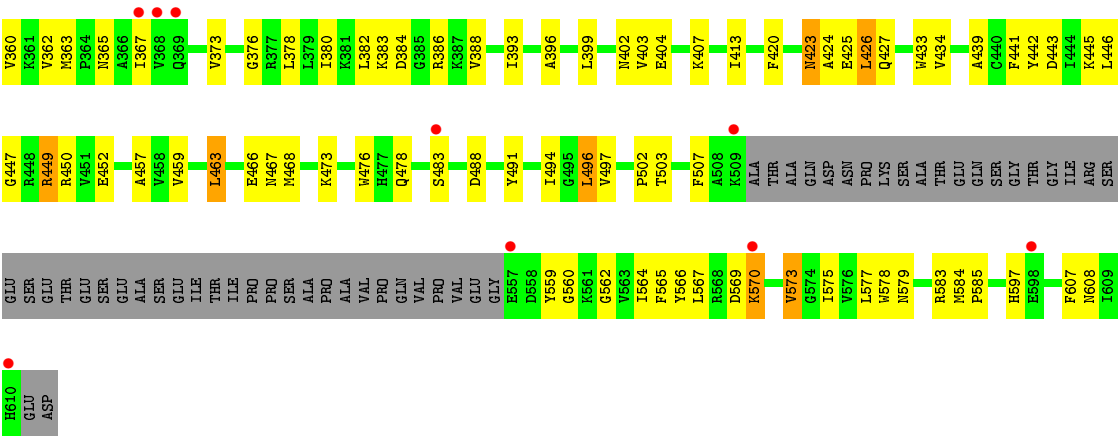
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Apoptosis-inducing factor 1, mitochondrial



- Molecule 1: Apoptosis-inducing factor 1, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 120.39Å 178.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.67 – 2.24 30.67 – 2.08	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.67-2.24) 80.4 (30.67-2.08)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.222 0.184 , 0.217	Depositor DCC
R_{free} test set	3035 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63021 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7518	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAD

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	0.59	0/3506	0.69	0/4736
1	B	0.62	0/3434	0.74	1/4638 (0.0%)
All	All	0.61	0/6940	0.71	1/9374 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3437	0	3478	128	0
1	B	3366	0	3408	109	0
2	A	53	0	30	5	0
2	B	53	0	30	7	0
3	A	44	0	26	5	0
3	B	44	0	26	7	0
4	A	257	0	0	8	0
4	B	264	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7518	0	6998	241	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 17.

All (241) 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:449:ARG:NH2	1:B:478:GLN:HE22	1.61	0.98
1:A:177:GLU:HG3	1:A:192:PHE:CD2	2.05	0.92
1:B:496:LEU:HB2	1:B:573:VAL:HG13	1.58	0.85
1:B:467:ASN:HD21	1:B:473:LYS:H	1.28	0.81
1:B:232:VAL:HG13	1:B:242:VAL:HB	1.63	0.79
1:B:449:ARG:HH22	1:B:478:GLN:HE22	1.26	0.78
1:A:231:LYS:H	1:A:245:ASN:ND2	1.83	0.75
1:A:234:HIS:HB3	1:A:243:LYS:HB3	1.69	0.74
1:A:451:VAL:HG22	1:A:456:HIS:CB	2.18	0.74
1:B:309:PHE:HB3	3:B:700:NAD:C3N	2.19	0.73
1:B:304:VAL:HG11	1:B:311:GLY:HA2	1.70	0.73
1:B:279:ARG:HG3	1:B:378:LEU:HD21	1.70	0.72
1:B:177:GLU:HG3	1:B:192:PHE:CD2	2.23	0.72
1:B:150:ARG:NH1	1:B:221:ASN:O	2.23	0.71
1:B:178:LEU:HD22	1:B:202:ILE:HD12	1.75	0.68
1:A:305:ILE:HD13	1:A:368:VAL:HG21	1.75	0.68
1:A:152:ARG:HD3	1:A:466:GLU:HG2	1.75	0.67
1:A:451:VAL:HG22	1:A:456:HIS:CG	2.30	0.67
1:A:467:ASN:ND2	1:A:473:LYS:H	1.93	0.67
1:A:309:PHE:HB3	3:A:700:NAD:C3N	2.24	0.66
1:B:467:ASN:ND2	1:B:473:LYS:H	1.93	0.66
1:B:165:PRO:HA	1:B:228:THR:HB	1.79	0.65
1:A:299:VAL:HB	1:A:391:ASP:HB2	1.80	0.64
1:A:131:VAL:O	1:A:252:PHE:HA	1.97	0.64
