WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:00 AM GMT

PDB ID	:	2Z1Q
Title	:	Crystal structure of acyl CoA dehydrogenase
Authors	:	Hikima, T.; Kawano, Y.; Nodake, Y.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-11
Resolution	:	2.30 Å(reported)

The following versions of software and data (see references (i)) 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
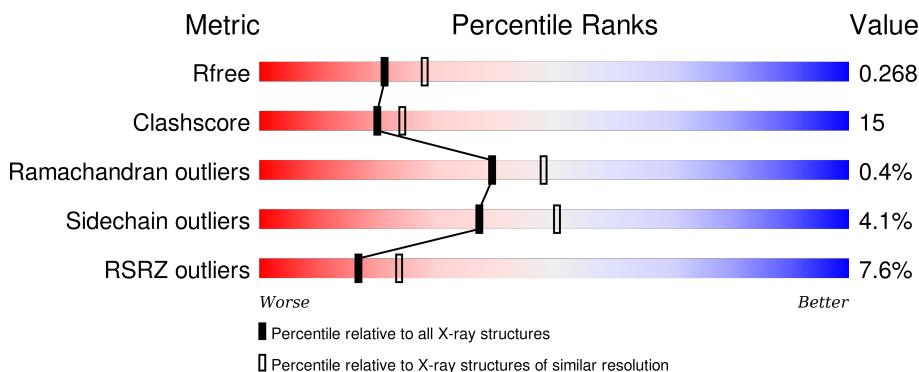
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
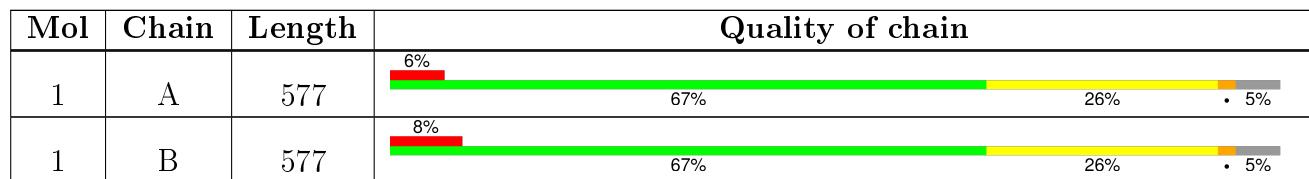
The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.268
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		4.1%
RSRZ outliers		7.6%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	577	6% / 67% 26% • 5%
1	B	577	8% / 67% 26% • 5%

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	FAD	A	700	-	-	-	X
2	FAD	B	701	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8961 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.
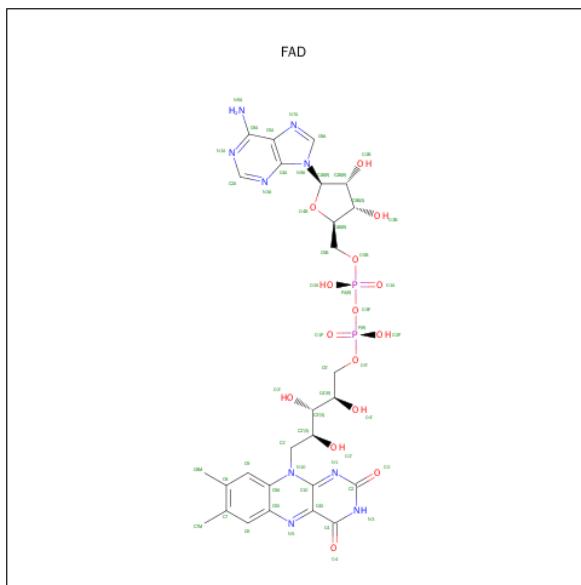
- Molecule 1 is a protein called Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4190	2665	730	787	8			
1	B	549	Total	C	N	O	S	0	0	0
			4211	2679	734	790	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	GLY	VAL	CONFLICT	UNP Q5SJW0
B	554	GLY	VAL	CONFLICT	UNP Q5SJW0

