



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:26 am GMT

PDB ID : 3SX2  
Title : Crystal structure of a putative 3-ketoacyl-(acyl-carrier-protein) reductase from Mycobacterium paratuberculosis in complex with NAD  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-07-14  
Resolution : 1.50 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

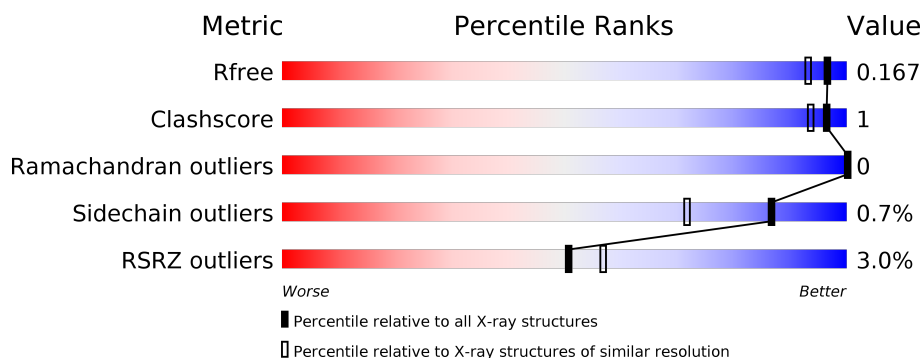
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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	278	<div> <div>3%</div> <div>93%</div> <div>8%</div> </div>
1	B	278	<div> <div>4%</div> <div>90%</div> <div>8%</div> </div>
1	C	278	<div> <div>3%</div> <div>90%</div> <div>8%</div> </div>
1	D	278	<div> <div>3%</div> <div>93%</div> <div>8%</div> </div>
1	E	278	<div> <div>4%</div> <div>88%</div> <div>8%</div> </div>
1	F	278	<div> <div>4%</div> <div>95%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	278	
1	H	278	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	B	301	X	-	-	X
3	MPD	E	302	X	-	-	-
3	MPD	H	301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17297 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 Putative 3-ketoacyl-(acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	8	0
			1971	1244	344	375	8			
1	B	257	Total	C	N	O	S	0	7	0
			1872	1183	329	354	6			
1	C	257	Total	C	N	O	S	0	8	0
			1885	1192	328	359	6			
1	D	269	Total	C	N	O	S	0	11	0
			1981	1253	344	376	8			
1	E	256	Total	C	N	O	S	0	5	0
			1838	1157	324	351	6			
1	F	274	Total	C	N	O	S	0	11	0
			2018	1274	349	387	8			
1	G	267	Total	C	N	O	S	0	8	0
			1953	1231	340	374	8			
1	H	249	Total	C	N	O	S	0	6	0
			1824	1151	320	348	5			

There are 16 discrepancies between the modelled and reference sequences:

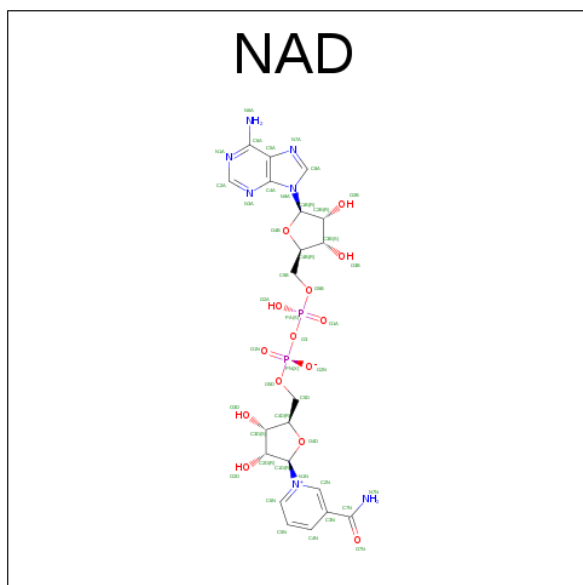
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
A	0	SER	-	EXPRESSION TAG	UNP Q73W00
B	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
B	0	SER	-	EXPRESSION TAG	UNP Q73W00
C	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
C	0	SER	-	EXPRESSION TAG	UNP Q73W00
D	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
D	0	SER	-	EXPRESSION TAG	UNP Q73W00
E	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
E	0	SER	-	EXPRESSION TAG	UNP Q73W00
F	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
F	0	SER	-	EXPRESSION TAG	UNP Q73W00
G	-1	GLY	-	EXPRESSION TAG	UNP Q73W00

