



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:36 am GMT

PDB ID : 3IC9  
Title : The structure of dihydrolipoamide dehydrogenase from *Colwellia psychrerythraea* 34H.  
Authors : Tan, K.; Rakowski, E.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-07-17  
Resolution : 2.15 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

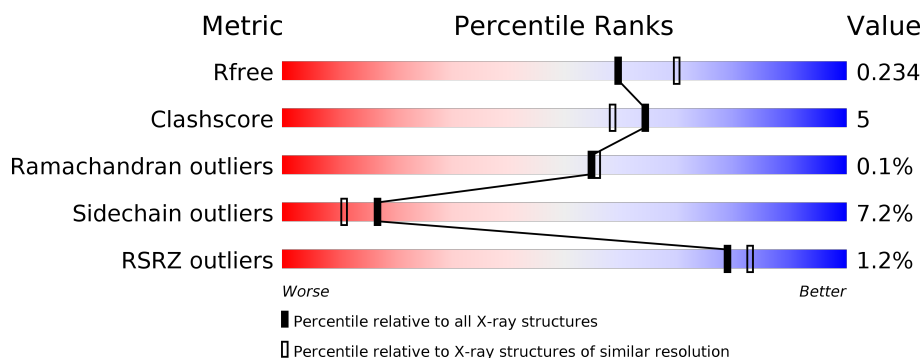
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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  $\geq 3$ , 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	492	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	492	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	492	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	492	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16087 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 dihydrolipoamide dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	Se	0	3	0
			3719	2341	648	716	2	12			
1	B	481	Total	C	N	O	S	Se	0	8	0
			3745	2362	649	720	2	12			
1	C	483	Total	C	N	O	S	Se	0	1	0
			3718	2339	648	717	2	12			
1	D	481	Total	C	N	O	S	Se	0	1	0
			3708	2334	648	712	2	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q488E0
A	-1	ASN	-	expression tag	UNP Q488E0
A	0	ALA	-	expression tag	UNP Q488E0
B	-2	SER	-	expression tag	UNP Q488E0
B	-1	ASN	-	expression tag	UNP Q488E0
B	0	ALA	-	expression tag	UNP Q488E0
C	-2	SER	-	expression tag	UNP Q488E0
C	-1	ASN	-	expression tag	UNP Q488E0
C	0	ALA	-	expression tag	UNP Q488E0
D	-2	SER	-	expression tag	UNP Q488E0
D	-1	ASN	-	expression tag	UNP Q488E0
D	0	ALA	-	expression tag	UNP Q488E0

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		

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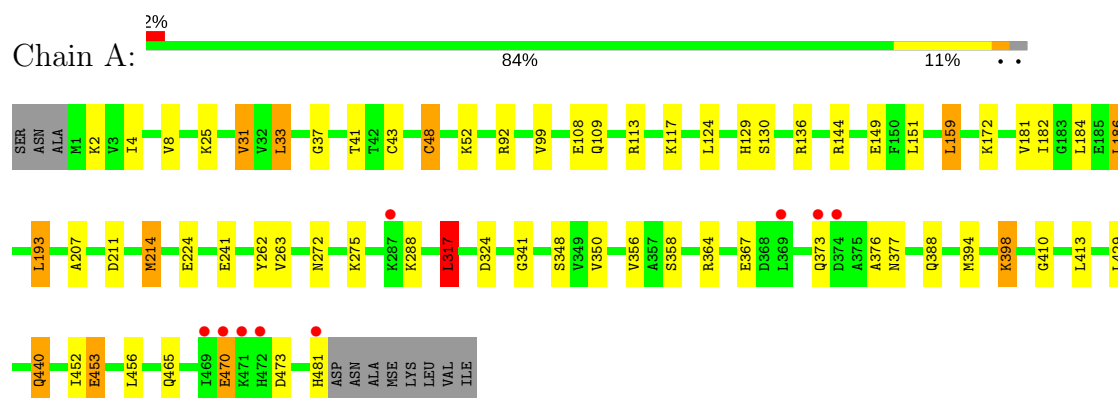
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	240	Total 240	O 240	0	0
4	C	273	Total 273	O 273	0	0
4	D	235	Total 235	O 235	0	0

