



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:09 PM GMT

PDB ID : 1IY8  
Title : Crystal Structure of Levodione Reductase  
Authors : Sogabe, S.; Fukami, T.; Shiratori, Y.; Yoshizumi, A.; Wada, M.  
Deposited on : 2002-07-25  
Resolution : 1.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

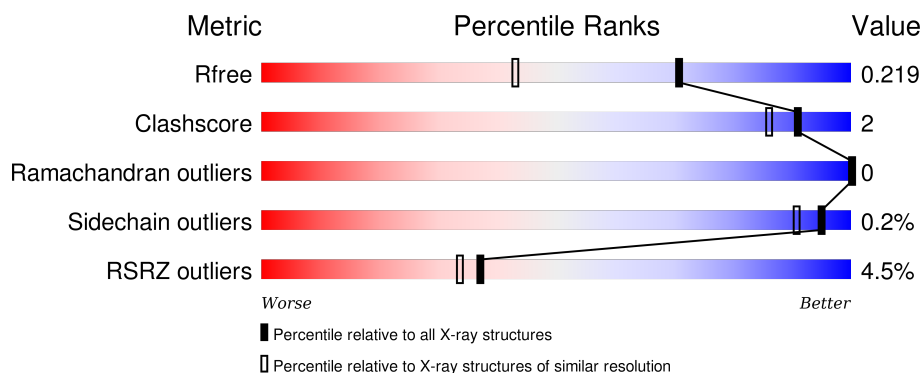
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	267	<div> <div>4%</div> <div>90%</div> <div>6%</div> </div>
1	B	267	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
1	C	267	<div> <div>3%</div> <div>92%</div> <div>5%</div> </div>
1	D	267	<div> <div>6%</div> <div>92%</div> <div>5%</div> </div>
1	E	267	<div> <div>2%</div> <div>94%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	267	 5% 91% 5% •
1	G	267	 2% 91% 6% •
1	H	267	 7% 90% 6% •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16602 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 LEVODIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	B	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	C	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	D	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	E	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	F	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	G	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			
1	H	258	Total	C	N	O	S	0	0	0
			1904	1189	332	379	4			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	G	1	Total C O 8 6 2	0	0
3	H	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0
4	B	114	Total O 114 114	0	0
4	C	125	Total O 125 125	0	0
4	D	117	Total O 117 117	0	0

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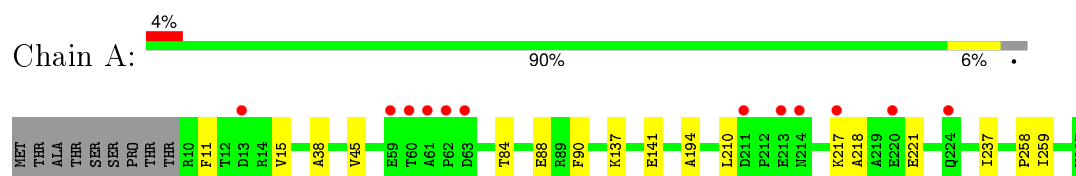
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	130	Total 130	O 130	0	0
4	F	117	Total 117	O 117	0	0
4	G	127	Total 127	O 127	0	0
4	H	103	Total 103	O 103	0	0

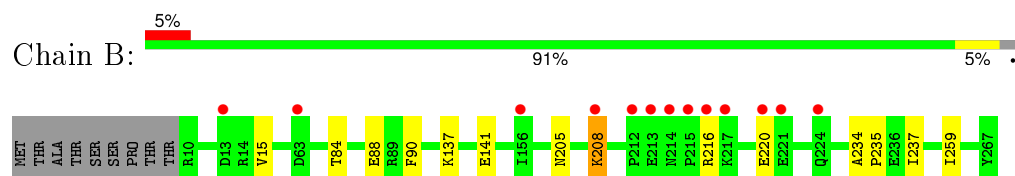
### 3 Residue-property plots [i](#)

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.