1:B:262:THR:HG23	1:B:402:ASN:HD21	1.61	0.63
1:B:449:ARG:HH22	1:B:478:GLN:NE2	1.95	0.63
1:A:467:ASN:HD21	1:A:473:LYS:H	1.45	0.63
1:A:309:PHE:HB3	3:A:700:NAD:C4N	2.28	0.63
1:B:445:LYS:HE2	1:B:476:TRP:CH2	2.33	0.63
1:A:293:GLU:OE2	1:A:297:ARG:NH2	2.32	0.62
1:B:439:ALA:O	1:B:450:ARG:HG3	1.98	0.62
1:A:231:LYS:H	1:A:245:ASN:HD22	1.45	0.62
1:B:304:VAL:CG1	1:B:311:GLY:HA2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ARG:NH2	1:A:478:GLN:OE1	2.32	0.61
1:B:261:GLY:HA3	1:B:399:LEU:HG	1.80	0.61
1:A:583:ARG:NH2	1:A:608:ASN:HB2	2.15	0.61
1:B:425:GLU:O	1:B:426:LEU:HB2	1.99	0.61
1:A:503:THR:HA	1:A:565:PHE:O	2.00	0.61
1:B:173:PRO:O	1:B:178:LEU:HB2	2.00	0.61
1:B:577:LEU:HD21	1:B:607:PHE:CE1	2.36	0.60
1:B:334:PRO:O	1:B:365:ASN:HA	2.01	0.60
1:A:453:HIS:NE2	4:A:643:HOH:O	2.31	0.60
1:A:263:PRO:HG3	1:A:284:ARG:HB2	1.83	0.59
1:A:152:ARG:HD3	1:A:466:GLU:HA	1.84	0.59
1:A:174:LEU:HB2	2:A:1611:FAD:HM72	1.85	0.59
1:B:152:ARG:HD3	1:B:466:GLU:HA	1.83	0.59
1:A:437:ASP:O	1:A:450:ARG:HD2	2.03	0.59
1:B:279:ARG:NH1	1:B:376:GLY:O	2.35	0.59
1:A:176:LYS:HB3	1:A:177:GLU:OE2	2.03	0.58
1:B:138:GLY:HA2	1:B:160:ILE:CG2	2.33	0.58
1:B:478:GLN:HB2	1:B:494:ILE:HD11	1.86	0.57
1:A:148:SER:HB2	1:A:462:ARG:HA	1.87	0.57
1:A:583:ARG:HD2	1:A:607:PHE:HA	1.87	0.57
1:A:299:VAL:HB	1:A:391:ASP:CB	2.35	0.57
1:B:131:VAL:HG21	1:B:159:LEU:HB2	1.87	0.57
1:B:339:MET:HE3	1:B:339:MET:HA	1.86	0.56
1:A:406:ALA:HB2	1:A:413:ILE:HD11	1.87	0.56
1:B:496:LEU:CB	1:B:573:VAL:HG13	2.31	0.56
1:A:227:LEU:HD22	1:A:230:LYS:HG3	1.87	0.56
1:A:157:ARG:NH1	1:A:219:ILE:O	2.38	0.55
1:B:171:ARG:N	1:B:172:PRO:CD	2.69	0.55
1:A:172:PRO:HA	2:A:1611:FAD:N5	2.21	0.55
1:B:315:ALA:HB1	1:B:360:VAL:HG11	1.89	0.55
1:A:449:ARG:HD3	1:A:496:LEU:HD11	1.89	0.54
1:A:347:LEU:HD11	1:A:578:TRP:CE2	2.43	0.54
1:A:505:GLY:HA2	1:A:563:VAL:O	2.08	0.54
1:B:457:ALA:HB2	2:B:1611:FAD:H5'2	1.89	0.54
1:A:148:SER:OG	1:A:466:GLU:HG3	2.08	0.54
1:A:211:VAL:O	1:A:225:ALA:HA	2.08	0.54
1:A:232:VAL:HG13	1:A:242:VAL:HB	1.89	0.54
1:B:254:LYS:HD2	1:B:433:TRP:CZ3	2.42	0.54
1:A:455:ASP:HB3	1:A:480:MET:O	2.08	0.54
1:B:352:MET:HG3	1:B:362:VAL:HG11	1.91	0.53
1:A:509:LYS:O	1:A:510:ALA:CB	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HG	1:B:202:ILE:HD11	1.90	0.53
1:A:179:TRP:CG	1:A:317:ALA:HB1	2.44	0.53