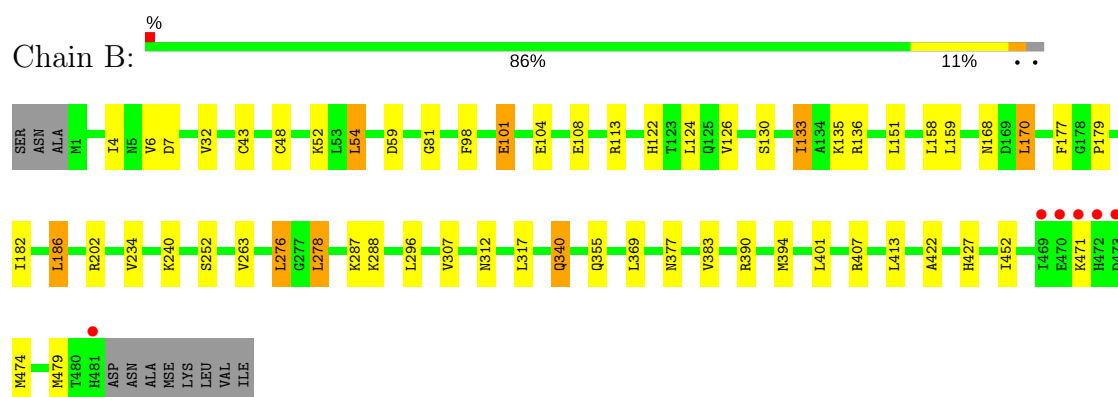
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

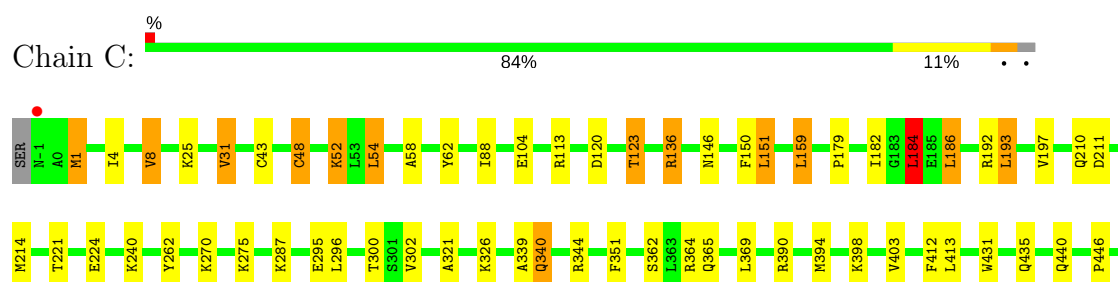
- Molecule 1: dihydrolipoamide dehydrogenase

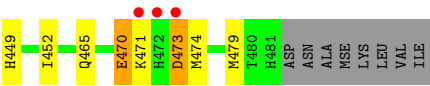


- Molecule 1: dihydrolipoamide dehydrogenase

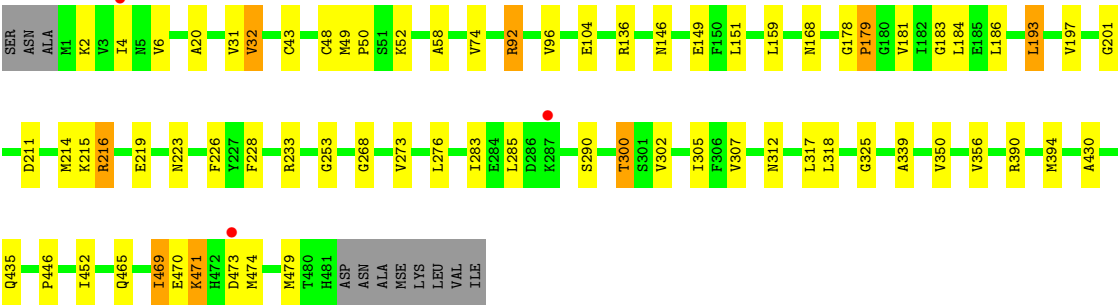
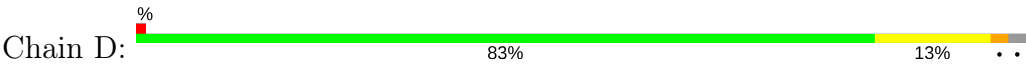