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0
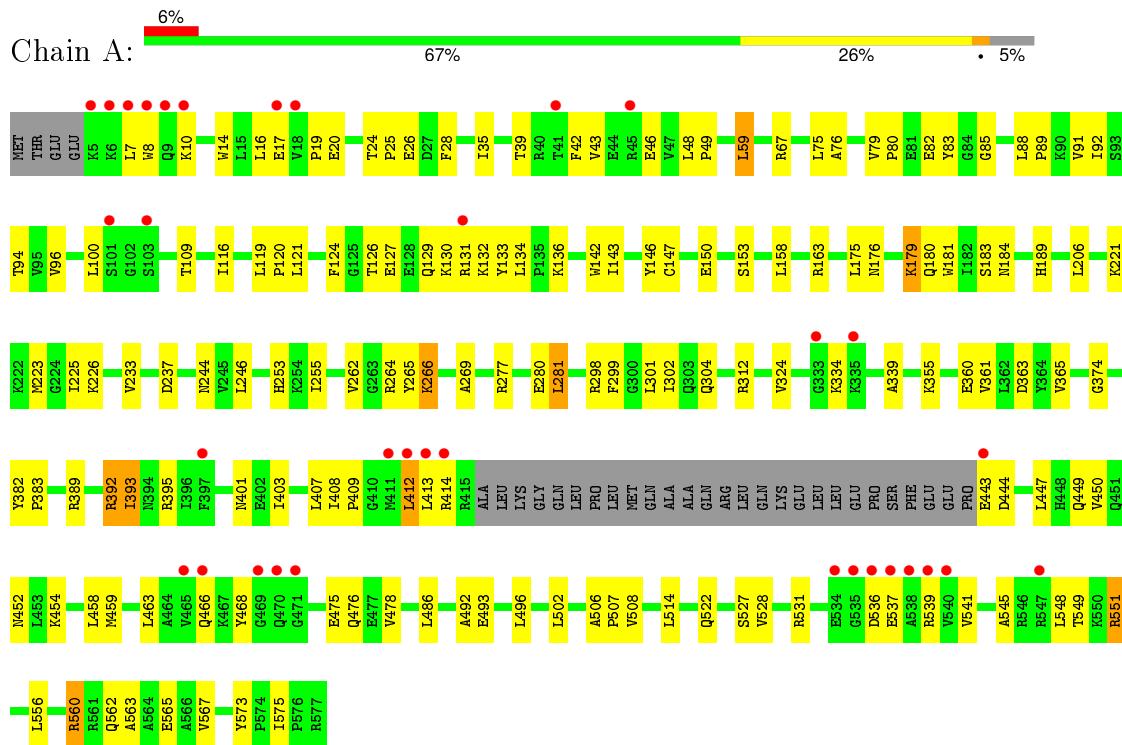
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	233	233	233	0	0
3	B	221	221	221	0	0
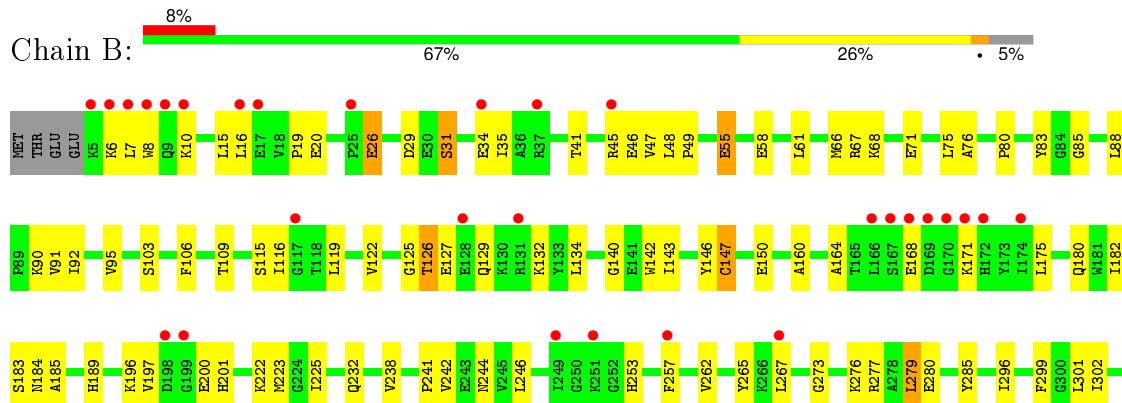
3 Residue-property plots (i)
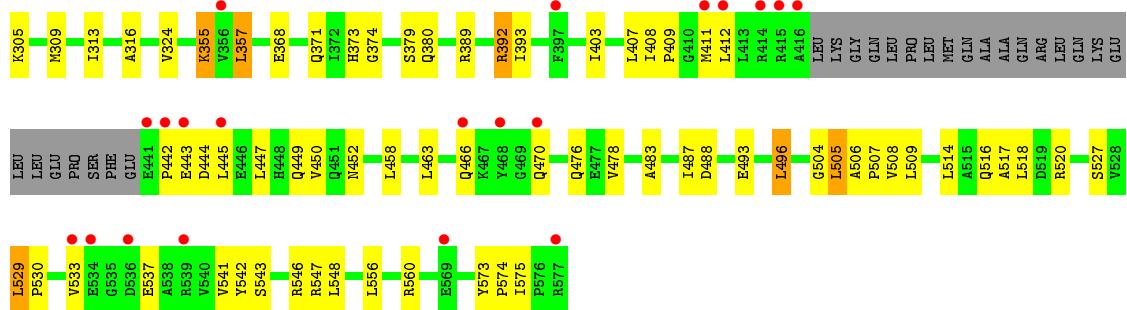
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Acyl-CoA dehydrogenase

- Molecule 1: Acyl-CoA dehydrogenase

K305 M309 I313 A316 V324 K355 V356 L357 E368 Q371 I372 H373 G374 S379 Q380 R389 R392 I393 F397 I403 L407 I408 P409 G410 M411 L412 L413 R414 R415 A416 LEU LYS GLY GLN LEU PRO LEU MET GLN ALA ALA GLN ARG LEU GLN LYS GLU

LEU LEU GLU PRO SER PHE GLU E441 P442 E443 D444 L445 E446 L447 H448 Q449 V450 Q451 N452 L458 L463 Q466 K467 Y468 G469 Q470 Q476 E477 V478 A483 I487 D488 E493 L496 G504 L505 A506 P507 V508 L509 L514 A515 Q516 A517 L518 D519 R520 S527 V528

L529 P530 V533 E534 G535 D536 E537 A538 R539 V540 V541 Y542 S543 R546 R547 L548 L556 R560 E569 Y573 P574 I575 P576 R577

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.85Å 128.85Å 136.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 2.30 37.09 – 2.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.30) 99.8 (37.09-2.03)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.03Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.269 0.219 , 0.268	Depositor DCC
R_{free} test set	5957 reflections (11.39%)	DCC
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.4	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	2 of 84394 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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.*

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[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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.38	0/4261	0.58	0/5760
1	B	0.37	1/4283 (0.0%)	0.56	0/5790
All	All	0.37	1/8544 (0.0%)	0.57	0/11550

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	CYS	CB-SG	-5.28	1.73	1.81

There are no bond angle outliers.