1:A:505:GLY:O	1:A:541:THR:HA	2.08	0.53
1:B:150:ARG:HD2	1:B:224:VAL:HG23	1.90	0.52
1:A:269:ILE:HG13	1:A:280:THR:HG21	1.92	0.52
1:A:149:ILE:HG13	1:A:465:GLY:HA2	1.92	0.52
1:B:380:ILE:HD11	1:B:393:ILE:HG12	1.92	0.52
1:B:138:GLY:HA2	1:B:160:ILE:HG21	1.92	0.52
1:B:404:GLU:HG2	4:B:791:HOH:O	2.10	0.52
1:A:189:THR:HB	1:A:191:GLN:HG3	1.93	0.51
1:A:152:ARG:CD	1:A:466:GLU:HG2	2.40	0.51
1:B:423:ASN:HD22	1:B:423:ASN:C	2.13	0.51
1:A:295:ILE:HD13	1:A:392:HIS:CE1	2.44	0.51
1:A:423:ASN:ND2	1:A:427:GLN:H	2.09	0.51
1:B:276:VAL:HG12	1:B:373:VAL:HG23	1.93	0.51
1:A:135:LEU:HD22	1:A:256:LEU:HB3	1.93	0.51
1:A:147:ARG:HD3	4:A:1021:HOH:O	2.10	0.51
1:A:423:ASN:C	1:A:423:ASN:HD22	2.14	0.51
2:B:1611:FAD:H1'1	3:B:700:NAD:H1D	1.92	0.50
1:B:307:GLY:HA3	1:B:333:PHE:CG	2.46	0.50
1:B:583:ARG:NH2	1:B:608:ASN:HB2	2.27	0.50
1:B:256:LEU:HB2	1:B:468:MET:SD	2.51	0.50
1:A:138:GLY:HA3	1:A:162:SER:HB2	1.93	0.50
1:A:445:LYS:HE3	1:A:478:GLN:HE21	1.77	0.50
1:B:306:GLY:HA3	1:B:396:ALA:O	2.13	0.49
1:B:382:LEU:HD12	1:B:386:ARG:HB2	1.94	0.49
1:A:155:GLY:HA2	1:A:221:ASN:O	2.12	0.49
1:A:483:SER:HB3	1:A:491:TYR:CE2	2.48	0.49
1:A:406:ALA:CB	1:A:413:ILE:HD11	2.43	0.49
1:A:241:MET:HA	1:A:251:THR:HA	1.95	0.49
1:B:420:PHE:HB2	1:B:434:VAL:HG21	1.93	0.49
1:A:445:LYS:HE3	1:A:478:GLN:NE2	2.28	0.48
1:A:433:TRP:CE3	1:A:468:MET:HG2	2.48	0.48
1:B:559:TYR:O	1:B:578:TRP:CD1	2.65	0.48
1:B:227:LEU:HD13	1:B:230:LYS:HG3	1.95	0.48
1:B:420:PHE:CB	1:B:434:VAL:HG21	2.42	0.48
1:A:354:LYS:HE2	4:A:686:HOH:O	2.12	0.48
1:B:424:ALA:HA	1:B:442:TYR:O	2.13	0.48
1:A:493:ALA:HA	1:A:575:ILE:O	2.14	0.48
1:A:171:ARG:N	1:A:172:PRO:CD	2.76	0.48
1:B:131:VAL:HG21	1:B:159:LEU:CB	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:O	1:B:179:TRP:NE1	2.39	0.48
1:B:342:ILE:HG23	1:B:497:VAL:HG12	1.96	0.48
1:A:354:LYS:HD2	1:A:488:ASP:HB2	1.96	0.48
1:B:569:ASP:O	1:B:570:LYS:HG2	2.14	0.48
1:B:216:LEU:HD22	1:B:225:ALA:HB3	1.96	0.48
1:A:420:PHE:CB	1:A:434:VAL:HG21	2.44	0.48
1:B:330:ILE:HD13	1:B:388:VAL:HG13	1.96	0.47
1:A:253:GLU:O	1:A:431:ASN:HB3	2.14	0.47
1:A:443:ASP:OD2	1:A:445:LYS:HD2	2.14	0.47
1:A:437:ASP:OD2	1:A:452:GLU:HA	2.15	0.47
1:A:241:MET:HG2	1:A:242:VAL:N	2.30	0.47
1:B:338:ASN:HD21	1:B:362:VAL:HG11	1.79	0.47
1:B:252:PHE:CD1	1:B:255:CYS:HB2	2.49	0.47
