



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:53 pm GMT

PDB ID : 1MFP  
Title : E. coli Enoyl Reductase in complex with NAD and SB611113  
Authors : Seefeld, M.A.; Miller, W.H.; Newlander, K.A.; Burgess, W.J.; DeWolf Jr., W.E.; Elkins, P.A.; Head, M.S.; Jakas, D.R.; Janson, C.A.; Keller, P.M.; Manley, P.J.; Moore, T.D.; Payne, D.J.; Pearson, S.; Polizzi, B.J.; Qiu, X.; Rittenhouse, S.F.; Uzinskas, I.N.; Wallis, N.G.; Huffman, W.F.  
Deposited on : 2002-08-13  
Resolution : 2.33 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

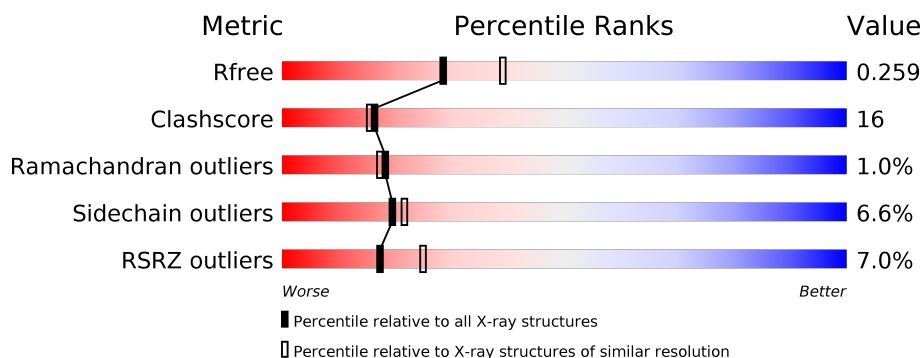
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	262	<div> <div>9%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	B	262	<div> <div>5%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

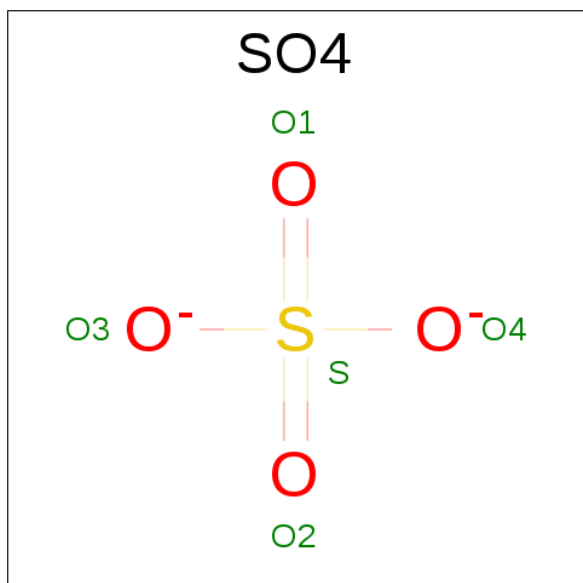
There are 5 unique types of molecules in this entry. The entry contains 4180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 enoyl-[acyl-carrier-protein] reductase [Nadh].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	B	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



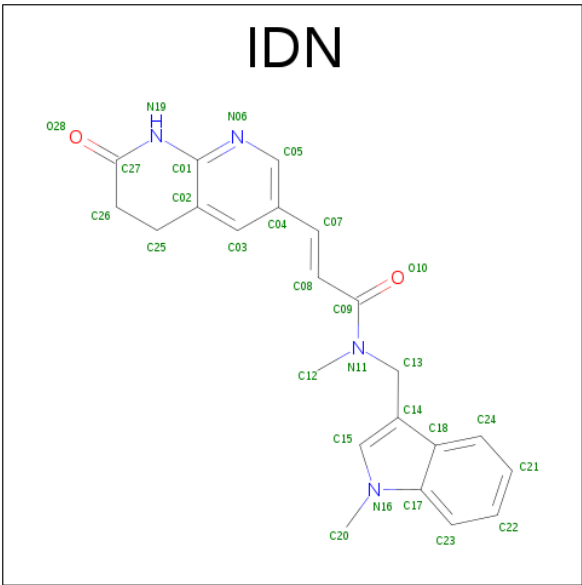
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 4 is (E)-N-METHYL-N-(1-METHYL-1H-INDOL-3-YLMETHYL)-3-(7-OXO-5,6,7,8-TETRAHYDRO-[1,8]NAPHTHYRIDIN-3-YL)-ACRYLAMIDE (three-letter code: IDN) (formula: C<sub>22</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			28	22	4	2		