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	4190	0	4245	126	0
1	B	4211	0	4270	134	0
2	A	53	0	30	9	0
2	B	53	0	30	9	0
3	A	233	0	0	4	0
3	B	221	0	0	5	0
All	All	8961	0	8575	253	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 15.

All (253) 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:147:CYS:HB3	1:A:179:LYS:HG2	1.37	1.06
1:B:299:PHE:HB2	1:B:302:ILE:HD13	1.50	0.91
1:B:143:ILE:H	1:B:189:HIS:HD2	1.21	0.87
1:B:126:THR:HG22	1:B:129:GLN:HG2	1.59	0.84
1:A:299:PHE:HB2	1:A:302:ILE:HD13	1.59	0.83
1:B:47:VAL:HG11	1:B:103:SER:HB2	1.61	0.83
1:A:147:CYS:HB3	1:A:179:LYS:CG	2.13	0.79
1:A:127:GLU:O	1:A:131:ARG:HG3	1.81	0.79
1:B:88:LEU:HB3	1:B:92:ILE:HD12	1.67	0.77
1:A:363:ASP:OD2	1:A:395:ARG:HD2	1.84	0.76
1:B:126:THR:H	1:B:129:GLN:NE2	1.84	0.76
1:B:403:ILE:O	1:B:407:LEU:HD13	1.86	0.75
1:B:445:LEU:H	1:B:445:LEU:HD12	1.53	0.73
1:B:147:CYS:SG	1:B:182:ILE:HG12	2.29	0.73
1:A:556:LEU:HD12	1:B:527:SER:HB2	1.69	0.72
1:A:527:SER:HB2	1:B:556:LEU:HD12	1.72	0.71
1:B:504:GLY:O	1:B:507:PRO:HD2	1.90	0.71
1:B:125:GLY:HA2	1:B:129:GLN:HE21	1.56	0.70
1:A:176:ASN:ND2	1:A:237:ASP:H	1.90	0.68
1:B:126:THR:HG22	1:B:129:GLN:H	1.59	0.67
1:B:29:ASP:OD1	1:B:31:SER:HB3	1.94	0.67
1:A:181:TRP:HH2	1:B:379:SER:HB2	1.60	0.67
1:A:478:VAL:HG22	1:A:528:VAL:HG13	1.78	0.66
1:A:225:ILE:HD11	2:A:700:FAD:HM73	1.78	0.65
1:B:408:ILE:HB	1:B:409:PRO:HD3	1.77	0.65
1:B:109:THR:HA	1:B:184:ASN:HD21	1.62	0.64
1:A:143:ILE:H	1:A:189:HIS:HD2	1.44	0.64
1:A:302:ILE:N	1:A:302:ILE:HD12	2.12	0.64
1:A:450:VAL:HG21	1:A:496:LEU:HD12	1.80	0.64
1:A:181:TRP:CH2	1:B:379:SER:HB2	2.33	0.64
1:B:116:ILE:HB	1:B:146:TYR:CG	2.32	0.63
1:A:158:LEU:HD11	1:A:253:HIS:HB3	1.80	0.63
1:A:299:PHE:CB	1:A:302:ILE:HD13	2.28	0.63
1:B:150:GLU:OE2	1:B:160:ALA:HB1	1.99	0.63
1:A:392:ARG:HH12	1:B:371:GLN:HE22	1.46	0.63
1:A:179:LYS:HB2	1:A:233:VAL:HB	1.80	0.62
1:A:302:ILE:HD11	2:B:701:FAD:O2B	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:HD3	1:A:392:ARG:O	1.99	0.62
1:A:277:ARG:O	1:A:281:LEU:HD22	1.99	0.62
1:A:312:ARG:HB3	1:A:361:VAL:HG22	1.82	0.61
1:A:124:PHE:CD2	1:A:255:ILE:HG12	2.35	0.61
1:B:241:PRO:HD2	1:B:244:ASN:ND2	2.15	0.61
1:B:45:ARG:HG3	1:B:46:GLU:HG2	1.80	0.61
1:B:241:PRO:HD2	1:B:244:ASN:HD22	1.66	0.61
1:A:408:ILE:HB	1:A:409:PRO:HD3	1.81	0.60
1:A:76:ALA:HB1	1:A:85:GLY:HA2	1.83	0.60
1:A:262:VAL:O	1:A:266:LYS:HB2	2.01	0.60
1:A:374:GLY:HA3	2:B:701:FAD:O1A	2.01	0.60
1:A:478:VAL:HG22	1:A:528:VAL:CG1	2.31	0.60
1:B:470:GLN:CD	1:B:470:GLN:H	2.04	0.60
1:A:48:LEU:HB3	1:A:49:PRO:HD3	1.83	0.60
1:A:120:PRO:HG2	3:A:762:HOH:O	2.01	0.59
1:A:463:LEU:HA	1:A:466:GLN:HG2	1.85	0.59
1:B:506:ALA:HB3	1:B:507:PRO:HD3	1.85	0.59
1:B:302:ILE:HD12	1:B:302:ILE:H	1.67	0.58
1:A:109:THR:HA	1:A:184:ASN:HD21	1.68	0.58
1:B:68:LYS:O	1:B:71:GLU:HG2	2.02	0.58
1:B:116:ILE:HD12	1:B:146:TYR:HB3	1.84	0.58
1:A:392:ARG:HH12	1:B:371:GLN:NE2	2.01	0.58
1:A:522:GLN:HG3	1:A:549:THR:HG21	1.85	0.58
1:B:575:ILE:HD12	1:B:575:ILE:N	2.18	0.58
1:B:15:LEU:HD13	1:B:15:LEU:O	2.03	0.57