1:B:258:ALA:O	2:B:1611:FAD:H52A	2.15	0.47
1:A:445:LYS:CE	1:A:478:GLN:HE21	2.28	0.46
1:A:173:PRO:HG2	1:A:202:ILE:HG22	1.97	0.46
1:A:192:PHE:CZ	1:A:200:ARG:HG2	2.50	0.46
1:B:354:LYS:HD2	1:B:488:ASP:HB2	1.97	0.46
1:A:263:PRO:CG	1:A:284:ARG:HB2	2.45	0.46
1:B:338:ASN:HD22	1:B:338:ASN:H	1.62	0.46
1:A:292:LEU:HD13	1:A:394:VAL:HG22	1.97	0.46
1:B:310:LEU:HD22	1:B:314:LEU:HG	1.97	0.46
1:A:380:ILE:HD11	1:A:393:ILE:HG12	1.98	0.46
1:A:272:ALA:HB1	1:A:276:VAL:HG11	1.98	0.46
1:A:496:LEU:HB3	1:A:501:LEU:HD11	1.97	0.46
1:B:384:ASP:OD1	1:B:386:ARG:HD3	2.17	0.45
1:A:483:SER:HB3	1:A:491:TYR:CZ	2.51	0.45
1:A:235:LEU:O	1:A:409:GLY:HA2	2.16	0.45
1:B:446:LEU:HD22	1:B:573:VAL:HG22	1.97	0.45
1:A:494:ILE:O	1:A:574:GLY:HA2	2.17	0.45
1:A:295:ILE:HG21	1:A:392:HIS:CG	2.51	0.45
1:B:503:THR:HA	1:B:565:PHE:O	2.16	0.45
1:B:131:VAL:O	1:B:252:PHE:HA	2.17	0.45
1:A:380:ILE:HG12	1:A:393:ILE:HD11	1.98	0.45
1:B:423:ASN:ND2	1:B:427:GLN:H	2.14	0.45
1:B:189:THR:HB	1:B:191:GLN:HG3	1.99	0.45
1:A:587:ALA:O	1:A:591:ILE:HG12	2.17	0.45
1:B:502:PRO:HD2	1:B:567:LEU:O	2.17	0.45
1:A:141:ALA:HB2	1:A:436:GLY:HA3	1.99	0.44
1:B:441:PHE:CZ	1:B:449:ARG:HG3	2.52	0.44
1:A:420:PHE:HB2	1:A:434:VAL:HG11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:HG11	1:B:219:ILE:HG21	1.98	0.44
1:A:295:ILE:O	1:A:299:VAL:HG22	2.17	0.44
1:A:236:ASP:HB3	1:A:241:MET:HB3	2.00	0.44
1:A:174:LEU:HD23	1:A:178:LEU:HD12	1.99	0.44
1:A:149:ILE:HG13	1:A:465:GLY:CA	2.47	0.44
1:B:560:GLY:O	1:B:579:ASN:HB2	2.17	0.44
1:A:483:SER:HA	4:A:776:HOH:O	2.17	0.44
1:A:605:LYS:HG3	1:A:610:HIS:CD2	2.52	0.44
1:B:129:SER:O	1:B:250:ILE:HA	2.18	0.44
1:A:177:GLU:HB2	1:A:192:PHE:HB2	2.00	0.44
1:B:483:SER:HB3	1:B:491:TYR:CE2	2.52	0.44
1:B:152:ARG:CD	1:B:466:GLU:HG2	2.48	0.44
1:A:597:HIS:HE1	4:A:641:HOH:O	2.01	0.44
1:A:451:VAL:CG2	1:A:456:HIS:HB2	2.49	0.43
1:B:175:SER:HB3	2:B:1611:FAD:HM73	2.00	0.43
1:A:422:VAL:HB	1:A:426:LEU:C	2.38	0.43
1:A:290:ARG:NH1	4:A:1059:HOH:O	2.51	0.43
1:B:367:ILE:O	1:B:383:LYS:N	2.40	0.43
1:A:406:ALA:HA	1:A:411:LEU:HB2	2.00	0.43
1:B:230:LYS:HB3	1:B:244:LEU:HD13	2.00	0.43
1:B:564:ILE:O	1:B:575:ILE:HA	2.18	0.43
1:A:178:LEU:HD11	1:A:202:ILE:HG21	2.01	0.42
1:B:363:MET:HB3	1:B:386:ARG:HH11	1.84	0.42
1:B:566:TYR:CD1	1:B:566:TYR:N	2.87	0.42
1:B:449:ARG:HH21	1:B:478:GLN:HE22	1.55	0.42