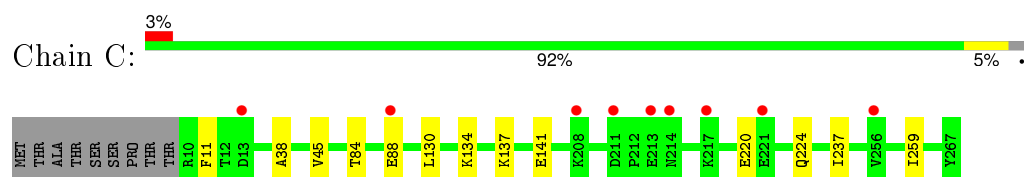
#### • Molecule 1: LEVODIONE REDUCTASE



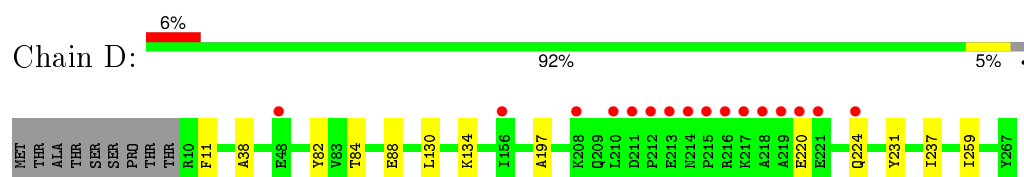
#### • Molecule 1: LEVODIONE REDUCTASE



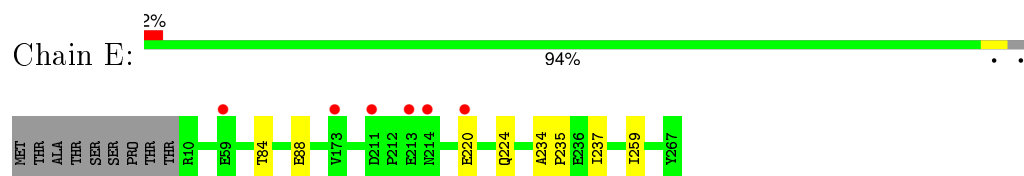
#### • Molecule 1: LEVODIONE REDUCTASE



#### • Molecule 1: LEVODIONE REDUCTASE



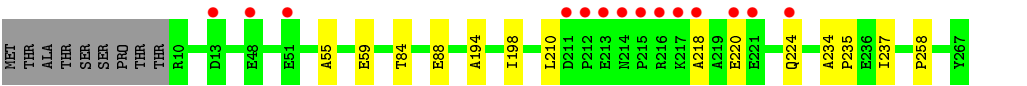
#### • Molecule 1: LEVODIONE REDUCTASE



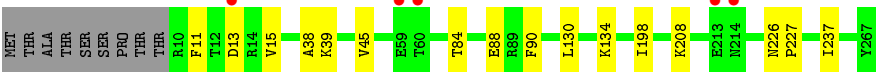
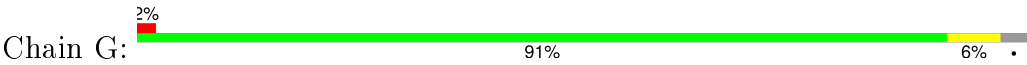
#### • Molecule 1: LEVODIONE REDUCTASE



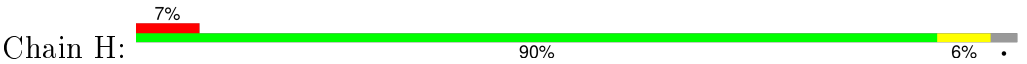




• Molecule 1: LEVODIONE REDUCTASE



• Molecule 1: LEVODIONE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.67Å 79.18Å 112.67Å 103.87° 91.40° 105.48°	Depositor
Resolution (Å)	40.00 – 1.60 48.23 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.60) 84.6 (48.23-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.219 0.199 , 0.219	Depositor DCC
$R_{free}$ test set	13160 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 261097 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16602	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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, 0.375 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: MRD, 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	0.31	0/1931	0.61	0/2617
1	B	0.31	0/1931	0.61	0/2617
1	C	0.31	0/1931	0.61	0/2617
1	D	0.31	0/1931	0.61	0/2617
1	E	0.31	0/1931	0.61	0/2617
1	F	0.30	0/1931	0.61	0/2617
1	G	0.31	0/1931	0.62	0/2617
1	H	0.30	0/1931	0.60	0/2617
All	All	0.31	0/15448	0.61	0/20936

There are no bond length outliers.

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	1904	0	1894	10	0
1	B	1904	0	1894	8	0
1	C	1904	0	1894	8	0
1	D	1904	0	1894	6	0
1	E	1904	0	1894	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1904	0	1894	9	0
1	G	1904	0	1894	12	0
1	H	1904	0	1894	10	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	8	0	14	0	0
3	E	8	0	14	0	0
3	F	8	0	14	0	0
3	G	8	0	14	0	0
3	H	8	0	14	0	0
4	A	121	0	0	0	0
4	B	114	0	0	0	0
4	C	125	0	0	0	0
4	D	117	0	0	0	0
4	E	130	0	0	0	0
4	F	117	0	0	0	0
4	G	127	0	0	0	0
4	H	103	0	0	0	0
All	All	16602	0	15472	67	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 2.