- Molecule 1: dihydrolipoamide dehydrogenase





● Molecule 1: dihydrolipoamide dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.50Å 246.35Å 73.66Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	43.90 – 2.15 43.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.90-2.15) 98.1 (43.90-2.15)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.186 , 0.233 0.188 , 0.234	Depositor DCC
$R_{free}$ test set	6975 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 16.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for l,k,-h 0.266 for h,-k,-l 0.049 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NA, 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	0.60	0/3777	0.71	4/5083 (0.1%)
1	B	0.61	0/3818	0.70	1/5137 (0.0%)
1	C	0.64	0/3769	0.71	2/5072 (0.0%)
1	D	0.62	0/3760	0.70	0/5060
All	All	0.62	0/15124	0.71	7/20352 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	LEU	CA-CB-CG	5.79	128.60	115.30
1	A	324	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	344	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	33	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	193	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	184	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	54	LEU	CB-CG-CD2	5.00	119.51	111.00

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	3719	0	3709	31	0
1	B	3745	0	3753	32	0
1	C	3718	0	3701	45	0
1	D	3708	0	3699	41	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	233	0	0	2	0
4	B	240	0	0	1	0
4	C	273	0	0	4	0
4	D	235	0	0	1	0
All	All	16087	0	14986	139	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 5.