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	EXPRESSION TAG	UNP Q73W00
H	-1	GLY	-	EXPRESSION TAG	UNP Q73W00
H	0	SER	-	EXPRESSION TAG	UNP Q73W00

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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 (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	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	H	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	234	Total O 234 234	0	0
4	B	188	Total O 188 188	0	0
4	C	188	Total O 188 188	0	0
4	D	179	Total O 179 179	0	0
4	E	145	Total O 145 145	0	0
4	F	216	Total O 216 216	0	0
4	G	245	Total O 245 245	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	168	Total 168	O 168	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.

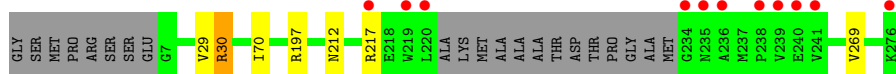
- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

Chain A: 




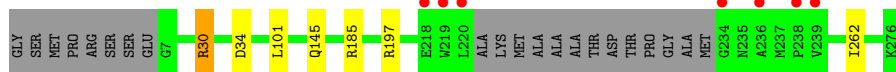
- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

Chain B: 



- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

Chain C: 




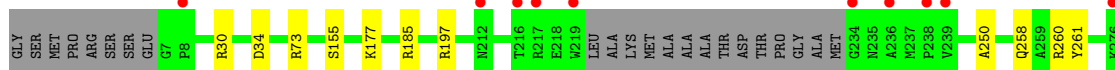
- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

Chain D: 



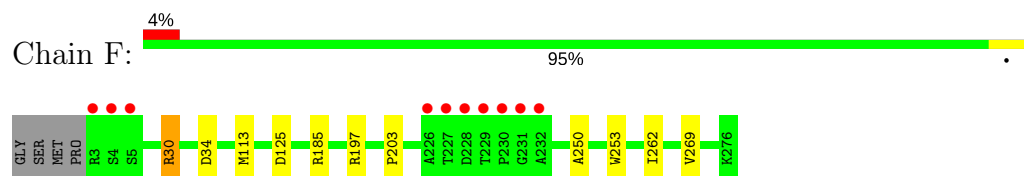
- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

Chain E: 