All (67) 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:H:216:ARG:HH12	1:H:220:GLU:HG3	1.58	0.66
1:F:198:ILE:HD12	1:F:237:ILE:HD11	1.78	0.66
1:G:198:ILE:HD12	1:G:237:ILE:HD11	1.84	0.58
1:H:237:ILE:HD13	1:H:259:ILE:HG21	1.86	0.57
1:C:237:ILE:HD13	1:C:259:ILE:HG21	1.86	0.56
1:C:137:LYS:O	1:C:141:GLU:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:ILE:HD13	1:E:259:ILE:HG21	1.89	0.55
1:E:84:THR:O	1:E:88:GLU:HG3	2.07	0.55
1:B:84:THR:O	1:B:88:GLU:HG3	2.07	0.54
1:G:237:ILE:HD12	1:G:237:ILE:N	2.24	0.53
1:B:208:LYS:NZ	1:B:208:LYS:HB2	2.23	0.53
1:F:84:THR:O	1:F:88:GLU:HG3	2.10	0.52
1:B:237:ILE:HD13	1:B:259:ILE:HG21	1.90	0.52
1:C:84:THR:O	1:C:88:GLU:HG3	2.09	0.52
1:B:137:LYS:O	1:B:141:GLU:HG3	2.09	0.52
1:A:217:LYS:O	1:A:221:GLU:HG3	2.10	0.52
1:D:237:ILE:HD13	1:D:259:ILE:HG21	1.92	0.51
1:H:84:THR:O	1:H:88:GLU:HG3	2.11	0.51
1:B:216:ARG:O	1:B:220:GLU:HG2	2.11	0.50
1:A:137:LYS:O	1:A:141:GLU:HG3	2.12	0.49
1:A:84:THR:O	1:A:88:GLU:HG3	2.12	0.49
1:G:11:PHE:HB3	1:G:38:ALA:HB2	1.95	0.49
1:G:45:VAL:HG13	2:G:7268:NAD:C2A	2.43	0.49
1:D:84:THR:O	1:D:88:GLU:HG3	2.13	0.49
1:H:220:GLU:O	1:H:224:GLN:HG2	2.13	0.48
1:C:220:GLU:O	1:C:224:GLN:HG2	2.12	0.48
1:F:237:ILE:N	1:F:237:ILE:HD12	2.29	0.48
1:F:198:ILE:CD1	1:F:237:ILE:HD11	2.43	0.48
1:G:45:VAL:HG13	2:G:7268:NAD:N1A	2.29	0.47
1:A:237:ILE:HD13	1:A:259:ILE:HG21	1.95	0.47
1:H:194:ALA:HB3	1:H:258:PRO:HA	1.95	0.47
1:H:216:ARG:NH1	1:H:220:GLU:HG3	2.28	0.47
1:G:84:THR:O	1:G:88:GLU:HG3	2.15	0.47
1:B:15:VAL:HG21	1:B:90:PHE:HB3	1.97	0.46
1:F:220:GLU:O	1:F:224:GLN:HG2	2.14	0.46
1:C:11:PHE:HB3	1:C:38:ALA:HB2	1.97	0.46
1:E:220:GLU:O	1:E:224:GLN:HG2	2.16	0.46
1:C:45:VAL:HG13	2:C:3268:NAD:C2A	2.45	0.46
1:D:197:ALA:HB1	1:D:231:TYR:CE1	2.51	0.45
1:D:11:PHE:HB3	1:D:38:ALA:HB2	1.98	0.45
1:A:210:LEU:HD23	1:A:218:ALA:HB1	1.98	0.44
1:H:45:VAL:HG13	2:H:8268:NAD:C2A	2.48	0.44
1:C:45:VAL:HG13	2:C:3268:NAD:N1A	2.33	0.44
1:A:15:VAL:HG21	1:A:90:PHE:HB3	2.00	0.44
1:H:210:LEU:HD23	1:H:218:ALA:HB1	1.99	0.44
1:G:198:ILE:CD1	1:G:237:ILE:HD11	2.48	0.43
1:B:205:ASN:O	1:B:208:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:VAL:HG21	1:G:90:PHE:HB3	2.00	0.43