All (139) 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:D:390:ARG:HG3	1:D:394:MSE:HE2	1.44	0.98
1:A:394:MSE:HE1	1:A:452:ILE:HD11	1.47	0.96
1:B:394:MSE:HE1	1:B:452:ILE:HD11	1.56	0.85
1:B:126:VAL:CG1	1:B:130:SER:HB2	2.12	0.80
1:C:52:LYS:N	1:C:52:LYS:HD3	1.96	0.79
1:A:182:ILE:HG23	1:A:186:LEU:HD22	1.64	0.78
1:C:43:CYS:HG	1:C:48:CYS:HG	0.77	0.77
1:A:181:VAL:HG22	1:A:207:ALA:HA	1.66	0.77
1:A:440:GLN:H	1:A:440:GLN:HE21	1.29	0.77
1:C:300:THR:HG23	1:C:302:VAL:H	1.49	0.77
1:C:394:MSE:HE1	1:C:452:ILE:HD11	1.68	0.75
1:C:403:VAL:HG13	1:C:412:PHE:HE1	1.57	0.69
1:C:403:VAL:HG13	1:C:412:PHE:CE1	2.28	0.68
1:A:440:GLN:H	1:A:440:GLN:NE2	1.91	0.68
1:A:159:LEU:HD22	1:A:262:TYR:HB3	1.77	0.67
1:D:470:GLU:HB2	1:D:473:ASP:HB2	1.75	0.67
1:C:479:MSE:HE2	1:D:339:ALA:HB3	1.77	0.66
1:B:390:ARG:HG3	1:B:394:MSE:HE2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:LYS:NZ	1:D:474:MSE:HE3	2.10	0.65
1:B:43:CYS:HG	1:B:48:CYS:HG	1.45	0.65
1:C:52:LYS:HE3	1:C:351:PHE:CD2	2.31	0.65
1:C:390:ARG:HG3	1:C:394:MSE:HE2	1.78	0.65
1:D:179:PRO:HG3	1:D:201:GLY:HA3	1.78	0.65
1:C:435:GLN:OE1	1:D:435:GLN:NE2	2.31	0.63
1:D:471:LYS:HZ3	1:D:474:MSE:HE3	1.64	0.63
1:C:362:SER:H	1:C:365:GLN:NE2	1.95	0.63
1:A:144:ARG:HH21	1:A:272:ASN:HD22	1.47	0.63
1:D:43:CYS:HB2	1:D:318:LEU:HD13	1.81	0.62
1:B:158:LEU:HD12	1:B:263:VAL:HG23	1.82	0.62
1:C:120:ASP:OD1	1:C:123:THR:HG23	2.00	0.62
1:C:179:PRO:HG3	4:C:548:HOH:O	2.00	0.61
1:B:6:VAL:HG11	1:B:32:VAL:HG13	1.80	0.61
1:A:470:GLU:HB3	1:A:473:ASP:HB2	1.82	0.61
1:B:276[A]:LEU:HD21	1:B:278:LEU:HD13	1.83	0.60
1:D:394:MSE:HE1	1:D:452:ILE:HD11	1.83	0.60
1:A:350:VAL:HB	1:A:356:VAL:HB	1.84	0.59
1:A:43:CYS:HG	1:A:48:CYS:HG	1.43	0.59
1:A:109:GLN:HG2	4:A:617:HOH:O	2.02	0.58
1:C:179:PRO:O	1:C:184:LEU:HD22	2.03	0.58
1:C:449:HIS:CD2	1:D:318:LEU:HD22	2.38	0.58
1:B:126:VAL:HG12	1:B:130:SER:HB2	1.86	0.57
1:D:300:THR:HB	1:D:305:ILE:O	2.04	0.57
1:C:1:MSE:HB3	4:C:741:HOH:O	2.05	0.57
1:B:355:GLN:HB2	1:B:422:ALA:HB3	1.87	0.56
1:C:224:GLU:OE1	1:C:398:LYS:HE3	2.06	0.56
1:D:216:ARG:NH1	1:D:219:GLU:OE1	2.39	0.55
1:D:43:CYS:CB	1:D:318:LEU:HD13	2.36	0.55
1:B:7:ASP:OD1	1:B:135:LYS:HE2	2.06	0.55
1:D:273:VAL:HA	1:D:276:LEU:HD22	1.90	0.54
1:C:470:GLU:CD	1:C:470:GLU:N	2.62	0.54
1:C:182:ILE:HG23	1:C:186:LEU:HD22	1.90	0.53
1:D:58:ALA:HA	1:D:193:LEU:HD13	1.89	0.53
1:C:339:ALA:HB3	1:D:479:MSE:HE2	1.89	0.53
1:C:470:GLU:H	1:C:470:GLU:CD	2.12	0.53
1:B:471:LYS:O	1:B:474:MSE:HB2	2.09	0.53
1:A:341:GLY:HA2	1:B:479:MSE:HG2	1.90	0.52
1:A:144:ARG:HH21	1:A:272:ASN:ND2	2.07	0.52
1:A:159:LEU:HD22	1:A:262:TYR:CB	2.39	0.52
1:B:394:MSE:HE1	1:B:452:ILE:CD1	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:VAL:HG11	1:D:32:VAL:HG22	1.93	0.51
1:C:221:THR:HG23	1:C:398:LYS:HE2	1.93	0.51
1:B:296:LEU:HB3	1:B:340:GLN:CB	2.42	0.50
1:B:307:VAL:HG22	1:B:312:ASN:HB3	1.95	0.49
1:B:383:VAL:HG12	1:B:401:LEU:HB3	1.95	0.48
1:D:233[B]:ARG:HH12	1:D:253:GLY:HA2	1.78	0.48
1:D:471:LYS:HZ3	1:D:474:MSE:CE	2.25	0.48
1:A:182:ILE:HD12	4:A:556:HOH:O	2.13	0.48
1:D:181:VAL:HG22	1:D:350:VAL:HG22	1.95	0.48
1:C:435:GLN:CD	1:D:435:GLN:HE21	2.17	0.48
1:D:43:CYS:CB	1:D:48:CYS:HG	2.26	0.48
1:C:54:LEU:HD23	1:C:88:ILE:HD11	1.94	0.48
1:B:6:VAL:HG11	1:B:32:VAL:CG1	2.45	0.47