1:B:252:PHE:CE1	1:B:255:CYS:HB2	2.54	0.42
1:B:143:PHE:CZ	1:B:204:PHE:HB3	2.54	0.42
1:A:336:LYS:HA	1:A:365:ASN:HD21	1.84	0.42
1:B:426:LEU:HD22	1:B:463:LEU:HD13	2.00	0.42
1:A:493:ALA:HB1	1:A:497:VAL:HG21	1.99	0.42
1:A:296:SER:HA	1:A:302:ILE:HD11	2.01	0.42
1:B:452:GLU:HB3	3:B:700:NAD:O3D	2.19	0.42
1:B:179:TRP:CG	1:B:317:ALA:HB1	2.54	0.42
1:A:443:ASP:HB3	1:A:447:GLY:O	2.20	0.42
1:A:563:VAL:HG23	1:A:577:LEU:HD23	2.00	0.42
1:B:171:ARG:HD3	2:B:1611:FAD:HM82	2.00	0.42
1:A:140:THR:HG1	1:A:204:PHE:HZ	1.67	0.42
1:A:424:ALA:HA	1:A:442:TYR:O	2.19	0.42
1:B:146:ALA:O	1:B:150:ARG:HG3	2.20	0.42
1:A:172:PRO:HA	2:A:1611:FAD:C5X	2.50	0.42
1:A:315:ALA:HB1	1:A:360:VAL:HG11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ARG:NH2	1:B:478:GLN:NE2	2.44	0.42
1:A:449:ARG:HD2	4:A:718:HOH:O	2.20	0.42
1:B:443:ASP:O	1:B:447:GLY:N	2.46	0.42
1:B:403:VAL:HA	1:B:420:PHE:CZ	2.55	0.42
1:B:310:LEU:HB3	1:B:396:ALA:HB1	2.01	0.41
1:A:150:ARG:NH2	1:A:221:ASN:O	2.39	0.41
1:B:269:ILE:HG21	1:B:280:THR:HG21	2.01	0.41
1:B:149:ILE:O	1:B:153:ASP:N	2.51	0.41
1:A:170:MET:HE2	1:A:170:MET:HB3	1.85	0.41
1:A:451:VAL:HG22	1:A:456:HIS:HB2	1.98	0.41
3:B:700:NAD:H8A	4:B:996:HOH:O	2.20	0.41
1:A:322:SER:HB2	1:A:327:ILE:O	2.19	0.41
1:B:135:LEU:HD22	1:B:256:LEU:HB3	2.02	0.41
1:A:597:HIS:CE1	4:A:641:HOH:O	2.73	0.41
1:A:382:LEU:HD12	1:A:386:ARG:HB2	2.02	0.41
1:A:133:PHE:HA	1:A:254:LYS:O	2.20	0.41
1:B:507:PHE:CD2	1:B:562:GLY:HA3	2.55	0.41
2:B:1611:FAD:C1'	3:B:700:NAD:H1D	2.49	0.41
1:A:152:ARG:HD3	1:A:466:GLU:CG	2.48	0.41
1:A:266:LEU:HD13	1:A:397:VAL:HG11	2.02	0.41
1:B:459:VAL:O	1:B:463:LEU:HB2	2.20	0.41
1:A:441:PHE:O	1:A:448:ARG:HA	2.21	0.41
1:A:355:VAL:O	1:A:358:GLU:HB2	2.20	0.41
1:B:309:PHE:HB3	3:B:700:NAD:C4N	2.49	0.41
2:A:1611:FAD:C1'	3:A:700:NAD:H1D	2.51	0.41
1:A:261:GLY:HA3	1:A:399:LEU:HG	2.02	0.41
1:B:584:MET:N	1:B:585:PRO:CD	2.84	0.41
1:A:332:LEU:HA	1:A:363:MET:O	2.21	0.41
1:A:338:ASN:HD22	1:A:338:ASN:H	1.68	0.41
1:B:302:ILE:HG13	1:B:327:ILE:HD11	2.02	0.41
1:B:137:GLY:HA2	2:B:1611:FAD:O4B	2.21	0.41
1:B:262:THR:CG2	1:B:402:ASN:HD21	2.31	0.41
1:A:256:LEU:HB2	1:A:468:MET:SD	2.61	0.41
1:B:266:LEU:HD11	3:B:700:NAD:N1A	2.36	0.40
1:A:397:VAL:HA	3:A:700:NAD:O4B	2.22	0.40
1:A:306:GLY:HA2	3:A:700:NAD:H1B	2.03	0.40