1:D:220:GLU:O	1:D:224:GLN:HG2	2.19	0.43
1:A:11:PHE:HB3	1:A:38:ALA:HB2	2.01	0.43
1:E:234:ALA:HB3	1:E:235:PRO:HD3	2.01	0.42
1:H:15:VAL:HG21	1:H:90:PHE:HB3	2.00	0.42
1:G:13:ASP:HA	1:G:39:LYS:HZ3	1.84	0.42
1:B:234:ALA:HB3	1:B:235:PRO:HD3	2.01	0.42
1:G:130:LEU:O	1:G:134:LYS:HG2	2.20	0.42
1:D:130:LEU:O	1:D:134:LYS:HG2	2.20	0.42
1:F:55:ALA:O	1:F:59:GLU:HG3	2.20	0.41
1:G:208:LYS:HB2	1:G:208:LYS:HE2	1.94	0.41
1:A:45:VAL:HG13	2:A:1268:NAD:C2A	2.51	0.41
1:A:194:ALA:HB3	1:A:258:PRO:HA	2.03	0.41
1:H:197:ALA:HB1	1:H:231:TYR:CE2	2.56	0.41
1:A:45:VAL:HG13	2:A:1268:NAD:N1A	2.36	0.40
1:F:194:ALA:HB3	1:F:258:PRO:HA	2.04	0.40
1:G:226:ASN:HA	1:G:227:PRO:HD3	1.96	0.40
1:C:130:LEU:O	1:C:134:LYS:HG2	2.21	0.40
1:F:234:ALA:HB3	1:F:235:PRO:HD3	2.03	0.40
1:F:210:LEU:HD23	1:F:218:ALA:HB1	2.02	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	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	B	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	C	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	D	256/267 (96%)	248 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
1	F	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
1	G	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
1	H	256/267 (96%)	247 (96%)	9 (4%)	0	100	100
All	All	2048/2136 (96%)	1981 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	195/203 (96%)	195 (100%)	0	100	100
1	B	195/203 (96%)	194 (100%)	1 (0%)	92	85
1	C	195/203 (96%)	195 (100%)	0	100	100
1	D	195/203 (96%)	194 (100%)	1 (0%)	92	85
1	E	195/203 (96%)	195 (100%)	0	100	100
1	F	195/203 (96%)	195 (100%)	0	100	100
1	G	195/203 (96%)	195 (100%)	0	100	100
1	H	195/203 (96%)	194 (100%)	1 (0%)	92	85
All	All	1560/1624 (96%)	1557 (100%)	3 (0%)	95	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	208	LYS
1	D	82	TYR
1	H	48	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	161	ASN
1	B	162	GLN
1	C	161	ASN
1	D	161	ASN
1	D	162	GLN
1	E	99	ASN
1	E	161	ASN
1	F	161	ASN
1	F	162	GLN
1	G	161	ASN
1	H	161	ASN
1	H	162	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](#)