1:D:300:THR:CG2	1:D:302:VAL:H	2.27	0.47
1:C:210:GLN:OE1	1:C:364:ARG:HG2	2.13	0.47
1:A:367:GLU:HG2	1:A:373:GLN:NE2	2.29	0.47
1:B:276[A]:LEU:CD2	1:B:278:LEU:HD13	2.43	0.47
1:A:224:GLU:OE1	1:A:398:LYS:HE3	2.15	0.46
1:B:240[B]:LYS:HA	1:B:240[B]:LYS:HD3	1.59	0.46
1:B:287:LYS:HE2	1:B:287:LYS:HB3	1.79	0.46
1:D:223:ASN:HA	1:D:226:PHE:O	2.15	0.46
1:C:300:THR:HG23	1:C:302:VAL:N	2.24	0.46
1:B:81:GLY:HA2	1:B:170:LEU:HD22	1.97	0.46
1:D:300:THR:HG23	1:D:302:VAL:H	1.79	0.46
1:B:276[A]:LEU:HD21	1:B:278:LEU:HD22	1.96	0.45
1:B:296:LEU:HB3	1:B:340:GLN:HB3	1.97	0.45
1:C:8:VAL:HA	1:C:136:ARG:O	2.17	0.45
1:D:469:ILE:HB	1:D:474:MSE:CE	2.47	0.45
1:C:58:ALA:HA	1:C:193:LEU:HD13	1.98	0.45
1:B:177:PHE:HE1	1:B:234:VAL:HG21	1.82	0.45
1:D:211:ASP:HB3	1:D:214:MSE:HG3	1.98	0.45
1:C:321:ALA:HB2	4:C:662:HOH:O	2.18	0.44
1:A:129:HIS:HD2	1:A:130:SER:OG	2.00	0.44
1:B:182:ILE:HG23	1:B:186:LEU:HD22	2.00	0.44
1:C:446:PRO:HG2	1:D:430:ALA:HB1	2.00	0.44
1:A:37:GLY:O	1:A:113[B]:ARG:NH2	2.50	0.44
1:B:98:PHE:O	1:B:101:GLU:HG3	2.17	0.44
1:A:172:LYS:HD3	1:A:172:LYS:HA	1.83	0.44
1:A:182:ILE:CG2	1:A:186:LEU:HD22	2.42	0.44
1:A:317:LEU:HD21	1:A:348:SER:HB3	1.99	0.43
1:A:410:GLY:HA3	1:A:440:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:THR:HG22	1:D:302:VAL:O	2.18	0.43
1:C:326:LYS:HE2	4:D:553:HOH:O	2.18	0.43
1:C:159:LEU:HD22	1:C:262:TYR:HB3	2.00	0.43
1:A:41:THR:HG23	1:A:99:VAL:HG11	2.01	0.43
1:B:126:VAL:HG13	1:B:130:SER:HB2	1.98	0.43
1:A:8:VAL:HB	1:A:31:VAL:HB	1.99	0.43
1:D:211:ASP:O	1:D:215:LYS:HG3	2.19	0.43
1:D:146:ASN:HB3	1:D:268:GLY:O	2.19	0.43
1:A:429:LEU:HD21	1:A:456:LEU:CD1	2.48	0.43
1:D:307:VAL:HG22	1:D:312:ASN:HB3	2.00	0.43
1:A:429:LEU:HD21	1:A:456:LEU:HD11	2.01	0.42
1:A:113[B]:ARG:HD2	1:A:113[B]:ARG:HA	1.70	0.42
1:C:150:PHE:CE1	1:C:151:LEU:HD13	2.54	0.42
1:C:440:GLN:HB3	1:C:474:MSE:SE	2.69	0.42
1:C:146:ASN:HB2	1:C:270:LYS:HB2	2.02	0.42
1:D:350:VAL:HB	1:D:356:VAL:HB	2.00	0.42
1:D:178:GLY:O	1:D:183:GLY:HA3	2.19	0.42
1:D:283:ILE:HG12	1:D:300:THR:HG21	2.02	0.42
1:D:20:ALA:HA	1:D:325:GLY:O	2.20	0.42
1:D:179:PRO:HB3	1:D:228:PHE:HE1	1.85	0.41
1:C:211:ASP:HB3	1:C:214:MSE:HB2	2.02	0.41
1:C:296:LEU:HB3	1:C:340:GLN:HG2	2.02	0.41
1:B:122:HIS:O	1:B:133:ILE:HA	2.20	0.41
1:B:377:ASN:ND2	1:B:407:ARG:HB3	2.36	0.41
1:D:49:MSE:HB2	1:D:50:PRO:CD	2.50	0.41
1:B:135:LYS:HD3	4:B:910:HOH:O	2.19	0.41
1:B:278:LEU:HA	1:B:278:LEU:HD12	1.93	0.41
1:C:1:MSE:HE3	1:C:1:MSE:HB2	1.88	0.41
1:C:431:TRP:CD1	1:D:446:PRO:HD2	2.56	0.41
1:A:25:LYS:HD3	1:A:31:VAL:HG13	2.02	0.41
1:C:8:VAL:O	1:C:31:VAL:HA	2.21	0.41
1:A:453:GLU:HG3	1:B:427:HIS:CD2	2.56	0.41
1:A:211:ASP:HB3	1:A:214:MSE:HG3	2.02	0.40
1:C:62:TYR:HB2	1:C:192:ARG:HB3	2.02	0.40
1:C:25:LYS:CD	1:C:31:VAL:HG13	2.51	0.40
1:C:295:GLU:HG2	4:C:944:HOH:O	2.22	0.40
1:C:473:ASP:OD1	1:C:473:ASP:N	2.55	0.40
1:C:435:GLN:CD	1:D:435:GLN:NE2	2.75	0.40
1:D:92:ARG:O	1:D:96:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/492 (98%)	466 (97%)	15 (3%)	1 (0%)	51	50
1	B	487/492 (99%)	472 (97%)	15 (3%)	0	100	100
1	C	482/492 (98%)	464 (96%)	18 (4%)	0	100	100
1	D	480/492 (98%)	466 (97%)	13 (3%)	1 (0%)	51	50
All	All	1931/1968 (98%)	1868 (97%)	61 (3%)	2 (0%)	55	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ALA
1	D	179	PRO