1:B:76:ALA:HB1	1:B:85:GLY:HA2	1.85	0.57
1:A:39:THR:CG2	1:A:100:LEU:HG	2.35	0.56
1:A:506:ALA:HB3	1:A:507:PRO:HD3	1.86	0.56
2:A:700:FAD:O2B	1:B:302:ILE:HD11	2.05	0.56
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.71	0.56
1:A:450:VAL:HG11	1:A:493:GLU:HB2	1.87	0.56
1:A:545:ALA:O	1:A:549:THR:HG22	2.05	0.56
1:B:171:LYS:O	1:B:242:VAL:HG23	2.06	0.56
1:A:176:ASN:HD21	1:A:237:ASP:H	1.54	0.56
1:A:496:LEU:HD11	1:A:514:LEU:HD22	1.88	0.56
1:B:46:GLU:OE2	1:B:68:LYS:HD3	2.06	0.56
1:B:6:LYS:O	1:B:10:LYS:HG3	2.06	0.55
1:B:496:LEU:HD11	1:B:514:LEU:HD22	1.88	0.55
1:A:444:ASP:OD1	1:A:447:LEU:HD13	2.06	0.55
1:A:537:GLU:CD	1:A:537:GLU:H	2.09	0.55
1:B:182:ILE:N	1:B:182:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TRP:CE3	1:A:19:PRO:HA	2.42	0.55
1:B:302:ILE:HD12	1:B:302:ILE:N	2.21	0.55
1:A:7:LEU:HD11	1:A:16:LEU:HD12	1.89	0.55
1:B:16:LEU:N	1:B:16:LEU:HD22	2.23	0.54
1:A:7:LEU:HA	1:A:10:LYS:HE3	1.90	0.54
1:B:392:ARG:O	1:B:392:ARG:HD3	2.06	0.54
1:B:262:VAL:HA	1:B:265:TYR:CE2	2.42	0.54
1:B:225:ILE:HD11	2:B:701:FAD:HM73	1.89	0.54
1:B:171:LYS:C	1:B:242:VAL:HG23	2.28	0.53
1:A:563:ALA:O	1:A:567:VAL:HG23	2.08	0.53
1:A:536:ASP:HA	1:A:539:ARG:HG3	1.89	0.53
2:A:700:FAD:O3B	1:B:296:ILE:HD12	2.08	0.53
1:B:393:ILE:HD11	2:B:701:FAD:HM83	1.91	0.53
1:B:445:LEU:O	1:B:449:GLN:HG3	2.09	0.53
1:A:179:LYS:HE2	1:A:179:LYS:HA	1.90	0.53
1:A:412:LEU:HD12	1:A:486:LEU:HD11	1.90	0.52
1:B:35:ILE:HD12	1:B:92:ILE:CG2	2.39	0.52
1:A:26:GLU:HG2	1:A:502:LEU:HD13	1.91	0.52
1:A:119:LEU:N	1:A:120:PRO:HD2	2.24	0.52
2:B:701:FAD:O1A	2:B:701:FAD:O1P	2.27	0.51
1:A:444:ASP:HB3	1:A:447:LEU:HB2	1.91	0.51
1:A:452:ASN:HB3	1:A:548:LEU:O	2.11	0.51
1:A:361:VAL:O	1:A:365:VAL:HG23	2.10	0.51
1:A:556:LEU:O	1:A:560:ARG:HB2	2.11	0.51
1:B:573:TYR:CE1	1:B:575:ILE:HB	2.46	0.51
1:A:468:TYR:CE2	1:A:475:GLU:HG3	2.45	0.51
1:A:88:LEU:HB3	1:A:92:ILE:HD12	1.91	0.51
1:B:126:THR:H	1:B:129:GLN:HE21	1.57	0.51
1:B:164:ALA:O	1:B:197:VAL:HA	2.11	0.51
1:B:127:GLU:CD	1:B:127:GLU:H	2.14	0.51
1:B:299:PHE:HB2	1:B:302:ILE:CD1	2.32	0.50
1:B:67:ARG:HD2	1:B:140:GLY:O	2.12	0.50
1:A:412:LEU:HD21	1:A:458:LEU:HD23	1.94	0.50
1:A:508:VAL:HG21	1:A:562:GLN:NE2	2.27	0.50
1:B:516:GLN:NE2	1:B:560:ARG:HH21	2.10	0.50
1:A:334:LYS:HG2	1:A:339:ALA:HB1	1.93	0.50
1:B:463:LEU:HA	1:B:466:GLN:HG2	1.94	0.49
1:A:360:GLU:HA	1:A:363:ASP:OD2	2.13	0.49
1:B:505:LEU:HD13	1:B:508:VAL:HB	1.95	0.49
2:A:700:FAD:O1A	1:B:374:GLY:HA3	2.12	0.49
1:A:142:TRP:HA	1:A:189:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:H	1:A:129:GLN:NE2	2.10	0.49
1:A:82:GLU:CD	1:A:82:GLU:H	2.16	0.49
1:A:39:THR:HG23	1:A:100:LEU:HG	1.95	0.49
1:A:573:TYR:CE1	1:A:575:ILE:HB	2.48	0.49
1:A:206:LEU:HD22	1:A:246:LEU:HB2	1.95	0.49
1:A:355:LYS:HD3	1:A:355:LYS:C	2.32	0.49
1:A:449:GLN:OE1	1:A:551:ARG:HB2	2.13	0.49
1:B:476:GLN:NE2	2:B:701:FAD:N1A	2.59	0.48
1:B:505:LEU:HD12	1:B:509:LEU:HG	1.94	0.48
1:B:180:GLN:NE2	1:B:232:GLN:HE21	2.11	0.48
1:A:476:GLN:HB3	1:B:301:LEU:HG	1.96	0.48
1:B:35:ILE:HD12	1:B:92:ILE:HG21	1.94	0.48
1:B:183:SER:O	1:B:184:ASN:HB2	2.13	0.48