16 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	NAD	A	1268	-	38,48,48	2.65	9 (23%)	47,73,73	1.60	8 (17%)
3	MRD	A	1269	-	6,7,7	0.59	0	7,10,10	0.34	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	2268	-	38,48,48	2.65	8 (21%)	47,73,73	1.31	6 (12%)
3	MRD	B	2269	-	6,7,7	0.49	0	7,10,10	0.38	0
2	NAD	C	3268	-	38,48,48	2.54	9 (23%)	47,73,73	1.77	8 (17%)
3	MRD	C	3269	-	6,7,7	0.50	0	7,10,10	0.40	0
2	NAD	D	4268	-	38,48,48	2.51	9 (23%)	47,73,73	1.44	8 (17%)
3	MRD	D	4269	-	6,7,7	0.52	0	7,10,10	0.27	0
2	NAD	E	5268	-	38,48,48	2.59	9 (23%)	47,73,73	1.41	6 (12%)
3	MRD	E	5269	-	6,7,7	0.42	0	7,10,10	0.44	0
2	NAD	F	6268	-	38,48,48	2.53	8 (21%)	47,73,73	1.44	6 (12%)
3	MRD	F	6269	-	6,7,7	0.53	0	7,10,10	0.34	0
2	NAD	G	7268	-	38,48,48	2.53	9 (23%)	47,73,73	1.47	6 (12%)
3	MRD	G	7269	-	6,7,7	0.49	0	7,10,10	0.38	0
2	NAD	H	8268	-	38,48,48	2.64	9 (23%)	47,73,73	1.59	8 (17%)
3	MRD	H	8269	-	6,7,7	0.46	0	7,10,10	0.42	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
2	NAD	A	1268	-	-	0/22/62/62	0/5/5/5
3	MRD	A	1269	-	-	0/5/5/5	0/0/0/0
2	NAD	B	2268	-	-	0/22/62/62	0/5/5/5
3	MRD	B	2269	-	-	0/5/5/5	0/0/0/0
2	NAD	C	3268	-	-	0/22/62/62	0/5/5/5
3	MRD	C	3269	-	-	0/5/5/5	0/0/0/0
2	NAD	D	4268	-	-	0/22/62/62	0/5/5/5
3	MRD	D	4269	-	-	0/5/5/5	0/0/0/0
2	NAD	E	5268	-	-	0/22/62/62	0/5/5/5
3	MRD	E	5269	-	-	0/5/5/5	0/0/0/0
2	NAD	F	6268	-	-	0/22/62/62	0/5/5/5
3	MRD	F	6269	-	-	0/5/5/5	0/0/0/0
2	NAD	G	7268	-	-	0/22/62/62	0/5/5/5
3	MRD	G	7269	-	-	0/5/5/5	0/0/0/0
2	NAD	H	8268	-	-	0/22/62/62	0/5/5/5
3	MRD	H	8269	-	-	0/5/5/5	0/0/0/0