### 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	392/385 (102%)	358 (91%)	34 (9%)	12	6
1	B	397/385 (103%)	368 (93%)	29 (7%)	16	10
1	C	391/385 (102%)	364 (93%)	27 (7%)	18	12
1	D	390/385 (101%)	365 (94%)	25 (6%)	20	14
All	All	1570/1540 (102%)	1455 (93%)	115 (7%)	17	10

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	ILE
1	A	31	VAL
1	A	33	LEU
1	A	48	CYS
1	A	52	LYS
1	A	92	ARG
1	A	108	GLU
1	A	117	LYS
1	A	124	LEU
1	A	136	ARG
1	A	149	GLU
1	A	151	LEU
1	A	159	LEU
1	A	184	LEU
1	A	186	LEU
1	A	193	LEU
1	A	214	MSE
1	A	241	GLU
1	A	263	VAL
1	A	275	LYS
1	A	288	LYS
1	A	317	LEU
1	A	358	SER
1	A	364	ARG
1	A	377	ASN
1	A	388	GLN
1	A	398	LYS
1	A	413	LEU
1	A	440	GLN
1	A	453	GLU
1	A	465	GLN
1	A	470	GLU
1	A	481	HIS
1	B	4	ILE
1	B	52	LYS
1	B	54	LEU
1	B	59[A]	ASP
1	B	59[B]	ASP
1	B	101	GLU
1	B	104	GLU
1	B	108[A]	GLU
1	B	108[B]	GLU

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Mol	Chain	Res	Type
1	B	113	ARG
1	B	124	LEU
1	B	133	ILE
1	B	136	ARG
1	B	151	LEU
1	B	159	LEU
1	B	168	ASN
1	B	170	LEU
1	B	179	PRO
1	B	186	LEU
1	B	202	ARG
1	B	252	SER
1	B	276[A]	LEU
1	B	276[B]	LEU
1	B	278	LEU
1	B	288	LYS
1	B	317	LEU
1	B	340	GLN
1	B	369	LEU
1	B	413	LEU
1	C	1	MSE
1	C	4	ILE
1	C	8	VAL
1	C	31	VAL
1	C	48	CYS
1	C	52	LYS
1	C	54	LEU
1	C	104	GLU
1	C	113	ARG
1	C	123	THR
1	C	136	ARG
1	C	151	LEU
1	C	159	LEU
1	C	184	LEU
1	C	186	LEU
1	C	193	LEU
1	C	197	VAL
1	C	240	LYS
1	C	275	LYS
1	C	287	LYS
1	C	340	GLN
1	C	369	LEU