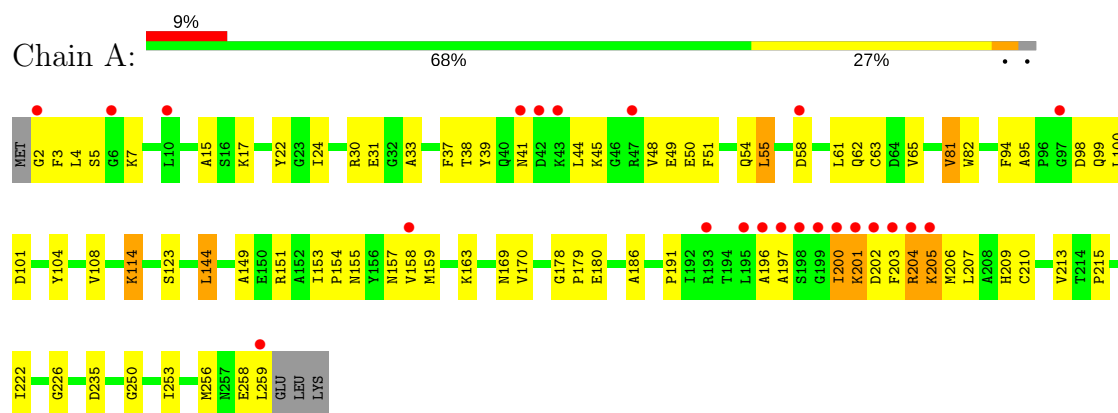
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	109	Total	O	0	0
			109	109		

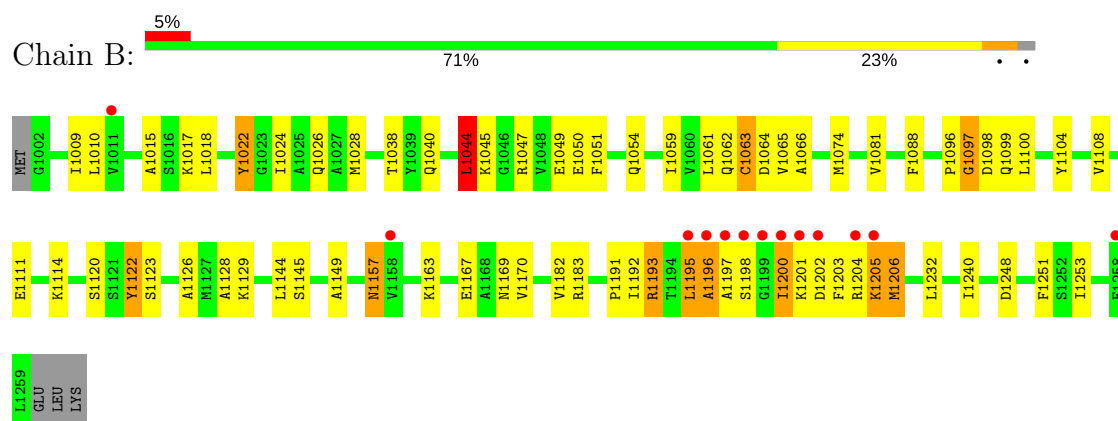
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: enoyl-[acyl-carrier-protein] reductase [Nadh]



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.60Å 79.60Å 325.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.33 19.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.33) 69.1 (19.90-2.33)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.86 (at 2.33Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.259 0.198 , 0.259	Depositor DCC
$R_{free}$ test set	923 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: IDN, SO4, 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	0.88	0/1950	0.93	2/2634 (0.1%)
1	B	0.93	1/1950 (0.1%)	0.93	2/2634 (0.1%)
All	All	0.91	1/3900 (0.0%)	0.93	4/5268 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1063	CYS	CB-SG	5.17	1.91	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	LEU	CA-CB-CG	-6.28	100.86	115.30
1	A	55	LEU	CA-CB-CG	-5.17	103.41	115.30
1	B	1195	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	1044	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	1022	TYR	Sidechain
1	B	1122	TYR	Sidechain