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2268	NAD	C4A-N3A	-4.51	1.28	1.35
2	C	3268	NAD	C4A-N3A	-4.21	1.29	1.35
2	E	5268	NAD	C4A-N3A	-4.15	1.29	1.35
2	D	4268	NAD	C4A-N3A	-4.13	1.29	1.35
2	F	6268	NAD	C4A-N3A	-3.96	1.29	1.35
2	G	7268	NAD	C4A-N3A	-3.85	1.29	1.35
2	H	8268	NAD	C4A-N3A	-3.82	1.29	1.35
2	A	1268	NAD	C4A-N3A	-3.63	1.30	1.35
2	F	6268	NAD	C3N-C7N	-3.24	1.45	1.50
2	H	8268	NAD	C3N-C7N	-2.94	1.45	1.50
2	D	4268	NAD	C3N-C7N	-2.79	1.46	1.50
2	E	5268	NAD	C5A-N7A	-2.54	1.30	1.39
2	G	7268	NAD	C3N-C7N	-2.48	1.46	1.50
2	B	2268	NAD	C3N-C7N	-2.46	1.46	1.50
2	A	1268	NAD	C3N-C7N	-2.46	1.46	1.50
2	C	3268	NAD	C5A-N7A	-2.39	1.31	1.39
2	G	7268	NAD	C5A-N7A	-2.32	1.31	1.39
2	H	8268	NAD	C5A-N7A	-2.32	1.31	1.39
2	E	5268	NAD	C3N-C7N	-2.31	1.46	1.50
2	A	1268	NAD	C5A-N7A	-2.26	1.31	1.39
2	C	3268	NAD	C3N-C7N	-2.26	1.47	1.50
2	F	6268	NAD	C5A-N7A	-2.24	1.31	1.39
2	D	4268	NAD	C5A-N7A	-2.23	1.31	1.39
2	B	2268	NAD	C5A-N7A	-2.20	1.31	1.39
2	E	5268	NAD	O4D-C1D	2.01	1.43	1.41
2	G	7268	NAD	O4B-C1B	2.01	1.43	1.41
2	A	1268	NAD	C8A-N7A	2.07	1.38	1.34
2	C	3268	NAD	C8A-N7A	2.15	1.38	1.34
2	H	8268	NAD	O4D-C1D	2.17	1.43	1.41
2	D	4268	NAD	O4B-C1B	2.50	1.44	1.41
2	H	8268	NAD	C5A-C4A	2.85	1.46	1.40
2	B	2268	NAD	C5A-C4A	2.96	1.47	1.40
2	G	7268	NAD	C5A-C4A	3.12	1.47	1.40
2	A	1268	NAD	C5A-C4A	3.14	1.47	1.40
2	C	3268	NAD	C5A-C4A	3.18	1.47	1.40
2	E	5268	NAD	C5A-C4A	3.27	1.47	1.40
2	F	6268	NAD	C5A-C4A	3.31	1.48	1.40
2	D	4268	NAD	C5A-C4A	3.38	1.48	1.40
2	D	4268	NAD	C2A-N3A	3.67	1.38	1.32
2	C	3268	NAD	C2A-N3A	3.73	1.38	1.32
2	A	1268	NAD	C2A-N3A	3.75	1.38	1.32
2	F	6268	NAD	C2A-N3A	3.83	1.39	1.32
2	B	2268	NAD	C2A-N3A	3.88	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8268	NAD	C2A-N3A	3.93	1.39	1.32
2	E	5268	NAD	C2A-N3A	3.94	1.39	1.32
2	G	7268	NAD	C2A-N3A	4.46	1.40	1.32
2	D	4268	NAD	C5N-C4N	5.75	1.50	1.38
2	G	7268	NAD	C5N-C4N	5.93	1.51	1.38
2	F	6268	NAD	C5N-C4N	6.17	1.51	1.38
2	A	1268	NAD	C5N-C4N	6.25	1.51	1.38
2	B	2268	NAD	C5N-C4N	6.30	1.51	1.38
2	H	8268	NAD	C5N-C4N	6.35	1.52	1.38
2	C	3268	NAD	C5N-C4N	6.36	1.52	1.38
2	E	5268	NAD	C5N-C4N	6.41	1.52	1.38
2	F	6268	NAD	C4N-C3N	6.82	1.51	1.39
2	D	4268	NAD	C4N-C3N	6.87	1.51	1.39
2	C	3268	NAD	C4N-C3N	7.00	1.51	1.39
2	E	5268	NAD	C4N-C3N	7.12	1.51	1.39
2	H	8268	NAD	C4N-C3N	7.14	1.51	1.39
2	G	7268	NAD	C4N-C3N	7.19	1.51	1.39
2	B	2268	NAD	C4N-C3N	7.36	1.51	1.39
2	A	1268	NAD	C4N-C3N	8.21	1.53	1.39
2	G	7268	NAD	C2N-C3N	8.36	1.51	1.39
2	D	4268	NAD	C2N-C3N	8.57	1.52	1.39
2	C	3268	NAD	C2N-C3N	8.81	1.52	1.39
2	F	6268	NAD	C2N-C3N	8.89	1.52	1.39
2	E	5268	NAD	C2N-C3N	8.94	1.52	1.39
2	A	1268	NAD	C2N-C3N	9.04	1.52	1.39
2	B	2268	NAD	C2N-C3N	9.55	1.53	1.39
2	H	8268	NAD	C2N-C3N	9.74	1.53	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3268	NAD	N3A-C2A-N1A	-6.09	124.23	128.89
