Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2016 – 05:50 PM EDT

PDB ID	:	5L46
Title	:	Crystal structure of human dimethylglycine-dehydrogenase
Authors	:	Hromic, A.; Pavkov-Keller, T.; Gruber, K.
Deposited on	:	2016-05-25
Resolution	:	3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

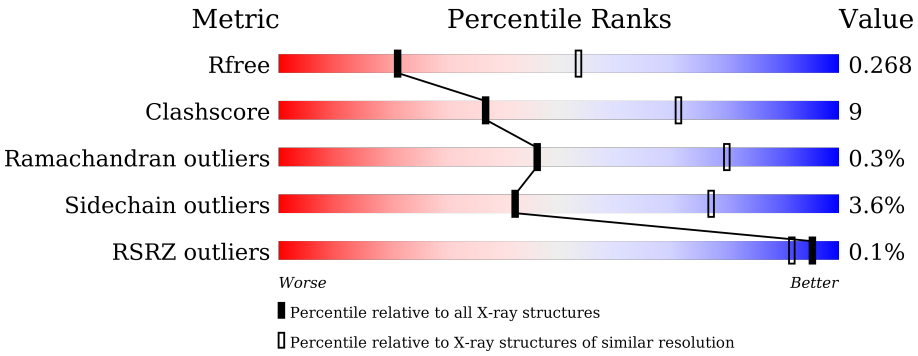
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.09 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	841	72% 23%
1	B	841	70% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12894 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.

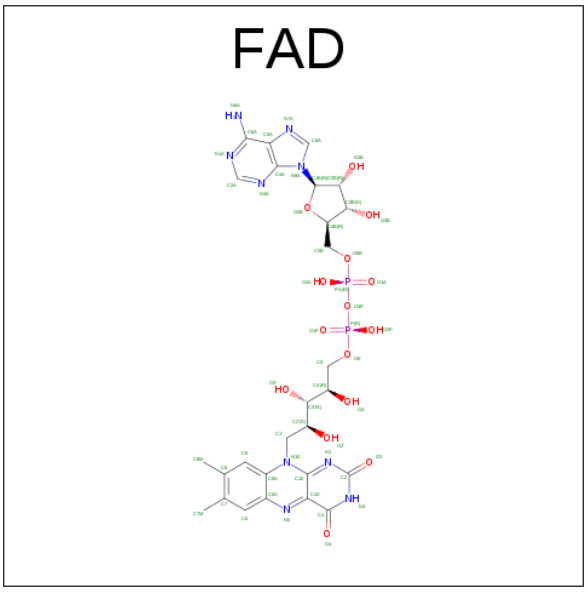
- Molecule 1 is a protein called Dimethylglycine dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6398	4099	1090	1186	23			
1	B	808	Total	C	N	O	S	0	0	0
			6384	4088	1088	1185	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP Q9UI17
A	279	PRO	SER	conflict	UNP Q9UI17
A	867	ARG	-	expression tag	UNP Q9UI17
A	868	PRO	-	expression tag	UNP Q9UI17
B	28	MET	-	initiating methionine	UNP Q9UI17
B	279	PRO	SER	conflict	UNP Q9UI17
B	867	ARG	-	expression tag	UNP Q9UI17
B	868	PRO	-	expression tag	UNP Q9UI17

- 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 water.

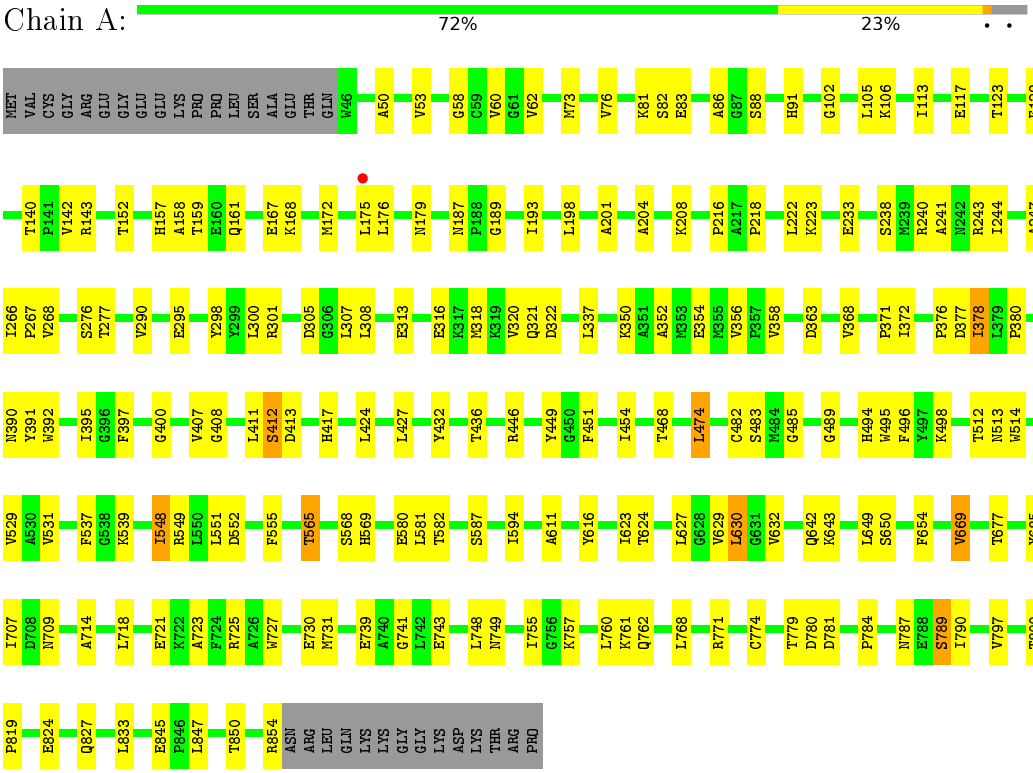
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	2	Total	O	0	0
			2	2		