## 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	1918	0	1909	68	0
1	B	1918	0	1909	60	0
2	B	5	0	0	0	0
3	A	44	0	26	2	0
3	B	44	0	26	3	0
4	A	28	0	22	6	0
4	B	28	0	22	5	0
5	A	86	0	0	4	0
5	B	109	0	0	3	0
All	All	4180	0	3914	126	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 16.

All (126) 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:1074:MET:SD	1:B:1074:MET:CE	2.04	1.45
1:B:1099:GLN:HE22	1:B:1108:VAL:HA	1.42	0.84
1:B:1191:PRO:HG3	1:B:1206:MET:HE2	1.60	0.83
1:A:202:ASP:OD2	1:A:204:ARG:HG2	1.82	0.80
1:B:1038:THR:HA	1:B:1061:LEU:O	1.83	0.79
1:A:99:GLN:HE22	1:A:108:VAL:HA	1.54	0.73
1:A:256:MET:HB3	1:A:259:LEU:HD13	1.71	0.71
1:B:1191:PRO:HG3	1:B:1206:MET:CE	2.20	0.70
1:A:197:ALA:HB1	1:A:203:PHE:CE2	2.27	0.70
1:A:17:LYS:HA	1:A:22:TYR:CD1	2.27	0.69
1:A:259:LEU:HD12	1:A:259:LEU:H	1.56	0.69
1:B:1192:ILE:HA	5:B:138:HOH:O	1.95	0.66
1:B:1024:ILE:O	1:B:1028:MET:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ALA:O	4:A:302:IDN:H251	1.96	0.64
1:A:155:ASN:HD22	1:A:201:LYS:HD3	1.63	0.64
1:B:1099:GLN:NE2	1:B:1108:VAL:HA	2.13	0.62
1:B:1050:GLU:OE2	1:B:1054:GLN:NE2	2.33	0.62
1:A:202:ASP:OD2	1:A:204:ARG:CG	2.48	0.61
1:A:108:VAL:O	1:B:1129:LYS:CE	2.48	0.61
1:A:180:GLU:OE1	5:A:382:HOH:O	2.16	0.61
1:A:205:LYS:HA	1:A:205:LYS:HE2	1.81	0.61
1:A:209:HIS:O	1:A:213:VAL:HG22	2.01	0.61
1:B:1206:MET:HE1	4:B:1302:IDN:H21	1.82	0.60
1:B:1017:LYS:HE2	1:B:1022:TYR:OH	2.02	0.59
1:B:1197:ALA:O	1:B:1200:ILE:HG12	2.02	0.59
1:B:1200:ILE:HD11	4:B:1302:IDN:H15	1.85	0.59
1:A:38:THR:HA	1:A:61:LEU:O	2.03	0.58
1:A:81:VAL:O	1:A:82:TRP:HD1	1.86	0.58
1:B:1205:LYS:HA	1:B:1205:LYS:NZ	2.19	0.58
1:B:1047:ARG:NH1	1:B:1051:PHE:CZ	2.72	0.58
1:B:1047:ARG:HE	1:B:1047:ARG:HA	1.68	0.57
1:A:108:VAL:O	1:B:1129:LYS:HE2	2.04	0.56
1:A:114:LYS:HD2	1:A:114:LYS:C	2.26	0.56
1:A:222:ILE:HG23	5:A:365:HOH:O	2.06	0.56
1:A:81:VAL:HG22	1:A:82:TRP:CD1	2.42	0.55
1:B:1045:LYS:O	1:B:1049:GLU:HG3	2.06	0.55
1:A:104:TYR:HD1	1:A:157:ASN:HB3	1.71	0.54
1:A:65:VAL:HG22	3:A:301:NAD:N1A	2.22	0.54
1:B:1047:ARG:CZ	1:B:1051:PHE:CZ	2.91	0.54