1:A:148:SER:HG	1:A:466:GLU:HG3	1.86	0.40
1:B:423:ASN:ND2	1:B:425:GLU:H	2.19	0.40
1:A:236:ASP:N	1:A:241:MET:O	2.39	0.40
1:B:186:VAL:HG23	1:B:191:GLN:O	2.21	0.40
1:B:597:HIS:HD2	4:B:805:HOH:O	2.05	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ILE:HD12	1:A:474:PRO:HB2	2.02	0.40
1:A:310:LEU:HD13	2:A:1611:FAD:HM73	2.04	0.40
1:A:586:ILE:HD13	1:A:606:LEU:O	2.22	0.40

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	439/511 (86%)	424 (97%)	15 (3%)	0	100	100
1	B	431/511 (84%)	411 (95%)	17 (4%)	3 (1%)	26	25
All	All	870/1022 (85%)	835 (96%)	32 (4%)	3 (0%)	46	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	GLY
1	B	183	ASP
1	B	182	ASP

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/417 (88%)	349 (96%)	16 (4%)	35	39
1	B	357/417 (86%)	337 (94%)	20 (6%)	26	25
All	All	722/834 (87%)	686 (95%)	36 (5%)	30	31

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	200	ARG
1	A	275	GLU
1	A	276	VAL
1	A	342	ILE
1	A	345	GLN
1	A	387	LYS
1	A	423	ASN
1	A	430	SER
1	A	432	ILE
1	A	445	LYS
1	A	449	ARG
1	A	496	LEU
1	A	557	GLU
1	A	567	LEU
1	A	598	GLU
1	B	178	LEU
1	B	182	ASP
1	B	187	THR
1	B	190	LEU
1	B	195	TRP
1	B	214	GLN
1	B	227	LEU
1	B	266	LEU
1	B	267	SER
1	B	293	GLU
1	B	295	ILE
1	B	310	LEU
1	B	407	LYS
1	B	413	ILE
1	B	423	ASN
1	B	426	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	463	LEU
1	B	496	LEU
1	B	570	LYS
1	B	573	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	249	GLN
1	A	338	ASN
1	A	365	ASN
1	A	423	ASN
1	A	456	HIS
1	A	467	ASN
1	A	610	HIS
1	B	205	GLN
1	B	338	ASN
1	B	345	GLN
1	B	365	ASN
1	B	402	ASN
1	B	423	ASN
1	B	456	HIS
1	B	467	ASN
1	B	478	GLN
1	B	596	GLN
1	B	597	HIS

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

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	1611	-	48,58,58	1.66	6 (12%)	54,89,89	3.80	13 (24%)
3	NAD	A	700	-	38,48,48	1.65	4 (10%)	47,73,73	2.44	9 (19%)
2	FAD	B	1611	-	48,58,58	1.73	7 (14%)	54,89,89	4.03	15 (27%)
3	NAD	B	700	-	38,48,48	1.57	4 (10%)	47,73,73	2.46	8 (17%)

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	1611	-	-	0/30/50/50	0/6/6/6
3	NAD	A	700	-	-	0/22/62/62	0/5/5/5
2	FAD	B	1611	-	-	0/30/50/50	0/6/6/6
3	NAD	B	700	-	-	0/22/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1611	FAD	C6-C5X	-8.73	1.28	1.41