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.

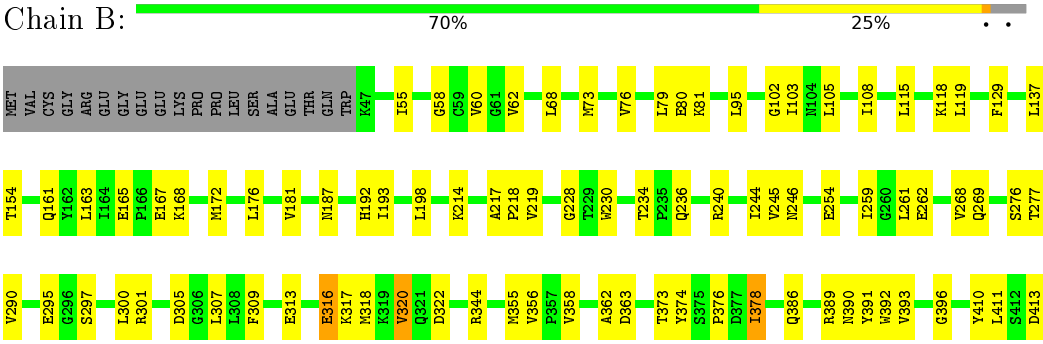
- Molecule 1: Dimethylglycine dehydrogenase, mitochondrial

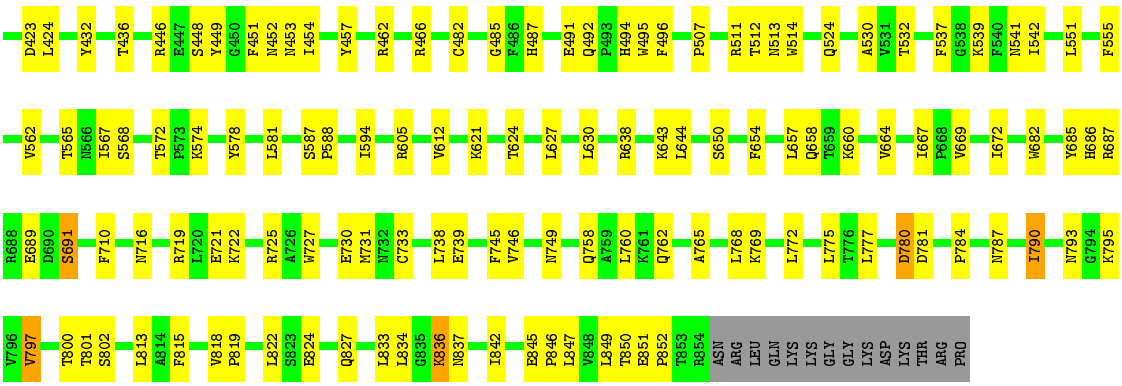
Chain A:



- Molecule 1: Dimethylglycine dehydrogenase, mitochondrial

Chain B:




D423 L424 Y432 T436 R446 E447 S448 Y449 G450 F451 N452 N453 I454 Y457 R462 R466 C482 G485 F486 H487 E491 Q492 P493 H494 W495 F496 P507 R511 T512 N513 W514 Q524 A530 V531 T532 F537 G538 K539 F540 N541 I542 L551 P555
V562 T565 N566 I567 S568 T572 P573 K574 Y578 L581 S587 P588 I594 R605 V612 K621 T624 L627 L630 R638 K643 L644 S650 F654 L657 Q658 T659 K660 V664 I667 P668 V669 I672 W682 Y685 H686 R687
R688 E689 D690 S691 F710 N716 R719 L720 E721 K722 R725 A726 W727 E730 M731 N732 C733 L738 E739 F745 V746 N749 Q758 A759 L760 K761 Q762 A765 L768 K769 L772 L775 T776 L777 D780 D781 P784 N787 I790 N793 G794 K795
V796 V797 T800 T801 S802 L813 A814 F815 V818 P819 L822 S823 E824 Q827 L833 L834 G835 K836 N837 I842 E845 P846 L847 V848 L849 T850 E851 P852 T853 R854 ASN ARG LEU GLN LYS LYS GLY GLY LYS ASP LYS THR ARG PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.38Å 119.87Å 86.47Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	58.65 – 3.09 58.65 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (58.65-3.09) 97.7 (58.65-3.09)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.179 , 0.269 0.181 , 0.268	Depositor DCC
R_{free} test set	1524 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.068 for h,-k,-l 0.030 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12894	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 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.49	1/6558 (0.0%)	0.66	0/8895
1	B	0.50	0/6542	0.64	1/8872 (0.0%)
All	All	0.50	1/13100 (0.0%)	0.65	1/17767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	774	CYS	CB-SG	-5.00	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	813	LEU	CA-CB-CG	5.69	128.39	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6398	0	6352	115	0
1	B	6384	0	6342	128	0
2	A	53	0	30	6	0
2	B	53	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	2	0	0	0	0
All	All	12894	0	12754	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 9.