1:B:1064:ASP:OD1	1:B:1066:ALA:HB3	2.08	0.53
1:B:1182:VAL:HG12	1:B:1183:ARG:O	2.09	0.53
1:A:250:GLY:O	1:A:253:ILE:HG13	2.09	0.53
1:B:1104:TYR:HD1	1:B:1157:ASN:HB3	1.74	0.53
1:B:1044:LEU:HD23	5:B:181:HOH:O	2.08	0.52
1:B:1193:ARG:O	1:B:1193:ARG:HG3	2.09	0.52
1:B:1063:CYS:HB2	1:B:1074:MET:HG3	1.92	0.52
1:A:50:GLU:O	1:A:54:GLN:HG3	2.10	0.51
1:B:1010:LEU:HB3	1:B:1088:PHE:HB3	1.92	0.51
1:B:1065:VAL:HB	1:B:1123:SER:HB2	1.93	0.51
1:A:201:LYS:HG3	1:A:202:ASP:N	2.26	0.50
1:B:1017:LYS:HG2	1:B:1022:TYR:CZ	2.46	0.50
1:A:204:ARG:HG2	1:A:205:LYS:H	1.76	0.50
1:B:1010:LEU:HD11	1:B:1038:THR:HG23	1.92	0.50
1:A:149:ALA:HB2	1:A:163:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:ARG:HE	1:B:1047:ARG:CA	2.25	0.50
1:B:1253:ILE:HD12	1:B:1253:ILE:C	2.31	0.50
1:B:1099:GLN:C	1:B:1100:LEU:HD23	2.32	0.49
1:A:24:ILE:HG12	1:A:226:GLY:HA2	1.93	0.49
3:B:1301:NAD:C4N	4:B:1302:IDN:H122	2.43	0.49
1:A:178:GLY:N	1:A:179:PRO:CD	2.75	0.49
1:A:170:VAL:HG21	1:A:186:ALA:HB2	1.93	0.49
1:B:1196:ALA:O	4:B:1302:IDN:H03	2.12	0.49
1:B:1201:LYS:HG3	1:B:1202:ASP:N	2.28	0.49
1:B:1015:ALA:HB2	3:B:1301:NAD:O3B	2.13	0.49
1:B:1022:TYR:OH	1:B:1026:GLN:NE2	2.46	0.48
1:A:258:GLU:HG2	1:A:259:LEU:HD12	1.95	0.48
1:B:1183:ARG:HD2	1:B:1240:ILE:O	2.13	0.48
1:B:1248:ASP:OD2	1:B:1251:PHE:HB3	2.14	0.48
1:A:3:PHE:CZ	1:A:31:GLU:HG3	2.49	0.48
1:A:37:PHE:CD1	1:A:37:PHE:N	2.81	0.48
1:B:1167:GLU:O	1:B:1170:VAL:HB	2.13	0.48
1:A:200:ILE:HB	4:A:302:IDN:H203	1.96	0.48
1:A:155:ASN:HD22	1:A:201:LYS:CD	2.26	0.47
1:B:1128:ALA:O	1:B:1129:LYS:C	2.53	0.47
1:A:200:ILE:HG21	4:A:302:IDN:H203	1.96	0.47
1:A:99:GLN:NE2	1:A:108:VAL:HA	2.26	0.47
1:A:159:MET:CE	1:A:163:LYS:HE2	2.45	0.46
1:A:30:ARG:NE	1:A:31:GLU:OE2	2.46	0.46
1:A:191:PRO:HG2	1:A:210:CYS:SG	2.56	0.46
1:A:62:GLN:NE2	1:A:63:CYS:N	2.64	0.45
1:B:1009:ILE:HD13	1:B:1028:MET:CE	2.47	0.45
1:A:158:VAL:O	1:A:158:VAL:HG22	2.17	0.45
1:A:197:ALA:O	1:A:200:ILE:HD11	2.17	0.45
1:A:44:LEU:O	1:A:48:VAL:HG23	2.16	0.45
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.99	0.45
1:A:7:LYS:NZ	5:A:312:HOH:O	2.32	0.45