1:B:41:THR:O	1:B:45:ARG:HG2	2.12	0.48
1:A:537:GLU:O	1:A:541:VAL:HG23	2.13	0.48
1:A:88:LEU:HB3	1:A:89:PRO:HD2	1.95	0.48
1:B:574:PRO:HG2	1:B:575:ILE:HD12	1.95	0.48
1:B:7:LEU:HD13	1:B:7:LEU:C	2.34	0.48
1:B:575:ILE:H	1:B:575:ILE:HD12	1.77	0.48
3:A:857:HOH:O	2:B:701:FAD:PA	2.71	0.48
1:A:492:ALA:HB1	1:A:514:LEU:HD13	1.96	0.48
1:B:305:LYS:HB3	1:B:309:MET:CE	2.44	0.48
1:A:35:ILE:HD13	1:A:92:ILE:HG23	1.96	0.47
2:A:700:FAD:H9	2:A:700:FAD:H1'2	1.70	0.47
1:A:180:GLN:HG3	1:A:181:TRP:CD1	2.49	0.47
1:B:91:VAL:O	1:B:95:VAL:HG13	2.15	0.47
1:B:180:GLN:HE22	1:B:232:GLN:HE21	1.62	0.47
1:B:478:VAL:HG23	3:B:753:HOH:O	2.15	0.47
1:B:80:PRO:HB2	1:B:83:TYR:HD2	1.79	0.47
1:A:116:ILE:HB	1:A:146:TYR:CG	2.49	0.47
1:B:316:ALA:HA	1:B:357:LEU:HD13	1.95	0.47
1:A:302:ILE:CD1	1:A:302:ILE:N	2.79	0.46
1:A:392:ARG:HH22	1:B:371:GLN:HE21	1.62	0.46
1:A:183:SER:O	1:A:184:ASN:HB2	2.15	0.46
1:B:412:LEU:HD11	1:B:458:LEU:CD2	2.44	0.46
1:B:92:ILE:O	1:B:95:VAL:HG22	2.16	0.46
1:B:182:ILE:HG22	1:B:185:ALA:HB2	1.98	0.46
1:A:556:LEU:HD12	1:B:527:SER:CB	2.43	0.46
1:A:8:TRP:HB3	1:A:17:GLU:HB2	1.97	0.46
1:B:26:GLU:CD	1:B:26:GLU:H	2.18	0.46
1:B:66:MET:HE3	1:B:106:PHE:HZ	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:HA	1:B:201:HIS:O	2.15	0.46
1:B:48:LEU:HB3	1:B:49:PRO:HD3	1.98	0.45
1:A:136:LYS:HE2	3:A:720:HOH:O	2.15	0.45
2:A:700:FAD:O1A	2:A:700:FAD:O1P	2.34	0.45
1:B:276:LYS:O	1:B:280:GLU:HG3	2.17	0.45
1:A:301:LEU:HG	1:B:476:GLN:HB3	1.98	0.45
1:B:279:LEU:HD12	1:B:313:ILE:HD12	1.98	0.45
1:A:478:VAL:HA	1:A:528:VAL:HG11	1.98	0.45
1:B:305:LYS:HD3	1:B:368:GLU:OE1	2.16	0.45
1:A:80:PRO:HB2	1:A:83:TYR:HD2	1.82	0.45
1:B:267:LEU:HD23	1:B:355:LYS:CD	2.46	0.45
2:A:700:FAD:O3B	1:B:302:ILE:HG12	2.17	0.44
1:A:262:VAL:HA	1:A:265:TYR:CE1	2.52	0.44
1:B:305:LYS:HB3	1:B:309:MET:HE2	2.00	0.44
1:B:122:VAL:HG22	1:B:134:LEU:HD21	1.99	0.44
1:B:143:ILE:H	1:B:189:HIS:CD2	2.13	0.44
1:B:449:GLN:HB3	1:B:518:LEU:HD21	2.00	0.44
1:B:529:LEU:HA	1:B:529:LEU:HD12	1.84	0.44
1:B:533:VAL:HG11	1:B:541:VAL:HG21	1.99	0.44
1:A:42:PHE:O	1:A:46:GLU:HB2	2.18	0.44
1:A:14:TRP:O	1:A:454:LYS:HE2	2.17	0.44
1:A:334:LYS:HE2	1:A:339:ALA:HB1	2.00	0.44
1:B:273:GLY:O	1:B:277:ARG:HG2	2.17	0.44
1:A:393:ILE:HD11	2:A:700:FAD:HM83	1.99	0.44
1:B:142:TRP:HA	1:B:189:HIS:CD2	2.53	0.44
1:A:298:ARG:NH1	1:A:565:GLU:OE2	2.50	0.43
1:A:150:GLU:HG2	1:A:179:LYS:HE2	1.99	0.43
1:A:264:ARG:HG3	1:A:355:LYS:HG3	1.99	0.43
1:B:529:LEU:N	1:B:530:PRO:CD	2.81	0.43
1:A:94:THR:HG23	1:A:269:ALA:HB2	1.99	0.43
1:B:520:ARG:HD3	3:B:886:HOH:O	2.19	0.43
1:B:543:SER:O	1:B:547:ARG:HG2	2.18	0.43
1:A:91:VAL:HA	1:A:324:VAL:HG11	2.00	0.43
1:B:452:ASN:HB3	1:B:548:LEU:O	2.18	0.43
1:B:180:GLN:HE22	1:B:232:GLN:NE2	2.17	0.43
1:B:66:MET:HE2	1:B:75:LEU:HD21	2.01	0.43
1:A:25:PRO:HA	1:A:28:PHE:CE2	2.54	0.43
1:A:121:LEU:HD21	1:A:133:TYR:HB2	1.99	0.43
1:A:403:ILE:O	1:A:407:LEU:HG	2.17	0.43
1:B:8:TRP:CZ2	1:B:20:GLU:HB2	2.53	0.43
1:A:96:VAL:CG1	1:A:100:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:NZ	1:A:401:ASN:ND2	2.67	0.43