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:290:VAL:HG13	1:B:301:ARG:HB3	1.54	0.90
1:B:487:HIS:CD2	1:B:492:GLN:HE21	2.01	0.78
1:A:290:VAL:HG13	1:A:301:ARG:HB3	1.66	0.76
1:A:755:ILE:HD11	1:B:793:ASN:HD21	1.53	0.74
1:B:115:LEU:HA	1:B:118:LYS:HE2	1.71	0.72
1:A:73:MET:HG2	1:A:76:VAL:HG22	1.72	0.71
1:B:730:GLU:OE2	1:B:802:SER:OG	2.08	0.70
1:A:677:THR:HG22	1:A:718:LEU:HD13	1.76	0.68
1:B:143:ARG:NH2	1:B:453:ASN:O	2.28	0.67
1:B:73:MET:HG2	1:B:76:VAL:HG22	1.77	0.66
1:B:176:LEU:HD11	1:B:355:MET:HG3	1.78	0.65
1:B:687:ARG:HG3	1:B:689:GLU:HG2	1.80	0.64
1:A:277:THR:HG23	1:A:305:ASP:HB3	1.77	0.64
1:A:723:ALA:O	1:A:725:ARG:NH1	2.30	0.63
1:A:787:ASN:N	1:A:800:THR:O	2.29	0.63
1:A:337:LEU:HD11	1:A:368:VAL:HG13	1.80	0.63
1:A:152:THR:O	1:A:789:SER:OG	2.15	0.63
1:B:487:HIS:HD2	1:B:492:GLN:HE21	1.44	0.62
1:B:356:VAL:HG12	1:B:358:VAL:HG22	1.80	0.62
1:B:562:VAL:HG11	1:B:588:PRO:HG3	1.81	0.62
1:B:686:HIS:NE2	1:B:691:SER:OG	2.32	0.62
1:A:408:GLY:O	1:A:412:SER:HB3	2.01	0.61
1:A:413:ASP:O	1:A:417:HIS:ND1	2.32	0.61
1:A:739:GLU:HB3	1:A:768:LEU:HD22	1.82	0.61
1:A:251:TRP:CE3	2:A:901:FAD:H8A	2.36	0.60
1:A:267:PRO:HB2	1:A:321:GLN:HB2	1.83	0.60
1:A:721:GLU:HG2	1:A:847:LEU:HD23	1.83	0.59
1:A:313:GLU:HG2	1:A:449:TYR:HE2	1.68	0.59
1:B:137:LEU:HD11	1:B:176:LEU:HD21	1.85	0.58
1:B:234:THR:HG22	1:B:236:GLN:H	1.67	0.58
1:B:219:VAL:H	2:B:901:FAD:H61A	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HD22	1:B:555:PHE:HE2	1.70	0.57
1:A:81:LYS:HG3	1:A:218:PRO:HB3	1.85	0.57
1:B:81:LYS:HG3	1:B:218:PRO:HB3	1.87	0.56
1:A:380:PRO:HG2	1:A:427:LEU:HD11	1.87	0.56
1:A:485:GLY:HA3	1:A:494:HIS:CE1	2.41	0.56
1:B:161:GLN:HG3	1:B:187:ASN:OD1	2.05	0.56
1:A:175:LEU:HD13	1:A:358:VAL:HG11	1.87	0.55
1:A:630:LEU:HD12	1:A:686:HIS:CE1	2.42	0.55
1:B:80:GLU:HA	2:B:901:FAD:H8A	1.89	0.55
1:B:300:LEU:HD21	1:B:307:LEU:HD22	1.87	0.55
1:A:850:THR:O	1:A:854:ARG:HG3	2.07	0.54
1:B:262:GLU:N	1:B:262:GLU:OE1	2.35	0.54
1:A:468:THR:OG1	1:A:489:GLY:O	2.26	0.54
1:B:716:ASN:O	1:B:719:ARG:HG3	2.08	0.54
1:A:397:PHE:HZ	1:A:407:VAL:HG11	1.73	0.54
1:A:581:LEU:HB2	1:A:594:ILE:O	2.08	0.54
1:A:356:VAL:HG12	1:A:358:VAL:HG22	1.89	0.53
1:B:638:ARG:HD3	1:B:650:SER:HA	1.90	0.53
1:A:784:PRO:HA	1:A:833:LEU:HD21	1.90	0.53
1:A:193:ILE:HG21	1:A:198:LEU:HD22	1.89	0.53
1:A:266:ILE:HD11	1:A:320:VAL:HB	1.89	0.53
1:B:277:THR:HG23	1:B:305:ASP:HB3	1.91	0.53
1:B:511:ARG:NH1	1:B:780:ASP:O	2.42	0.52
1:A:131:GLN:NE2	1:A:189:GLY:O	2.42	0.52
1:A:143:ARG:NE	1:A:295:GLU:OE2	2.29	0.52
1:A:137:LEU:HD11	1:A:176:LEU:HD21	1.92	0.52
1:A:83:GLU:HG3	1:A:86:ALA:HB2	1.92	0.52
1:B:787:ASN:N	1:B:800:THR:O	2.35	0.52
1:B:721:GLU:HG2	1:B:847:LEU:HD23	1.91	0.52
1:A:518:VAL:HG13	1:A:714:ALA:HA	1.92	0.51
1:B:228:GLY:O	1:B:390:ASN:ND2	2.30	0.51
1:B:244:ILE:HG13	1:B:391:TYR:HD1	1.73	0.51
1:B:836:LYS:HE3	1:B:837:ASN:H	1.74	0.51
1:B:245:VAL:HG22	1:B:392:TRP:HB2	1.91	0.51
1:B:482:CYS:HB3	1:B:496:PHE:CD1	2.46	0.51
1:A:161:GLN:HG3	1:A:187:ASN:OD1	2.11	0.51
1:B:259:ILE:HG13	1:B:261:LEU:HG	1.92	0.51
1:B:449:TYR:O	1:B:452:ASN:HB2	2.10	0.51
1:A:630:LEU:HD12	1:A:686:HIS:HE1	1.76	0.51
1:B:487:HIS:CE1	1:B:494:HIS:HE2	2.28	0.51
1:B:790:ILE:HD11	1:B:818:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:LYS:NZ	1:B:769:LYS:HB3	2.26	0.50
1:A:265:LEU:HD11	1:A:395:ILE:HD12	1.94	0.50
1:B:539:LYS:HD3	1:B:627:LEU:HB2	1.93	0.50
1:A:582:THR:HB	1:A:594:ILE:HB	1.94	0.50
1:B:268:VAL:HG12	1:B:320:VAL:HG12	1.93	0.50
1:A:432:TYR:HB3	1:A:436:THR:OG1	2.12	0.50
1:B:739:GLU:HB3	1:B:768:LEU:HD22	1.94	0.49
1:A:240:ARG:NH2	1:B:765:ALA:O	2.45	0.49
1:B:386:GLN:HB2	1:B:605:ARG:HB2	1.95	0.49
1:A:204:ALA:O	1:A:208:LYS:HB2	2.12	0.49