2	A	1611	FAD	C6-C5X	-8.33	1.29	1.41
2	B	1611	FAD	C6-C7	-3.29	1.28	1.37
2	A	1611	FAD	C6-C7	-3.13	1.29	1.37
3	A	700	NAD	O4B-C4B	-2.80	1.38	1.45
2	B	1611	FAD	C1'-N10	-2.75	1.45	1.48
3	B	700	NAD	O4B-C4B	-2.31	1.39	1.45
2	B	1611	FAD	C10-N10	2.14	1.41	1.39
2	A	1611	FAD	C9A-N10	2.15	1.41	1.38
2	B	1611	FAD	C4X-N5	2.27	1.36	1.33
2	A	1611	FAD	C10-N10	2.34	1.41	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	C2A-N1A	2.53	1.38	1.33
2	B	1611	FAD	C5A-C4A	2.57	1.46	1.40
2	A	1611	FAD	C5A-C4A	2.87	1.47	1.40
3	A	700	NAD	C2A-N1A	2.87	1.39	1.33
2	B	1611	FAD	C9A-C5X	3.12	1.49	1.42
2	A	1611	FAD	C9A-C5X	3.40	1.49	1.42
3	B	700	NAD	C2A-N3A	3.42	1.38	1.32
3	A	700	NAD	C2A-N3A	3.44	1.38	1.32
3	B	700	NAD	O7N-C7N	6.91	1.38	1.24
3	A	700	NAD	O7N-C7N	7.06	1.39	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	NAD	N3A-C2A-N1A	-13.23	118.77	128.89
3	B	700	NAD	N3A-C2A-N1A	-12.94	118.99	128.89
2	B	1611	FAD	C6-C5X-C9A	-11.69	103.61	118.98
2	A	1611	FAD	C6-C5X-C9A	-10.49	105.19	118.98
2	B	1611	FAD	N3A-C2A-N1A	-9.77	121.41	128.89
2	A	1611	FAD	N3A-C2A-N1A	-7.48	123.17	128.89
2	A	1611	FAD	C6-C7-C8	-6.58	107.48	120.04
2	B	1611	FAD	C6-C7-C8	-6.12	108.36	120.04
2	B	1611	FAD	C4-C4X-C10	-5.40	116.48	119.94
2	A	1611	FAD	C4-C4X-C10	-4.78	116.88	119.94
2	B	1611	FAD	C1B-N9A-C4A	-4.21	120.59	126.94
3	B	700	NAD	O7N-C7N-C3N	-3.90	115.33	119.59
2	A	1611	FAD	C4A-C5A-N7A	-3.64	106.13	109.48
3	B	700	NAD	C1B-N9A-C4A	-3.54	121.60	126.94
3	B	700	NAD	C2B-C1B-N9A	-3.51	108.93	114.29
2	B	1611	FAD	C4A-C5A-N7A	-3.25	106.49	109.48
3	A	700	NAD	O5B-C5B-C4B	-3.22	97.25	109.12
2	A	1611	FAD	C4X-C4-N3	-2.98	119.52	123.59
3	A	700	NAD	C1B-N9A-C4A	-2.87	122.61	126.94
3	A	700	NAD	O7N-C7N-C3N	-2.70	116.64	119.59
3	B	700	NAD	O5B-C5B-C4B	-2.67	99.27	109.12
2	B	1611	FAD	C4X-C4-N3	-2.22	120.55	123.59
3	B	700	NAD	C2A-N1A-C6A	2.00	122.34	118.77
3	A	700	NAD	C2A-N1A-C6A	2.01	122.36	118.77
2	A	1611	FAD	C4-C4X-N5	2.09	121.26	118.72
2	B	1611	FAD	O2A-PA-O1A	2.12	124.02	112.53
3	B	700	NAD	O2N-PN-O1N	2.13	124.05	112.53
3	A	700	NAD	C4D-O4D-C1D	2.21	112.14	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1611	FAD	C4X-N5-C5X	2.23	119.33	116.76
2	A	1611	FAD	C1'-N10-C9A	2.33	121.48	118.86
3	A	700	NAD	C2N-C3N-C4N	2.39	120.95	118.29
2	B	1611	FAD	C4-C4X-N5	2.44	121.68	118.72