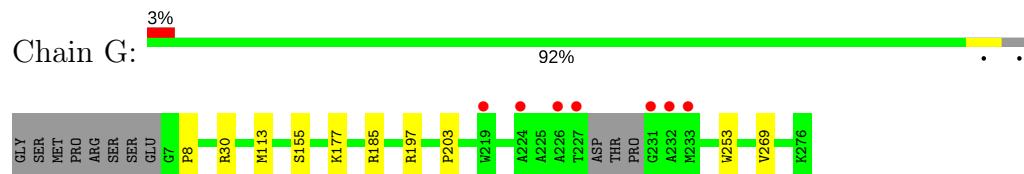


- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase

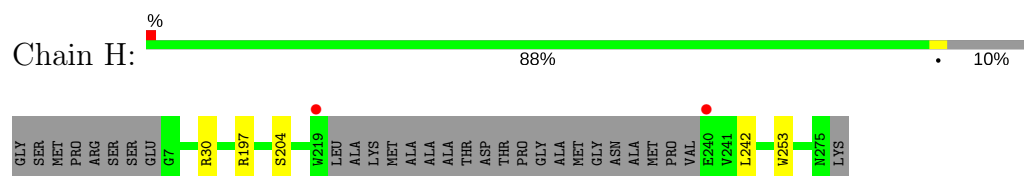




- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase



- Molecule 1: Putative 3-ketoacyl-(acyl-carrier-protein) reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.46Å 70.76Å 125.68Å 97.01° 93.92° 86.91°	Depositor
Resolution (Å)	20.00 – 1.50 19.51 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-1.50) 91.1 (19.51-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.140 , 0.159 0.149 , 0.167	Depositor DCC
$R_{free}$ test set	16842 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.3	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	0.97	EDS
Total number of atoms	17297	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 3.94% 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: MPD, 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	0.76	2/2023 (0.1%)	0.79	1/2759 (0.0%)
1	B	0.65	0/1919	0.76	1/2622 (0.0%)
1	C	0.70	0/1937	0.78	3/2648 (0.1%)
1	D	0.70	0/2039	0.77	3/2783 (0.1%)
1	E	0.61	0/1877	0.70	0/2565
1	F	0.71	0/2082	0.80	3/2843 (0.1%)
1	G	0.71	0/2004	0.80	3/2736 (0.1%)
1	H	0.64	0/1867	0.73	0/2550
All	All	0.69	2/15748 (0.0%)	0.77	14/21506 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CB-CG	-6.89	1.39	1.52
1	A	214	GLU	CB-CG	-5.18	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	30	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	C	185	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	F	30	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	D	30	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	30	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	30	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	G	30	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	B	30	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	G	185	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	F	185	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	D	30	ARG	NE-CZ-NH1	-5.77	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	30	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	D	185	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	185	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	1971	0	2000	4	0
1	B	1872	0	1897	5	0
1	C	1885	0	1895	4	0
1	D	1981	0	2005	5	0
1	E	1838	0	1846	8	0
1	F	2018	0	2032	7	0
1	G	1953	0	1972	6	0
1	H	1824	0	1846	5	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	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	0	0
2	H	44	0	26	1	0
3	B	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	H	8	0	14	0	0
4	A	234	0	0	1	0
4	B	188	0	0	1	0
4	C	188	0	0	1	0
4	D	179	0	0	1	0
4	E	145	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	216	0	0	2	0
4	G	245	0	0	1	0
4	H	168	0	0	1	0
All	All	17297	0	15771	37	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 1.

All (37) 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:E:185[A]:ARG:NH2	4:E:1519:HOH:O	1.69	1.25
1:F:125[B]:ASP:OD1	4:F:1308:HOH:O	1.88	0.90
1:A:125[B]:ASP:OD2	4:A:1393:HOH:O	2.03	0.77
1:H:30:ARG:HD3	4:H:526:HOH:O	1.89	0.71
1:C:101:LEU:H	1:C:145:GLN:HE22	1.44	0.64
1:F:30:ARG:HD3	4:F:434:HOH:O	2.06	0.55
1:D:163[B]:VAL:O	1:D:163[B]:VAL:HG23	2.07	0.55
1:G:8:PRO:HB2	4:G:910:HOH:O	2.11	0.50
1:C:30:ARG:HH12	1:C:34:ASP:CG	2.15	0.49
1:F:253[B]:TRP:CH2	1:F:262[B]:ILE:CD1	2.96	0.48
1:E:73:ARG:NH2	4:E:1547:HOH:O	2.47	0.48
1:B:30:ARG:HD3	4:B:493:HOH:O	2.13	0.48
1:F:30:ARG:HH12	1:F:34:ASP:CG	2.17	0.47
1:D:30:ARG:HD3	4:D:709:HOH:O	2.14	0.46
1:A:253[B]:TRP:CZ2	1:D:250:ALA:HA	2.50	0.45
1:E:30:ARG:HH12	1:E:34:ASP:CG	2.19	0.45
1:B:30:ARG:HH11	1:B:30:ARG:HG3	1.82	0.44
1:C:30:ARG:HD3	4:C:1103:HOH:O	2.16	0.44
1:G:155:SER:HA	1:G:177:LYS:HD2	2.00	0.44
1:G:203:PRO:HA	1:G:269:VAL:O	2.18	0.44
1:E:261:TYR:CD2	1:H:242:LEU:HD22	2.53	0.44
1:E:260:ARG:NE	1:E:261:TYR:CE2	2.86	0.44
1:G:113:MET:HB2	1:G:113:MET:HE3	1.70	0.44
1:F:203:PRO:HA	1:F:269:VAL:O	2.18	0.43
1:F:250:ALA:HA	1:G:253[B]:TRP:CZ2	2.54	0.43
1:D:7:GLY:N	1:D:10:THR:HG1	2.16	0.42
1:E:250:ALA:HA	1:H:253[B]:TRP:CZ2	2.55	0.42
1:D:203:PRO:HA	1:D:269:VAL:O	2.19	0.42
1:F:262[A]:ILE:HD11	1:G:269:VAL:HG13	2.01	0.42
1:E:258:GLN:NE2	1:H:30:ARG:HH21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASN:OD1	1:B:217:ARG:NH1	2.50	0.42
1:H:204[A]:SER:O	2:H:300:NAD:H4N	2.20	0.42
1:E:155:SER:HA	1:E:177:LYS:HD2	2.02	0.42
1:A:30:ARG:HH12	1:A:34:ASP:CG	2.23	0.41
1:B:29[A]:VAL:HG13	1:B:70:ILE:HD11	2.03	0.41
1:A:113:MET:HE3	1:A:113:MET:HB2	1.68	0.41
1:B:269:VAL:HG13	1:C:262[A]:ILE:HD11	2.02	0.41