2	H	8268	NAD	N3A-C2A-N1A	-5.79	124.46	128.89
2	A	1268	NAD	N3A-C2A-N1A	-5.73	124.51	128.89
2	E	5268	NAD	N3A-C2A-N1A	-5.42	124.74	128.89
2	G	7268	NAD	N3A-C2A-N1A	-5.17	124.94	128.89
2	F	6268	NAD	N3A-C2A-N1A	-4.52	125.43	128.89
2	B	2268	NAD	N3A-C2A-N1A	-4.33	125.58	128.89
2	C	3268	NAD	O7N-C7N-C3N	-4.31	114.88	119.59
2	D	4268	NAD	N3A-C2A-N1A	-4.04	125.80	128.89
2	A	1268	NAD	C1B-N9A-C4A	-3.76	121.26	126.94
2	A	1268	NAD	C5N-C4N-C3N	-3.72	115.65	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8268	NAD	C5N-C4N-C3N	-3.71	115.67	120.33
2	F	6268	NAD	O7N-C7N-C3N	-3.58	115.67	119.59
2	B	2268	NAD	C5N-C4N-C3N	-3.50	115.93	120.33
2	F	6268	NAD	C5N-C4N-C3N	-3.23	116.27	120.33
2	D	4268	NAD	C1B-N9A-C4A	-3.21	122.09	126.94
2	G	7268	NAD	C5N-C4N-C3N	-3.18	116.33	120.33
2	C	3268	NAD	C1B-N9A-C4A	-3.16	122.17	126.94
2	D	4268	NAD	O7N-C7N-C3N	-3.15	116.15	119.59
2	C	3268	NAD	C5N-C4N-C3N	-3.14	116.39	120.33
2	E	5268	NAD	C5N-C4N-C3N	-3.01	116.55	120.33
2	H	8268	NAD	O7N-C7N-C3N	-2.82	116.51	119.59
2	C	3268	NAD	C4B-O4B-C1B	-2.77	106.67	109.72
2	D	4268	NAD	C4B-O4B-C1B	-2.68	106.77	109.72
2	E	5268	NAD	C4B-O4B-C1B	-2.63	106.83	109.72
2	F	6268	NAD	C1B-N9A-C4A	-2.59	123.03	126.94
2	H	8268	NAD	C4B-O4B-C1B	-2.52	106.95	109.72
2	H	8268	NAD	C2B-C1B-N9A	-2.51	110.46	114.29
2	G	7268	NAD	C1B-N9A-C4A	-2.51	123.16	126.94
2	G	7268	NAD	C4B-O4B-C1B	-2.50	106.97	109.72
2	D	4268	NAD	C5N-C4N-C3N	-2.48	117.22	120.33
2	B	2268	NAD	C4B-O4B-C1B	-2.43	107.04	109.72
2	B	2268	NAD	O7N-C7N-C3N	-2.39	116.98	119.59
2	A	1268	NAD	PN-O3-PA	-2.25	126.40	132.73
2	A	1268	NAD	C4B-O4B-C1B	-2.21	107.29	109.72
2	E	5268	NAD	C1B-N9A-C4A	-2.07	123.82	126.94
2	H	8268	NAD	C1B-N9A-C4A	-2.07	123.82	126.94
2	A	1268	NAD	C2B-C1B-N9A	-2.00	111.23	114.29
2	D	4268	NAD	C2A-N1A-C6A	2.14	122.59	118.77
2	B	2268	NAD	C4A-C5A-N7A	2.26	111.56	109.48
2	D	4268	NAD	C3N-C7N-N7N	2.30	120.33	117.82
2	B	2268	NAD	C2A-N1A-C6A	2.38	123.02	118.77
2	G	7268	NAD	C2A-N1A-C6A	2.55	123.32	118.77
2	H	8268	NAD	C2A-N1A-C6A	2.59	123.40	118.77
2	F	6268	NAD	C4A-C5A-N7A	2.76	112.02	109.48
2	A	1268	NAD	C2A-N1A-C6A	2.77	123.72	118.77
2	E	5268	NAD	C4A-C5A-N7A	2.78	112.04	109.48
2	F	6268	NAD	C3N-C7N-N7N	2.87	120.96	117.82
2	D	4268	NAD	C4A-C5A-N7A	2.91	112.16	109.48
2	E	5268	NAD	C2A-N1A-C6A	2.99	124.11	118.77
2	C	3268	NAD	C2A-N1A-C6A	3.06	124.23	118.77
2	H	8268	NAD	C4A-C5A-N7A	3.19	112.42	109.48
2	C	3268	NAD	C4A-C5A-N7A	3.34	112.55	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7268	NAD	C4A-C5A-N7A	3.38	112.59	109.48
2	A	1268	NAD	C4A-C5A-N7A	3.50	112.70	109.48
2	C	3268	NAD	C3N-C7N-N7N	3.71	121.88	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1268	NAD	2	0
2	C	3268	NAD	2	0
2	G	7268	NAD	2	0
2	H	8268	NAD	1	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 ⓘ