1:B:1017:LYS:HG2	1:B:1022:TYR:CE2	2.52	0.44
1:B:1047:ARG:HA	1:B:1047:ARG:NE	2.31	0.44
1:A:65:VAL:HB	1:A:123:SER:HB2	2.00	0.44
1:B:1200:ILE:CD1	4:B:1302:IDN:H15	2.48	0.44
1:B:1114:LYS:HD3	1:B:1114:LYS:C	2.38	0.44
1:A:48:VAL:HA	1:A:51:PHE:CD1	2.52	0.44
1:B:1145:SER:HA	1:B:1163:LYS:HD2	2.00	0.43
1:B:1059:ILE:HD11	1:B:1081:VAL:HG11	1.99	0.43
1:A:200:ILE:CB	4:A:302:IDN:H203	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:O	1:B:1129:LYS:HE3	2.17	0.43
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.68	0.43
1:B:1196:ALA:HB2	3:B:1301:NAD:O1A	2.18	0.43
1:B:1122:TYR:CE2	1:B:1126:ALA:HB2	2.54	0.42
1:A:200:ILE:CG2	4:A:302:IDN:H203	2.49	0.42
1:A:94:PHE:HA	4:A:302:IDN:N06	2.34	0.42
1:B:1232:LEU:HD23	1:B:1232:LEU:HA	1.82	0.42
1:B:1059:ILE:CD1	1:B:1081:VAL:HG11	2.49	0.42
1:B:1047:ARG:HH21	1:B:1050:GLU:HB3	1.85	0.42
1:A:153:ILE:HA	1:A:154:PRO:HD3	1.95	0.42
1:A:235:ASP:OD2	5:A:345:HOH:O	2.21	0.42
1:A:2:GLY:N	1:A:5:SER:HG	2.17	0.42
1:A:94:PHE:CG	1:A:95:ALA:N	2.88	0.42
1:A:15:ALA:HB2	3:A:301:NAD:O3B	2.20	0.41
1:B:1205:LYS:HA	1:B:1205:LYS:HZ3	1.84	0.41
1:A:259:LEU:CD1	1:A:259:LEU:H	2.29	0.41
1:A:39:TYR:HD2	1:A:41:ASN:O	2.02	0.41
1:A:205:LYS:HA	1:A:205:LYS:CE	2.49	0.41
1:B:1096:PRO:O	1:B:1097:GLY:C	2.59	0.41
1:A:30:ARG:NH2	1:A:31:GLU:OE2	2.50	0.41
1:B:1098:ASP:N	1:B:1098:ASP:OD1	2.53	0.41
1:A:203:PHE:O	1:A:206:MET:HB3	2.21	0.41
1:B:1149:ALA:HB2	1:B:1163:LYS:HB3	2.02	0.41
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.78	0.41
1:A:44:LEU:HD12	1:A:44:LEU:N	2.36	0.41
1:A:45:LYS:O	1:A:49:GLU:HG3	2.21	0.41
1:B:1197:ALA:HB1	1:B:1203:PHE:CE2	2.56	0.41
1:A:256:MET:CB	1:A:259:LEU:HD13	2.46	0.40
1:A:258:GLU:O	1:A:259:LEU:C	2.60	0.40
1:A:259:LEU:HD12	1:A:259:LEU:N	2.32	0.40
1:B:1040:GLN:NE2	5:B:165:HOH:O	2.55	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	256/262 (98%)	240 (94%)	15 (6%)	1 (0%)	38	42
1	B	256/262 (98%)	236 (92%)	16 (6%)	4 (2%)	11	9
All	All	512/524 (98%)	476 (93%)	31 (6%)	5 (1%)	18	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1196	ALA
1	B	1198	SER
1	A	201	LYS
1	B	1157	ASN
1	B	1097	GLY