1:A:131:ARG:NH1	1:A:131:ARG:HG2	2.34	0.42
1:A:35:ILE:HD13	1:A:92:ILE:CG2	2.49	0.42
1:A:24:THR:HB	1:A:25:PRO:HD2	2.00	0.42
1:B:8:TRP:CE3	1:B:19:PRO:HA	2.54	0.42
1:B:90:LYS:HD3	1:B:90:LYS:HA	1.84	0.42
1:A:59:LEU:HD11	1:A:226:LYS:O	2.19	0.42
1:B:444:ASP:OD1	1:B:447:LEU:HD12	2.19	0.42
1:A:304:GLN:HA	1:A:560:ARG:HG2	2.00	0.42
1:A:20:GLU:O	1:A:20:GLU:HG2	2.19	0.42
1:B:488:ASP:HB3	1:B:517:ALA:HB1	2.01	0.42
1:B:542:TYR:O	1:B:546:ARG:HG3	2.19	0.42
1:B:126:THR:CG2	1:B:129:GLN:HG2	2.39	0.42
1:B:66:MET:HE3	1:B:106:PHE:CZ	2.55	0.42
1:B:66:MET:CE	1:B:66:MET:HA	2.49	0.42
1:B:285:TYR:CE2	1:B:373:HIS:HA	2.55	0.42
1:A:150:GLU:HB2	1:A:153:SER:OG	2.20	0.42
1:A:223:MET:O	1:A:389:ARG:HD2	2.19	0.42
1:A:280:GLU:HG3	3:A:827:HOH:O	2.19	0.42
1:B:66:MET:CE	1:B:75:LEU:HD21	2.49	0.42
1:B:55:GLU:HG2	3:B:723:HOH:O	2.18	0.42
1:A:130:LYS:HB3	1:A:134:LEU:HD12	2.01	0.42
1:B:296:ILE:HA	1:B:299:PHE:CD1	2.55	0.42
1:B:393:ILE:CD1	2:B:701:FAD:HM83	2.50	0.42
1:A:450:VAL:HG12	1:A:454:LYS:HZ2	1.85	0.42
1:B:175:LEU:HB2	1:B:238:VAL:HB	2.01	0.42
1:B:129:GLN:NE2	3:B:756:HOH:O	2.52	0.42
1:B:182:ILE:CG2	1:B:185:ALA:HB2	2.50	0.42
1:A:79:VAL:O	1:A:85:GLY:HA3	2.19	0.42
1:A:459:MET:O	1:A:463:LEU:HD13	2.20	0.42
1:A:528:VAL:O	1:A:531:ARG:HB3	2.19	0.42
1:A:221:LYS:O	1:B:380:GLN:HG3	2.20	0.41
1:A:392:ARG:HD3	1:A:392:ARG:C	2.40	0.41
1:B:407:LEU:HD21	3:B:811:HOH:O	2.19	0.41
1:A:382:TYR:HA	1:A:383:PRO:HD3	1.92	0.41
1:B:450:VAL:HG11	1:B:493:GLU:HB2	2.02	0.41
1:A:120:PRO:HB3	1:A:255:ILE:CG2	2.50	0.41
1:A:43:VAL:CG1	1:A:100:LEU:HD23	2.51	0.41
1:B:115:SER:O	1:B:119:LEU:HB2	2.20	0.41
1:B:392:ARG:C	1:B:392:ARG:HD3	2.41	0.41
1:B:7:LEU:HD13	1:B:7:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ALA:O	1:B:487:ILE:HG13	2.21	0.41
1:A:302:ILE:HD11	2:B:701:FAD:N3A	2.35	0.41
1:B:91:VAL:HA	1:B:324:VAL:HG11	2.02	0.41
1:B:392:ARG:HD3	1:B:392:ARG:HA	1.92	0.41
1:A:452:ASN:HA	1:A:452:ASN:HD22	1.68	0.41
1:B:253:HIS:HB2	1:B:257:PHE:CE2	2.55	0.41
1:A:163:ARG:O	1:A:175:LEU:HA	2.21	0.41
1:B:223:MET:O	1:B:389:ARG:HD2	2.21	0.40
1:A:476:GLN:NE2	2:A:700:FAD:N1A	2.68	0.40
1:B:516:GLN:NE2	1:B:560:ARG:NH2	2.69	0.40
1:A:35:ILE:HG21	1:A:92:ILE:HG23	2.04	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	542/577 (94%)	515 (95%)	27 (5%)	0	100	100
1	B	545/577 (94%)	522 (96%)	19 (4%)	4 (1%)	26	31
All	All	1087/1154 (94%)	1037 (95%)	46 (4%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	PRO
1	B	58	GLU
1	B	200	GLU
1	B	443	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	425/455 (93%)	409 (96%)	16 (4%)	40	54
1	B	427/455 (94%)	408 (96%)	19 (4%)	35	46
All	All	852/910 (94%)	817 (96%)	35 (4%)	37	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	67	ARG
1	A	75	LEU
1	A	132	LYS
1	A	179	LYS
1	A	244	ASN
1	A	266	LYS
1	A	281	LEU
1	A	392	ARG
1	A	393	ILE
1	A	412	LEU
1	A	413	LEU
1	A	414	ARG
1	A	443	GLU
1	A	551	ARG
1	A	560	ARG
1	B	26	GLU
1	B	31	SER
1	B	34	GLU
1	B	55	GLU
1	B	61	LEU
1	B	126	THR
1	B	132	LYS
1	B	168	GLU
1	B	222	LYS
1	B	246	LEU
1	B	279	LEU