1:A:301:ARG:CZ	1:A:308:LEU:HD13	2.43	0.49
1:B:143:ARG:NE	1:B:295:GLU:OE2	2.40	0.49
1:B:539:LYS:HD2	1:B:624:THR:HA	1.94	0.49
1:B:313:GLU:HG2	1:B:449:TYR:HE2	1.78	0.49
1:A:498:LYS:HE3	1:A:520:SER:OG	2.12	0.49
1:B:276:SER:N	1:B:363:ASP:O	2.45	0.49
1:B:485:GLY:HA3	1:B:494:HIS:CE1	2.48	0.49
1:B:278:ILE:HG12	1:B:362:ALA:HB2	1.94	0.49
1:B:153:ARG:HA	1:B:787:ASN:O	2.13	0.49
1:B:827:GLN:HB3	1:B:842:ILE:HD12	1.93	0.49
1:A:669:VAL:HG23	1:A:686:HIS:HB3	1.94	0.49
1:B:524:GLN:HG2	1:B:530:ALA:HB2	1.94	0.48
1:A:244:ILE:HG13	1:A:391:TYR:HD1	1.78	0.48
1:A:569:HIS:CE1	1:A:580:GLU:HG3	2.48	0.48
1:A:548:ILE:O	1:A:552:ASP:HB2	2.13	0.48
1:B:154:THR:HG21	1:B:161:GLN:NE2	2.29	0.48
1:B:638:ARG:HG3	1:B:682:TRP:HH2	1.78	0.48
1:A:451:PHE:HA	1:A:454:ILE:HG23	1.94	0.48
1:B:432:TYR:HB3	1:B:436:THR:OG1	2.14	0.48
1:B:297:SER:HA	1:B:453:ASN:HD22	1.78	0.48
1:A:400:GLY:HA3	2:A:901:FAD:H4'	1.95	0.47
1:B:667:ILE:O	1:B:669:VAL:HG23	2.15	0.47
1:B:60:VAL:HG22	2:B:901:FAD:O2P	2.14	0.47
1:B:230:TRP:O	1:B:240:ARG:HA	2.15	0.47
1:B:664:VAL:O	1:B:667:ILE:HB	2.15	0.47
1:A:301:ARG:NH2	1:A:308:LEU:HD13	2.29	0.47
1:A:318:MET:SD	1:A:446:ARG:HG3	2.55	0.47
1:B:374:TYR:CE2	1:B:378:ILE:HG13	2.49	0.47
1:A:106:LYS:HD2	1:A:157:HIS:CE1	2.50	0.47
1:A:757:LYS:HE2	1:A:761:LYS:NZ	2.30	0.47
1:B:58:GLY:O	1:B:62:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TRP:CE2	1:A:514:TRP:HB3	2.50	0.47
1:A:551:LEU:HD22	1:A:555:PHE:HE2	1.79	0.46
1:A:781:ASP:N	1:A:781:ASP:OD1	2.48	0.46
1:B:495:TRP:CE2	1:B:514:TRP:HB3	2.51	0.46
1:B:644:LEU:HB3	1:B:664:VAL:HG13	1.97	0.46
1:B:95:LEU:HD23	1:B:192:HIS:HB3	1.96	0.46
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.71	0.46
1:B:781:ASP:N	1:B:781:ASP:OD1	2.48	0.46
1:B:797:VAL:O	1:B:819:PRO:HD3	2.16	0.46
1:A:482:CYS:HB3	1:A:496:PHE:CD1	2.50	0.46
1:B:411:LEU:HA	1:B:411:LEU:HD23	1.61	0.46
1:A:529:VAL:HG13	1:A:707:ILE:HG13	1.98	0.46
1:B:269:GLN:HB3	1:B:344:ARG:HH22	1.81	0.46
1:B:746:VAL:HG11	1:B:760:LEU:HD13	1.98	0.46
1:B:532:THR:HB	1:B:710:PHE:CE1	2.51	0.46
1:B:410:TYR:OH	1:B:424:LEU:HB2	2.17	0.45
1:A:790:ILE:HD11	1:A:818:VAL:HG12	1.98	0.45
1:B:572:THR:HG23	1:B:578:TYR:HB2	1.98	0.45
1:A:565:THR:HG23	1:A:582:THR:HG23	1.99	0.45
1:B:451:PHE:HA	1:B:454:ILE:HG23	1.99	0.45
1:B:581:LEU:HB2	1:B:594:ILE:O	2.17	0.45
1:A:730:GLU:OE2	1:A:802:SER:OG	2.22	0.45
1:B:845:GLU:H	1:B:845:GLU:HG2	1.55	0.45
1:A:222:LEU:O	1:A:223:LYS:HD2	2.17	0.45
1:A:424:LEU:HD13	1:A:427:LEU:HD22	1.98	0.45
1:A:376:PRO:HD2	1:A:432:TYR:CZ	2.52	0.45
1:B:168:LYS:O	1:B:172:MET:HG3	2.17	0.45
1:B:316:GLU:HG2	1:B:317:LYS:N	2.31	0.45
1:B:541:ASN:HB3	1:B:621:LYS:HG3	1.99	0.45
1:B:658:GLN:OE1	1:B:660:LYS:HE3	2.17	0.45
1:B:376:PRO:HD2	1:B:432:TYR:CZ	2.52	0.45
2:A:901:FAD:H9	2:A:901:FAD:H1'2	1.59	0.45
1:A:300:LEU:HD21	1:A:307:LEU:HD22	1.99	0.44
1:A:748:LEU:HD21	1:A:760:LEU:HD13	2.00	0.44
1:B:758:GLN:O	1:B:762:GLN:HG3	2.17	0.44
1:B:836:LYS:HE3	1:B:837:ASN:N	2.33	0.44
1:B:119:LEU:HA	1:B:119:LEU:HD12	1.79	0.44
1:B:300:LEU:HD12	1:B:309:PHE:HB3	1.99	0.44
1:A:780:ASP:HB3	1:A:781:ASP:OD1	2.18	0.44
1:A:384:PRO:HD3	1:A:392:TRP:CZ3	2.53	0.44
1:A:539:LYS:HD2	1:A:624:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.59	0.44
1:B:193:ILE:HD13	1:B:198:LEU:HD22	2.00	0.44
1:B:537:PHE:O	1:B:539:LYS:NZ	2.43	0.44
1:B:687:ARG:HG3	1:B:689:GLU:CG	2.47	0.43
1:A:268:VAL:O	1:A:371:PRO:HA	2.19	0.43
1:A:377:ASP:O	1:A:378:ILE:HG22	2.19	0.43
1:A:611:ALA:HA	1:A:616:TYR:HD2	1.84	0.43
1:A:797:VAL:O	1:A:819:PRO:HD3	2.18	0.43
1:B:137:LEU:HD13	1:B:181:VAL:HG22	1.99	0.43
1:B:313:GLU:OE2	1:B:344:ARG:NE	2.29	0.43
1:A:60:VAL:HG23	1:A:247:ALA:HB1	2.01	0.43