### 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	197/201 (98%)	184 (93%)	13 (7%)	19	22
1	B	197/201 (98%)	184 (93%)	13 (7%)	19	22
All	All	394/402 (98%)	368 (93%)	26 (7%)	19	22

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	81	VAL
1	A	98	ASP
1	A	100	LEU
1	A	101	ASP
1	A	114	LYS
1	A	144	LEU
1	A	151	ARG

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	200	ILE
1	A	204	ARG
1	A	205	LYS
1	A	215	PRO
1	B	1018	LEU
1	B	1044	LEU
1	B	1062	GLN
1	B	1111	GLU
1	B	1120	SER
1	B	1144	LEU
1	B	1169	ASN
1	B	1193	ARG
1	B	1195	LEU
1	B	1200	ILE
1	B	1204	ARG
1	B	1205	LYS
1	B	1206	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	62	GLN
1	A	99	GLN
1	A	169	ASN
1	A	175	ASN
1	A	257	ASN
1	B	1026	GLN
1	B	1040	GLN
1	B	1062	GLN
1	B	1099	GLN
1	B	1169	ASN
1	B	1257	ASN

### 5.3.3 RNA ⓘ

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](#)

5 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	$\# Z  > 2$
3	NAD	A	301	-	41,48,48	1.61	11 (26%)	43,73,73	2.46	5 (11%)
4	IDN	A	302	-	27,31,31	2.88	15 (55%)	33,44,44	1.35	4 (12%)
3	NAD	B	1301	-	41,48,48	1.55	7 (17%)	43,73,73	2.49	5 (11%)
4	IDN	B	1302	-	27,31,31	2.56	12 (44%)	33,44,44	1.39	3 (9%)
2	SO4	B	1303	-	4,4,4	0.45	0	6,6,6	0.20	0