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Mol	Chain	Res	Type
1	B	355	LYS
1	B	357	LEU
1	B	392	ARG
1	B	411	MET
1	B	496	LEU
1	B	505	LEU
1	B	529	LEU
1	B	537	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	129	GLN
1	A	176	ASN
1	A	184	ASN
1	A	189	HIS
1	A	244	ASN
1	A	261	ASN
1	A	288	GLN
1	A	291	GLN
1	A	401	ASN
1	A	404	ASN
1	A	449	GLN
1	A	452	ASN
1	A	562	GLN
1	B	9	GLN
1	B	56	HIS
1	B	62	ASN
1	B	129	GLN
1	B	180	GLN
1	B	184	ASN
1	B	189	HIS
1	B	201	HIS
1	B	258	ASN
1	B	284	GLN
1	B	371	GLN
1	B	380	GLN
1	B	452	ASN
1	B	516	GLN
1	B	522	GLN
1	B	562	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 ⓘ

2 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	700	-	48,58,58	1.76	13 (27%)	54,89,89	4.32	23 (42%)
2	FAD	B	701	-	48,58,58	1.73	10 (20%)	54,89,89	4.46	22 (40%)

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	700	-	-	0/30/50/50	0/6/6/6
2	FAD	B	701	-	-	0/30/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C1'-N10	-3.72	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	FAD	C8A-N7A	-3.30	1.28	1.34
2	B	701	FAD	O4B-C4B	-3.23	1.37	1.45
2	B	701	FAD	C8A-N7A	-3.11	1.28	1.34
2	A	700	FAD	C1'-N10	-2.90	1.45	1.48
2	B	701	FAD	O5'-C5'	-2.58	1.34	1.44
2	A	700	FAD	C2'-C3'	-2.54	1.48	1.53
2	A	700	FAD	O4B-C4B	-2.54	1.39	1.45
2	A	700	FAD	O5'-C5'	-2.41	1.34	1.44
2	A	700	FAD	O4B-C1B	-2.28	1.38	1.41
2	B	701	FAD	O4B-C1B	-2.12	1.38	1.41
2	A	700	FAD	P-O2P	2.07	1.63	1.54
2	B	701	FAD	C9A-N10	2.12	1.41	1.38
2	A	700	FAD	C6-C5X	2.28	1.45	1.41
2	A	700	FAD	C3B-C4B	2.41	1.59	1.53
2	A	700	FAD	C9A-N10	2.47	1.42	1.38
2	B	701	FAD	C3B-C4B	2.59	1.60	1.53
2	B	701	FAD	C4-N3	2.75	1.38	1.33
2	A	700	FAD	C4-N3	2.93	1.38	1.33
2	A	700	FAD	C4-C4X	3.25	1.47	1.41
2	B	701	FAD	C4-C4X	3.80	1.48	1.41
2	B	701	FAD	C4X-C10	5.05	1.50	1.41
2	A	700	FAD	C4X-C10	5.77	1.51	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	C4B-O4B-C1B	-21.25	86.37	109.72
2	A	700	FAD	C4B-O4B-C1B	-20.36	87.34	109.72
2	B	701	FAD	N3A-C2A-N1A	-10.88	120.56	128.89
2	A	700	FAD	N3A-C2A-N1A	-10.25	121.05	128.89
2	A	700	FAD	O3P-PA-O5B	-9.77	77.02	102.94
2	B	701	FAD	O3P-PA-O5B	-9.21	78.50	102.94
2	B	701	FAD	P-O3P-PA	-6.43	114.66	132.73
2	A	700	FAD	P-O3P-PA	-5.90	116.15	132.73
2	B	701	FAD	C4-C4X-C10	-5.66	116.32	119.94
2	B	701	FAD	C4X-C10-N10	-5.43	117.32	120.52
2	A	700	FAD	C4-C4X-C10	-5.41	116.48	119.94
2	A	700	FAD	C4X-C10-N10	-4.73	117.73	120.52
2	B	701	FAD	O2A-PA-O3P	-4.69	83.82	105.09
2	A	700	FAD	O2A-PA-O3P	-4.57	84.34	105.09
2	B	701	FAD	C2B-C3B-C4B	-4.45	93.46	102.61
2	B	701	FAD	C4X-C4-N3	-4.37	117.61	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	FAD	C4X-C4-N3	-4.33	117.67	123.59
2	A	700	FAD	C2B-C3B-C4B	-4.20	93.98	102.61
2	A	700	FAD	C1'-C2'-C3'	-3.03	101.15	109.82
2	B	701	FAD	C1'-C2'-C3'	-3.03	101.16	109.82
2	B	701	FAD	O5B-C5B-C4B	-2.60	99.55	109.12
2	A	700	FAD	C4A-C5A-N7A	-2.51	107.17	109.48
2	B	701	FAD	C1'-N10-C9A	-2.32	116.26	118.86