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Mol	Chain	Res	Type
1	C	413	LEU
1	C	465	GLN
1	C	470	GLU
1	C	471	LYS
1	C	473	ASP
1	D	2	LYS
1	D	4	ILE
1	D	31	VAL
1	D	32	VAL
1	D	52	LYS
1	D	74	VAL
1	D	92	ARG
1	D	104	GLU
1	D	136	ARG
1	D	149	GLU
1	D	151	LEU
1	D	159	LEU
1	D	168	ASN
1	D	184	LEU
1	D	186	LEU
1	D	193	LEU
1	D	197	VAL
1	D	216	ARG
1	D	285	LEU
1	D	290	SER
1	D	300	THR
1	D	317	LEU
1	D	465	GLN
1	D	469	ILE
1	D	471	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	272	ASN
1	A	289	ASN
1	A	377	ASN
1	A	388	GLN
1	A	440	GLN
1	A	464	GLN
1	B	373	GLN

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	435	GLN
1	C	27	HIS
1	C	254	GLN
1	C	365	GLN
1	C	377	ASN
1	C	465	GLN
1	D	27	HIS
1	D	435	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	490	-	51,58,58	1.38	7 (13%)	54,89,89	2.06	6 (11%)
2	FAD	B	490	-	51,58,58	1.36	8 (15%)	54,89,89	2.12	7 (12%)
2	FAD	C	490	-	51,58,58	1.47	7 (13%)	54,89,89	2.15	7 (12%)
2	FAD	D	490	-	51,58,58	1.43	8 (15%)	54,89,89	1.96	7 (12%)