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
3	NAD	A	301	-	-	0/22/62/62	0/5/5/5
4	IDN	A	302	-	-	0/12/22/22	0/4/4/4
3	NAD	B	1301	-	-	0/22/62/62	0/5/5/5
4	IDN	B	1302	-	-	0/12/22/22	0/4/4/4
2	SO4	B	1303	-	-	0/0/0/0	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAD	C5A-N7A	-2.45	1.31	1.39
3	B	1301	NAD	C5A-N7A	-2.32	1.31	1.39
3	A	301	NAD	C2D-C1D	-2.03	1.50	1.53
3	A	301	NAD	O4B-C1B	2.25	1.44	1.41
4	B	1302	IDN	C25-C26	2.26	1.57	1.51
3	B	1301	NAD	C3N-C7N	2.27	1.54	1.50
4	A	302	IDN	C25-C26	2.28	1.57	1.51
3	B	1301	NAD	C6N-N1N	2.29	1.41	1.35
3	A	301	NAD	C4A-N3A	2.49	1.39	1.35
4	A	302	IDN	C08-C07	2.49	1.39	1.32
4	B	1302	IDN	C05-N06	2.57	1.39	1.34
4	A	302	IDN	C08-C09	2.60	1.52	1.48
3	A	301	NAD	C4N-C3N	2.63	1.43	1.39
3	A	301	NAD	C2A-N1A	2.65	1.38	1.33
3	A	301	NAD	C5N-C4N	2.67	1.44	1.38
4	A	302	IDN	C01-N06	2.73	1.39	1.35
3	A	301	NAD	C6N-N1N	2.74	1.42	1.35
4	A	302	IDN	C03-C04	2.78	1.44	1.39
3	B	1301	NAD	C4N-C3N	2.81	1.43	1.39
3	B	1301	NAD	C2A-N3A	2.84	1.36	1.32
4	B	1302	IDN	C27-N19	2.85	1.38	1.35
4	B	1302	IDN	C03-C04	2.94	1.44	1.39
4	A	302	IDN	C22-C21	2.95	1.45	1.38
4	B	1302	IDN	C22-C21	2.96	1.45	1.38
3	A	301	NAD	C3N-C7N	3.12	1.55	1.50
4	B	1302	IDN	C05-C04	3.15	1.44	1.39
4	A	302	IDN	C05-N06	3.18	1.41	1.34
4	A	302	IDN	C03-C02	3.21	1.45	1.39
4	B	1302	IDN	C03-C02	3.26	1.45	1.39
3	A	301	NAD	C2A-N3A	3.26	1.37	1.32
4	B	1302	IDN	C21-C24	3.28	1.44	1.36
4	A	302	IDN	C26-C27	3.30	1.57	1.50
4	B	1302	IDN	C26-C27	3.40	1.58	1.50
4	A	302	IDN	C21-C24	3.83	1.45	1.36
4	B	1302	IDN	C22-C23	3.89	1.45	1.36
4	A	302	IDN	C22-C23	3.90	1.45	1.36
3	B	1301	NAD	C2N-C3N	4.02	1.45	1.39
4	A	302	IDN	C05-C04	4.07	1.46	1.39
3	A	301	NAD	O4D-C1D	4.20	1.47	1.41
4	A	302	IDN	C27-N19	4.35	1.40	1.35
3	B	1301	NAD	O4D-C1D	4.66	1.47	1.41
4	B	1302	IDN	C09-N11	5.60	1.42	1.35
4	A	302	IDN	C02-C01	5.81	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	IDN	C02-C01	5.97	1.47	1.41
4	A	302	IDN	C09-N11	6.43	1.43	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAD	C4B-O4B-C1B	-11.86	97.15	109.77
3	A	301	NAD	C4B-O4B-C1B	-11.01	98.05	109.77
3	A	301	NAD	N3A-C2A-N1A	-8.99	121.03	128.86
3	B	1301	NAD	N3A-C2A-N1A	-7.94	121.94	128.86
4	B	1302	IDN	O10-C09-C08	-4.22	113.46	122.16
4	A	302	IDN	O10-C09-C08	-4.05	113.82	122.16
3	B	1301	NAD	C1B-N9A-C4A	-3.21	121.10	126.64
3	A	301	NAD	C1B-N9A-C4A	-3.01	121.43	126.64
4	A	302	IDN	C01-N19-C27	2.06	126.28	124.48
3	B	1301	NAD	N6A-C6A-N1A	2.06	122.86	118.77
4	A	302	IDN	C13-N11-C09	2.48	126.13	119.96
3	A	301	NAD	N6A-C6A-N1A	2.57	123.86	118.77
4	B	1302	IDN	C13-N11-C09	2.68	126.64	119.96
4	B	1302	IDN	O10-C09-N11	3.21	123.76	121.17
4	A	302	IDN	O10-C09-N11	3.52	124.01	121.17
3	A	301	NAD	C4A-C5A-N7A	3.99	113.27	109.41
3	B	1301	NAD	C4A-C5A-N7A	4.29	113.55	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAD	2	0
4	A	302	IDN	6	0
3	B	1301	NAD	3	0
4	B	1302	IDN	5	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<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	258/262 (98%)	0.24	23 (8%) 10 16	15, 28, 57, 85	0
1	B	258/262 (98%)	0.09	13 (5%) 30 41	14, 26, 57, 91	0
All	All	516/524 (98%)	0.17	36 (6%) 17 25	14, 27, 57, 91	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1196	ALA	6.8
1	B	1200	ILE	6.4
1	A	199	GLY	5.8
1	A	200	ILE	5.7
1	B	1198	SER	5.5
1	A	202	ASP	4.8
1	A	259	LEU	4.7
1	B	1205	LYS	4.7
1	B	1199	GLY	4.6
1	B	1201	LYS	4.0
1	A	43	LYS	4.0
1	B	1202	ASP	3.9
1	A	198	SER	3.8
1	A	47	ARG	3.7
1	B	1195	LEU	3.4
1	A	204	ARG	3.3
1	A	201	LYS	3.1
1	A	2	GLY	3.0
1	B	1197	ALA	3.0
1	A	158	VAL	3.0
1	A	41	ASN	2.9
1	A	196	ALA	2.9
1	A	193	ARG	2.7
1	A	97	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1158	VAL	2.6
1	B	1204	ARG	2.5
1	A	205	LYS	2.4
1	A	10	LEU	2.3
1	A	58	ASP	2.3
1	A	197	ALA	2.3
1	B	1011	VAL	2.2
1	A	203	PHE	2.2
1	A	195	LEU	2.2
1	A	6	GLY	2.2
1	A	42	ASP	2.2
1	B	1258	GLU	2.1

## 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
4	IDN	A	302	28/28	0.56	0.38	1.79	83,87,88,88	0
2	SO4	B	1303	5/5	0.98	0.17	1.32	45,47,47,47	0
4	IDN	B	1302	28/28	0.62	0.32	0.96	78,80,83,84	0
3	NAD	A	301	44/44	0.91	0.16	0.27	35,39,45,48	0
3	NAD	B	1301	44/44	0.94	0.14	-0.13	34,39,46,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.