2	A	700	FAD	O5B-C5B-C4B	-2.22	100.95	109.12
2	A	700	FAD	C1'-N10-C9A	-2.20	116.39	118.86
2	A	700	FAD	O4'-C4'-C5'	2.00	114.55	110.19
2	A	700	FAD	O2P-P-O3P	2.00	114.19	105.09
2	B	701	FAD	O2P-P-O3P	2.01	114.23	105.09
2	B	701	FAD	O2A-PA-O1A	2.12	124.00	112.53
2	B	701	FAD	C1B-N9A-C4A	2.23	130.30	126.94
2	A	700	FAD	C1B-N9A-C4A	3.16	131.70	126.94
2	A	700	FAD	C5X-C9A-N10	3.19	120.04	117.62
2	B	701	FAD	C4-C4X-N5	3.23	122.64	118.72
2	B	701	FAD	O4B-C1B-N9A	3.44	115.30	108.10
2	B	701	FAD	C5X-C9A-N10	3.73	120.45	117.62
2	A	700	FAD	C4-C4X-N5	3.73	123.25	118.72
2	B	701	FAD	C4X-N5-C5X	3.98	121.34	116.76
2	B	701	FAD	O4B-C4B-C5B	4.16	124.21	109.32
2	A	700	FAD	O4B-C1B-N9A	4.35	117.20	108.10
2	A	700	FAD	C4X-N5-C5X	4.48	121.92	116.76
2	A	700	FAD	O4B-C4B-C5B	4.49	125.37	109.32
2	A	700	FAD	C2B-C1B-N9A	5.42	122.58	114.29
2	B	701	FAD	C2B-C1B-N9A	6.51	124.23	114.29
2	A	700	FAD	C4-N3-C2	7.72	121.92	115.25
2	B	701	FAD	C4-N3-C2	8.08	122.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	FAD	9	0
2	B	701	FAD	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	546/577 (94%)	0.40	34 (6%)	24	32	17, 30, 60, 82	0
1	B	549/577 (95%)	0.52	49 (8%)	12	17	17, 33, 59, 82	0
All	All	1095/1154 (94%)	0.46	83 (7%)	17	24	17, 31, 60, 82	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	ALA	8.3
1	B	441	GLU	7.3
1	A	414	ARG	6.7
1	B	577	ARG	6.3
1	B	5	LYS	6.3
1	A	411	MET	5.8
1	A	7	LEU	5.8
1	A	536	ASP	5.7
1	B	443	GLU	5.4
1	B	442	PRO	5.1
1	A	335	LYS	5.0
1	B	7	LEU	5.0
1	A	412	LEU	4.8
1	A	443	GLU	4.7
1	A	539	ARG	4.6
1	B	415	ARG	4.6
1	A	534	GLU	4.5
1	A	470	GLN	4.4
1	A	537	GLU	4.4
1	B	169	ASP	4.4
1	A	131	ARG	4.3
1	A	333	GLY	4.2
1	A	540	VAL	4.1
1	A	535	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	18	VAL	4.1
1	A	469	GLY	3.8
1	B	170	GLY	3.7
1	B	171	LYS	3.7
1	B	174	ILE	3.5
1	B	168	GLU	3.5
1	B	470	GLN	3.5
1	A	466	GLN	3.5
1	B	414	ARG	3.4
1	A	8	TRP	3.3
1	A	538	ALA	3.2
1	A	9	GLN	3.2
1	A	413	LEU	3.1
1	B	6	LYS	3.1
1	B	9	GLN	3.0
1	B	199	GLY	3.0
1	A	103	SER	2.9
1	B	10	LYS	2.9
1	B	445	LEU	2.8
1	B	16	LEU	2.8
1	B	131	ARG	2.8
1	A	10	LYS	2.7
1	B	166	LEU	2.7
1	A	45	ARG	2.7
1	B	172	HIS	2.6
1	B	37	ARG	2.6
1	B	267	LEU	2.6
1	B	468	TYR	2.6
1	A	101	SER	2.5
1	A	397	PHE	2.5
1	B	356	VAL	2.4
1	B	569	GLU	2.4
1	B	8	TRP	2.4
1	B	17	GLU	2.3
1	A	547	ARG	2.3
1	B	257	PHE	2.3
1	A	17	GLU	2.3
1	A	6	LYS	2.2
1	A	41	THR	2.2
1	B	45	ARG	2.2
1	B	128	GLU	2.2
1	A	471	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	397	PHE	2.2
1	B	539	ARG	2.2
1	B	167	SER	2.1
1	A	5	LYS	2.1
1	B	412	LEU	2.1
1	A	465	VAL	2.1
1	B	198	ASP	2.1
1	B	411	MET	2.1
1	B	25	PRO	2.1
1	B	534	GLU	2.1
1	B	249	ILE	2.1
1	B	533	VAL	2.1
1	B	466	GLN	2.1
1	B	251	LYS	2.1
1	B	117	GLY	2.0
1	B	34	GLU	2.0
1	B	536	ASP	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(Å²)	Q<0.9
2	FAD	B	701	53/53	0.75	0.30	4.25	34,48,63,68	0
2	FAD	A	700	53/53	0.72	0.30	3.36	27,46,61,66	0

6.5 Other polymers (i)

There are no such residues in this entry.