1:B:738:LEU:HG	1:B:760:LEU:HD22	2.00	0.43
1:B:419:GLU:OE1	1:B:574:LYS:HB2	2.18	0.43
1:A:233:GLU:OE2	1:A:238:SER:HB3	2.18	0.43
1:A:58:GLY:O	1:A:62:VAL:HG23	2.19	0.43
1:A:267:PRO:HA	1:A:372:ILE:O	2.19	0.43
1:A:741:GLY:HA2	1:A:743:GLU:OE2	2.18	0.43
1:B:565:THR:O	1:B:657:LEU:HD13	2.19	0.43
1:B:672:ILE:HD12	1:B:685:TYR:HE2	1.83	0.43
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.52	0.43
1:B:725:ARG:HD3	1:B:772:LEU:HD23	2.01	0.43
1:A:113:ILE:O	1:A:117:GLU:HG3	2.19	0.42
1:A:82:SER:HA	1:A:216:PRO:HB3	2.00	0.42
1:A:60:VAL:HG22	2:A:901:FAD:O1P	2.19	0.42
1:B:512:THR:OG1	1:B:513:ASN:N	2.52	0.42
1:B:288:LEU:HA	1:B:289:PRO:HD3	1.91	0.42
1:B:413:ASP:O	1:B:417:HIS:ND1	2.39	0.42
1:B:727:TRP:HA	1:B:731:MET:HG2	2.01	0.42
1:A:376:PRO:HD2	1:A:432:TYR:CE2	2.55	0.42
1:A:60:VAL:HG13	2:A:901:FAD:O1P	2.19	0.42
1:B:485:GLY:HA3	1:B:494:HIS:NE2	2.34	0.42
1:B:457:TYR:CG	1:B:507:PRO:HB2	2.54	0.42
1:A:549:ARG:NH2	1:B:795:LYS:HE2	2.34	0.42
1:A:50:ALA:O	1:A:241:ALA:HA	2.19	0.42
1:A:642:GLN:HA	1:A:649:LEU:HD12	2.01	0.42
1:A:727:TRP:HA	1:A:731:MET:HG2	2.02	0.42
1:A:168:LYS:O	1:A:172:MET:HB2	2.20	0.42
1:A:512:THR:OG1	1:A:513:ASN:N	2.48	0.42
1:B:214:LYS:HD2	1:B:214:LYS:HA	1.81	0.42
1:B:246:ASN:HB3	1:B:393:VAL:HG12	2.01	0.42
1:B:567:ILE:HB	1:B:745:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:HG22	1:B:396:GLY:HA2	2.01	0.42
1:A:350:LYS:O	1:A:354:GLU:HG2	2.19	0.42
1:A:388:VAL:HG23	1:A:391:TYR:HB3	2.01	0.42
1:B:55:ILE:HG12	1:B:219:VAL:HG21	2.02	0.42
1:A:276:SER:N	1:A:363:ASP:O	2.50	0.42
1:A:611:ALA:HA	1:A:616:TYR:CD2	2.55	0.41
1:A:629:VAL:HG22	1:A:685:TYR:CD1	2.54	0.41
1:B:630:LEU:HA	1:B:630:LEU:HD23	1.94	0.41
1:B:851:GLU:HB3	1:B:852:PRO:HD3	2.01	0.41
1:A:123:THR:HG21	1:A:201:ALA:O	2.20	0.41
1:B:836:LYS:HA	1:B:836:LYS:HD2	1.64	0.41
1:A:739:GLU:HA	1:A:768:LEU:HD13	2.02	0.41
1:A:158:ALA:O	1:A:159:THR:C	2.58	0.41
1:B:466:ARG:NH2	1:B:491:GLU:OE1	2.50	0.41
1:B:103:ILE:HD11	1:B:153:ARG:CZ	2.50	0.41
1:B:727:TRP:CD1	1:B:731:MET:HG3	2.56	0.41
1:A:251:TRP:CD2	2:A:901:FAD:H8A	2.55	0.41
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.86	0.41
1:B:555:PHE:CZ	1:B:581:LEU:HD11	2.55	0.41
1:A:298:TYR:CZ	1:A:352:ALA:HA	2.56	0.41
1:A:669:VAL:CG2	1:A:686:HIS:HB3	2.51	0.41
1:A:818:VAL:HG23	1:A:819:PRO:O	2.21	0.41
1:B:722:LYS:HD2	1:B:850:THR:HG22	2.03	0.41
1:A:514:TRP:HE3	1:A:514:TRP:O	2.04	0.41
1:A:623:ILE:HG13	1:A:627:LEU:HD13	2.02	0.41
1:B:451:PHE:HD2	1:B:462:ARG:HD3	1.86	0.41
1:B:68:LEU:O	1:B:73:MET:HB3	2.21	0.41
1:A:140:THR:HG23	1:A:295:GLU:HG3	2.03	0.41
1:A:496:PHE:CE2	1:A:709:ASN:HB3	2.56	0.41
1:A:531:VAL:HG22	1:A:632:VAL:HG22	2.03	0.41
1:A:845:GLU:H	1:A:845:GLU:HG2	1.68	0.41
1:B:165:GLU:HB3	1:B:167:GLU:OE2	2.21	0.41
1:B:79:LEU:HB3	1:B:217:ALA:O	2.21	0.41
1:B:389:ARG:CZ	1:B:612:VAL:HG11	2.51	0.41
1:A:168:LYS:HE2	1:A:168:LYS:HB2	1.88	0.41
1:B:318:MET:SD	1:B:446:ARG:HG2	2.61	0.40
1:B:822:LEU:O	1:B:827:GLN:HG2	2.22	0.40
1:B:846:PRO:HG2	1:B:849:LEU:HD23	2.03	0.40
1:A:53:VAL:HG23	1:A:241:ALA:HB2	2.04	0.40
1:B:278:ILE:HG21	1:B:358:VAL:HB	2.04	0.40
1:B:423:ASP:HB2	1:B:733:CYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:HA	1:B:834:LEU:HD23	1.71	0.40
1:A:243:ARG:HA	1:A:390:ASN:HB3	2.04	0.40
1:A:824:GLU:HG2	1:A:827:GLN:HB2	2.03	0.40
1:A:88:SER:O	1:A:91:HIS:ND1	2.54	0.40
1:B:784:PRO:HA	1:B:833:LEU:HD21	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	807/841 (96%)	765 (95%)	39 (5%)	3 (0%)	39	75
1	B	806/841 (96%)	756 (94%)	48 (6%)	2 (0%)	52	84
All	All	1613/1682 (96%)	1521 (94%)	87 (5%)	5 (0%)	46	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ILE
1	B	378	ILE
1	A	537	PHE
1	B	102	GLY
1	A	102	GLY