### 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	258/267 (96%)	0.20	12 (4%) 35 32	9, 14, 21, 27	0
1	B	258/267 (96%)	0.29	13 (5%) 32 29	9, 15, 22, 26	0
1	C	258/267 (96%)	0.12	9 (3%) 48 44	9, 15, 21, 26	0
1	D	258/267 (96%)	0.26	16 (6%) 24 21	8, 14, 22, 27	0
1	E	258/267 (96%)	0.14	6 (2%) 64 62	9, 14, 22, 27	0
1	F	258/267 (96%)	0.29	14 (5%) 29 26	9, 15, 23, 27	0
1	G	258/267 (96%)	0.11	5 (1%) 70 68	9, 14, 21, 27	0
1	H	258/267 (96%)	0.34	18 (6%) 19 17	10, 15, 23, 27	0
All	All	2064/2136 (96%)	0.22	93 (4%) 37 34	8, 15, 22, 27	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	GLU	6.1
1	F	214	ASN	5.9
1	D	216	ARG	5.7
1	H	216	ARG	5.6
1	D	214	ASN	5.3
1	H	213	GLU	5.3
1	B	216	ARG	5.2
1	B	213	GLU	5.1
1	F	216	ARG	5.1
1	F	213	GLU	4.8
1	H	214	ASN	4.8
1	D	210	LEU	4.6
1	B	13	ASP	4.5
1	A	213	GLU	4.5
1	F	215	PRO	4.4
1	B	214	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	217	LYS	4.2
1	F	211	ASP	4.2
1	F	212	PRO	4.1
1	G	213	GLU	4.1
1	H	220	GLU	4.0
1	F	217	LYS	4.0
1	D	212	PRO	3.9
1	H	212	PRO	3.9
1	F	220	GLU	3.9
1	B	217	LYS	3.8
1	C	214	ASN	3.8
1	B	212	PRO	3.8
1	E	213	GLU	3.7
1	A	214	ASN	3.5
1	B	215	PRO	3.5
1	H	211	ASP	3.5
1	H	13	ASP	3.5
1	B	220	GLU	3.3
1	H	215	PRO	3.3
1	G	214	ASN	3.3
1	A	13	ASP	3.2
1	D	215	PRO	3.1
1	C	213	GLU	3.1
1	D	211	ASP	3.0
1	D	217	LYS	3.0
1	F	221	GLU	3.0
1	A	62	PRO	3.0
1	H	156	ILE	3.0
1	B	221	GLU	3.0
1	C	221	GLU	2.9
1	B	63	ASP	2.9
1	G	13	ASP	2.8
1	F	224	GLN	2.8
1	A	211	ASP	2.7
1	H	210	LEU	2.7
1	H	224	GLN	2.7
1	C	13	ASP	2.7
1	E	214	ASN	2.7
1	H	208	LYS	2.6
1	H	221	GLU	2.6
1	A	63	ASP	2.6
1	A	217	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	156	ILE	2.6
1	D	219	ALA	2.5
1	H	199	TRP	2.5
1	H	218	ALA	2.5
1	F	48	GLU	2.5
1	D	48	GLU	2.5
1	D	220	GLU	2.4
1	E	220	GLU	2.4
1	H	48	GLU	2.4
1	B	208	LYS	2.4
1	D	224	GLN	2.4
1	D	218	ALA	2.4
1	D	221	GLU	2.4
1	H	63	ASP	2.4
1	F	51	GLU	2.4
1	F	218	ALA	2.3
1	E	59	GLU	2.3
1	A	220	GLU	2.3
1	E	173	VAL	2.3
1	F	13	ASP	2.2
1	C	211	ASP	2.2
1	C	217	LYS	2.2
1	A	59	GLU	2.1
1	C	88	GLU	2.1
1	A	60	THR	2.1
1	E	211	ASP	2.1
1	G	59	GLU	2.1
1	B	224	GLN	2.1
1	A	224	GLN	2.1
1	C	256	VAL	2.0
1	G	60	THR	2.0
1	D	208	LYS	2.0
1	A	61	ALA	2.0
1	D	156	ILE	2.0
1	C	208	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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
3	MRD	B	2269	8/8	0.85	0.13	1.54	19,20,21,22	0
3	MRD	G	7269	8/8	0.87	0.10	0.31	17,19,21,21	0
3	MRD	F	6269	8/8	0.90	0.11	0.28	19,20,21,22	0
2	NAD	D	4268	44/44	0.94	0.09	-0.42	12,15,17,18	0
3	MRD	E	5269	8/8	0.91	0.09	-0.44	17,19,21,21	0
3	MRD	D	4269	8/8	0.93	0.09	-0.47	18,19,21,21	0
3	MRD	H	8269	8/8	0.90	0.09	-0.50	20,20,21,22	0
2	NAD	E	5268	44/44	0.95	0.08	-0.65	11,15,17,19	0
2	NAD	A	1268	44/44	0.96	0.08	-0.67	11,14,16,17	0
3	MRD	C	3269	8/8	0.93	0.08	-0.74	19,20,21,21	0
2	NAD	G	7268	44/44	0.96	0.08	-0.75	10,14,16,17	0
2	NAD	F	6268	44/44	0.95	0.08	-0.77	14,16,17,18	0
2	NAD	B	2268	44/44	0.95	0.08	-0.82	13,16,18,19	0
2	NAD	H	8268	44/44	0.95	0.07	-1.00	14,16,18,20	0
2	NAD	C	3268	44/44	0.96	0.08	-1.12	12,15,17,19	0
3	MRD	A	1269	8/8	0.95	0.07	-1.71	18,20,21,21	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.