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	490	-	-	0/28/50/50	0/6/6/6
2	FAD	B	490	-	-	0/28/50/50	0/6/6/6
2	FAD	C	490	-	-	0/28/50/50	0/6/6/6
2	FAD	D	490	-	-	0/28/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	490	FAD	O4B-C4B	-2.02	1.40	1.45
2	C	490	FAD	C2A-N1A	2.05	1.37	1.33
2	D	490	FAD	O4B-C1B	2.06	1.44	1.41
2	A	490	FAD	C5X-N5	2.08	1.38	1.35
2	C	490	FAD	C5X-N5	2.14	1.38	1.35
2	D	490	FAD	C5X-N5	2.24	1.38	1.35
2	B	490	FAD	C5X-N5	2.27	1.38	1.35
2	B	490	FAD	C2A-N1A	2.35	1.38	1.33
2	D	490	FAD	C2A-N1A	2.44	1.38	1.33
2	B	490	FAD	C4-N3	2.70	1.37	1.33
2	A	490	FAD	C4-N3	2.71	1.38	1.33
2	A	490	FAD	C2A-N1A	2.79	1.39	1.33
2	C	490	FAD	C2A-N3A	3.06	1.37	1.32
2	C	490	FAD	C4-N3	3.09	1.38	1.33
2	A	490	FAD	C2A-N3A	3.18	1.37	1.32
2	A	490	FAD	C4X-N5	3.25	1.38	1.33
2	B	490	FAD	C4X-N5	3.26	1.38	1.33
2	D	490	FAD	C1'-N10	3.38	1.51	1.48
2	D	490	FAD	C2A-N3A	3.41	1.37	1.32
2	B	490	FAD	C2A-N3A	3.50	1.38	1.32
2	D	490	FAD	C4X-N5	3.57	1.38	1.33
2	D	490	FAD	C4-N3	3.59	1.39	1.33
2	A	490	FAD	C1'-N10	3.61	1.52	1.48
2	C	490	FAD	C4X-N5	3.72	1.38	1.33
2	B	490	FAD	C1'-N10	3.83	1.52	1.48
2	D	490	FAD	C10-N1	3.89	1.38	1.33
2	B	490	FAD	C10-N1	4.29	1.39	1.33
2	A	490	FAD	C10-N1	4.33	1.39	1.33
2	C	490	FAD	C10-N1	4.42	1.39	1.33
2	C	490	FAD	C1'-N10	4.73	1.53	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	490	FAD	N3A-C2A-N1A	-11.62	118.74	128.86
2	B	490	FAD	N3A-C2A-N1A	-11.19	119.12	128.86
2	A	490	FAD	N3A-C2A-N1A	-10.65	119.58	128.86
2	D	490	FAD	N3A-C2A-N1A	-10.52	119.70	128.86
2	C	490	FAD	C1B-N9A-C4A	-2.91	121.60	126.64
2	B	490	FAD	C4X-C4-N3	-2.88	119.39	123.48
2	D	490	FAD	C4X-C4-N3	-2.27	120.26	123.48
2	A	490	FAD	C4X-C4-N3	-2.22	120.32	123.48
2	D	490	FAD	O3B-C3B-C4B	-2.22	104.61	111.09
2	B	490	FAD	C5X-C9A-N10	2.28	119.35	117.66
2	A	490	FAD	C4-C4X-N5	2.39	121.30	118.68
2	B	490	FAD	C4-C4X-N5	2.42	121.34	118.68
2	B	490	FAD	C1'-N10-C9A	2.89	121.00	118.35
2	C	490	FAD	C1'-N10-C10	2.93	121.51	118.50
2	C	490	FAD	C4-C4X-N5	3.09	122.07	118.68
2	D	490	FAD	C5X-C9A-N10	3.13	119.98	117.66
2	D	490	FAD	C4X-N5-C5X	3.18	120.12	116.76
2	C	490	FAD	C5X-C9A-N10	3.36	120.16	117.66
2	B	490	FAD	C4X-N5-C5X	3.56	120.52	116.76
2	D	490	FAD	C1'-N10-C9A	3.58	121.63	118.35
2	A	490	FAD	C1'-N10-C9A	3.69	121.73	118.35
2	C	490	FAD	C4X-N5-C5X	3.85	120.82	116.76
2	A	490	FAD	C4X-N5-C5X	4.30	121.30	116.76
2	D	490	FAD	C4-N3-C2	5.16	119.67	115.16
2	C	490	FAD	C4-N3-C2	5.24	119.75	115.16
2	A	490	FAD	C4-N3-C2	6.02	120.42	115.16
2	B	490	FAD	C4-N3-C2	6.77	121.08	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	469/492 (95%)	-0.30	9 (1%) 67 74	18, 26, 36, 55	0
1	B	469/492 (95%)	-0.39	6 (1%) 77 82	19, 27, 35, 60	0
1	C	471/492 (95%)	-0.36	4 (0%) 86 89	20, 26, 36, 58	0
1	D	469/492 (95%)	-0.34	3 (0%) 89 91	19, 26, 37, 53	0
All	All	1878/1968 (95%)	-0.35	22 (1%) 79 83	18, 26, 37, 60	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	HIS	4.7
1	A	481	HIS	4.3
1	C	-1	ASN	4.1
1	B	472	HIS	3.9
1	C	472	HIS	3.9
1	A	471	LYS	3.9
1	B	473	ASP	3.4
1	C	471	LYS	3.3
1	A	374	ASP	3.2
1	B	470	GLU	3.0
1	C	473	ASP	3.0
1	A	469	ILE	2.9
1	B	471	LYS	2.9
1	A	373	GLN	2.8
1	B	481	HIS	2.5
1	B	469	ILE	2.4
1	A	287	LYS	2.3
1	A	470	GLU	2.2
1	D	473	ASP	2.1
1	D	4	ILE	2.0
1	A	369	LEU	2.0
1	D	287	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FAD	B	490	53/53	0.98	0.09	-0.16	28,31,36,37	0
2	FAD	A	490	53/53	0.97	0.09	-0.19	28,31,33,34	0
2	FAD	C	490	53/53	0.98	0.09	-0.21	26,29,34,34	0
2	FAD	D	490	53/53	0.98	0.09	-0.47	26,30,33,33	0
3	NA	A	491	1/1	0.96	0.07	-0.67	36,36,36,36	0
3	NA	C	491	1/1	0.95	0.09	-0.69	33,33,33,33	0
3	NA	D	491	1/1	0.99	0.07	-1.38	29,29,29,29	0
3	NA	B	491	1/1	0.98	0.05	-4.97	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.