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	682/709 (96%)	657 (96%)	25 (4%)	41 76
1	B	681/709 (96%)	657 (96%)	24 (4%)	43 78
All	All	1363/1418 (96%)	1314 (96%)	49 (4%)	42 77

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	A	142	VAL
1	A	167	GLU
1	A	179	ASN
1	A	316	GLU
1	A	322	ASP
1	A	412	SER
1	A	474	LEU
1	A	483	SER
1	A	548	ILE
1	A	565	THR
1	A	568	SER
1	A	587	SER
1	A	630	LEU
1	A	643	LYS
1	A	650	SER
1	A	654	PHE
1	A	669	VAL
1	A	691	SER
1	A	749	ASN
1	A	762	GLN
1	A	771	ARG
1	A	779	THR
1	A	789	SER
1	A	801	THR
1	B	108	ILE
1	B	129	PHE
1	B	163	LEU
1	B	254	GLU
1	B	316	GLU
1	B	320	VAL
1	B	322	ASP
1	B	448	SER
1	B	542	ILE

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Mol	Chain	Res	Type
1	B	568	SER
1	B	587	SER
1	B	643	LYS
1	B	654	PHE
1	B	691	SER
1	B	749	ASN
1	B	775	LEU
1	B	777	LEU
1	B	780	ASP
1	B	790	ILE
1	B	797	VAL
1	B	801	THR
1	B	815	PHE
1	B	824	GLU
1	B	836	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	494	HIS
1	B	487	HIS
1	B	793	ASN