2	B	1611	FAD	C2A-N1A-C6A	2.54	123.31	118.77
2	A	1611	FAD	C4X-N5-C5X	2.83	120.02	116.76
2	A	1611	FAD	C7M-C7-C6	3.01	128.45	120.28
2	B	1611	FAD	C7M-C7-C6	3.05	128.56	120.28
3	A	700	NAD	C3N-C7N-N7N	3.63	121.80	117.82
3	A	700	NAD	O4D-C1D-N1N	3.90	112.42	108.13
3	B	700	NAD	C3N-C7N-N7N	4.62	122.87	117.82
2	B	1611	FAD	C4-N3-C2	6.92	121.22	115.25
2	A	1611	FAD	C4-N3-C2	8.31	122.43	115.25
2	A	1611	FAD	C6-C5X-N5	11.42	133.65	118.96
2	B	1611	FAD	C6-C5X-N5	12.21	134.67	118.96
2	A	1611	FAD	C7-C6-C5X	16.43	147.76	120.92
2	B	1611	FAD	C7-C6-C5X	16.82	148.38	120.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1611	FAD	5	0
3	A	700	NAD	5	0
2	B	1611	FAD	7	0
3	B	700	NAD	7	0

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	445/511 (87%)	0.23	27 (6%)	25 25	28, 46, 72, 84	0
1	B	435/511 (85%)	0.32	27 (6%)	24 25	27, 46, 79, 93	0
All	All	880/1022 (86%)	0.28	54 (6%)	25 25	27, 46, 77, 93	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	TRP	11.6
1	A	195	TRP	8.5
1	B	182	ASP	5.7
1	A	128	PRO	5.6
1	A	510	ALA	5.3
1	A	197	GLY	5.2
1	A	196	ASN	5.0
1	B	197	GLY	4.8
1	B	184	PRO	4.3
1	B	274	ALA	4.3
1	A	509	LYS	4.2
1	A	198	LYS	4.0
1	B	509	LYS	3.9
1	B	271	ARG	3.7
1	A	536	GLU	3.5
1	B	272	ALA	3.5
1	B	209	PHE	3.4
1	A	375	GLY	3.3
1	A	194	GLN	3.3
1	B	324	ALA	3.3
1	B	557	GLU	3.3
1	A	598	GLU	3.2
1	A	610	HIS	3.2
1	B	368	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	220	GLU	2.9
1	B	198	LYS	2.9
1	A	222	GLY	2.9
1	B	196	ASN	2.8
1	B	268	ALA	2.7
1	A	221	ASN	2.7
1	B	369	GLN	2.6
1	A	543	PRO	2.6
1	B	570	LYS	2.6
1	A	300	LYS	2.5
1	A	199	GLU	2.5
1	B	598	GLU	2.4
1	A	209	PHE	2.3
1	B	310	LEU	2.3
1	B	270	ASP	2.3
1	A	256	LEU	2.3
1	A	434	VAL	2.3
1	B	193	ARG	2.3
1	A	257	ILE	2.3
1	B	247	GLY	2.2
1	A	154	PRO	2.2
1	A	135	LEU	2.2
1	B	320	ARG	2.2
1	A	219	ILE	2.1
1	B	483	SER	2.1
1	B	367	ILE	2.1
1	A	323	GLN	2.1
1	B	610	HIS	2.1
1	A	136	ILE	2.0
1	B	199	GLU	2.0

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 [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(\AA^2)	Q<0.9
3	NAD	B	700	44/44	0.91	0.18	0.29	30,39,56,57	0
2	FAD	B	1611	53/53	0.97	0.18	0.26	32,35,37,41	0
2	FAD	A	1611	53/53	0.97	0.15	-0.19	33,36,42,44	0
3	NAD	A	700	44/44	0.96	0.11	-0.60	30,37,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.