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	901	1	52,58,58	1.46	9 (17%)	52,89,89	2.51	13 (25%)
2	FAD	B	901	1	52,58,58	1.40	7 (13%)	52,89,89	2.51	14 (26%)

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	901	1	-	1/30/50/50	0/6/6/6
2	FAD	B	901	1	-	0/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C2-N3	-2.10	1.33	1.38
2	A	901	FAD	O4B-C1B	2.17	1.44	1.41
2	B	901	FAD	O4B-C1B	2.21	1.44	1.41
2	A	901	FAD	C9A-N10	2.22	1.42	1.38
2	A	901	FAD	C5A-C4A	2.49	1.46	1.40
2	A	901	FAD	C8-C7	2.95	1.48	1.41
2	B	901	FAD	C9A-N10	2.96	1.43	1.38
2	B	901	FAD	C8-C7	2.99	1.49	1.41
2	B	901	FAD	C4-C4X	3.15	1.47	1.41
2	A	901	FAD	C9A-C5X	3.19	1.49	1.42
2	A	901	FAD	C4-C4X	3.67	1.48	1.41
2	B	901	FAD	C5A-C4A	3.67	1.48	1.40
2	B	901	FAD	C4X-C10	3.77	1.47	1.40
2	B	901	FAD	C9A-C5X	3.86	1.50	1.42
2	A	901	FAD	C10-N10	4.43	1.44	1.39
2	A	901	FAD	C4X-C10	4.72	1.49	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	FAD	C1'-N10-C9A	-7.93	109.63	118.83
2	A	901	FAD	N3A-C2A-N1A	-7.38	123.07	128.87
2	B	901	FAD	N3A-C2A-N1A	-6.21	123.99	128.87
2	B	901	FAD	C4X-C4-N3	-4.60	117.51	123.52
2	B	901	FAD	C4B-O4B-C1B	-4.19	105.20	109.64
2	A	901	FAD	O4'-C4'-C5'	-3.64	102.16	110.09
2	A	901	FAD	C4X-C4-N3	-3.60	118.81	123.52
2	B	901	FAD	C4-C4X-C10	-3.19	117.90	119.94
2	B	901	FAD	N3-C2-N1	-3.06	122.54	127.69
2	A	901	FAD	C4-C4X-C10	-2.80	118.15	119.94
2	A	901	FAD	C4X-C10-N10	-2.68	118.57	120.52
2	A	901	FAD	N3-C2-N1	-2.59	123.33	127.69
2	A	901	FAD	N6A-C6A-N1A	2.03	121.92	118.52
2	B	901	FAD	C5X-C9A-N10	2.09	119.14	117.58
2	B	901	FAD	C6-C5X-C9A	2.38	121.73	119.11
2	B	901	FAD	C4X-N5-C5X	2.56	119.73	116.72
2	A	901	FAD	O2'-C2'-C1'	2.57	116.28	109.93
2	A	901	FAD	O4B-C1B-N9A	2.73	113.26	108.11
2	A	901	FAD	C4X-N5-C5X	3.26	120.57	116.72
2	B	901	FAD	C1B-N9A-C4A	3.33	130.53	126.81
2	B	901	FAD	C1'-C2'-C3'	3.38	119.48	109.82
2	B	901	FAD	N6A-C6A-N1A	3.48	124.35	118.52
2	B	901	FAD	O4B-C1B-N9A	5.36	118.23	108.11
2	A	901	FAD	C5X-C9A-N10	6.51	122.45	117.58
2	B	901	FAD	C1'-N10-C9A	6.68	126.58	118.83
2	A	901	FAD	C4-N3-C2	7.54	121.45	115.16
2	B	901	FAD	C4-N3-C2	8.66	122.38	115.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	FAD	C2'-C1'-N10-C9A

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	6	0
2	B	901	FAD	3	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	809/841 (96%)	-0.34	1 (0%) 95 91	7, 36, 61, 98	0
1	B	808/841 (96%)	-0.36	0 100 100	10, 36, 62, 105	0
All	All	1617/1682 (96%)	-0.35	1 (0%) 95 91	7, 36, 62, 105	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	2.2

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	B	901	53/53	0.95	0.17	-0.36	34,34,34,34	0
2	FAD	A	901	53/53	0.95	0.17	-0.42	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.