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	272/278 (98%)	266 (98%)	6 (2%)	0	100	100
1	B	260/278 (94%)	253 (97%)	7 (3%)	0	100	100
1	C	261/278 (94%)	252 (97%)	9 (3%)	0	100	100
1	D	276/278 (99%)	268 (97%)	8 (3%)	0	100	100
1	E	257/278 (92%)	249 (97%)	8 (3%)	0	100	100
1	F	283/278 (102%)	275 (97%)	8 (3%)	0	100	100
1	G	271/278 (98%)	265 (98%)	6 (2%)	0	100	100
1	H	251/278 (90%)	244 (97%)	7 (3%)	0	100	100
All	All	2131/2224 (96%)	2072 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	202/206 (98%)	201 (100%)	1 (0%)	91	80
1	B	192/206 (93%)	191 (100%)	1 (0%)	91	80
1	C	193/206 (94%)	192 (100%)	1 (0%)	91	80
1	D	202/206 (98%)	200 (99%)	2 (1%)	80	60
1	E	186/206 (90%)	185 (100%)	1 (0%)	91	80
1	F	207/206 (100%)	205 (99%)	2 (1%)	80	60
1	G	199/206 (97%)	198 (100%)	1 (0%)	91	80
1	H	188/206 (91%)	187 (100%)	1 (0%)	91	80
All	All	1569/1648 (95%)	1559 (99%)	10 (1%)	87	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	B	197	ARG
1	C	197	ARG
1	D	113	MET
1	D	197	ARG
1	E	197	ARG
1	F	113	MET
1	F	197	ARG
1	G	197	ARG
1	H	197	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	194	GLN
1	B	23	GLN
1	C	23	GLN
1	C	92	GLN
1	C	145	GLN
1	D	23	GLN
1	D	258	GLN

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Mol	Chain	Res	Type
1	E	23	GLN
1	E	212	ASN
1	E	258	GLN
1	F	23	GLN
1	G	23	GLN
1	H	23	GLN
1	H	92	GLN
1	H	258	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](#)

13 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	300	-	41,48,48	1.73	9 (21%)	43,73,73	1.71	8 (18%)
2	NAD	B	300	-	41,48,48	1.97	11 (26%)	43,73,73	2.04	6 (13%)
3	MPD	B	301	-	7,7,7	0.34	0	9,10,10	0.86	0
2	NAD	C	300	-	41,48,48	1.98	12 (29%)	43,73,73	1.89	7 (16%)
2	NAD	D	300	-	41,48,48	2.10	14 (34%)	43,73,73	1.99	9 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPD	D	302	-	7,7,7	0.33	0	9,10,10	0.53	0
2	NAD	E	300	-	41,48,48	2.19	13 (31%)	43,73,73	1.99	7 (16%)
3	MPD	E	302	-	7,7,7	0.32	0	9,10,10	0.62	0
2	NAD	F	300	-	41,48,48	1.86	11 (26%)	43,73,73	1.56	5 (11%)
3	MPD	F	302	-	7,7,7	0.36	0	9,10,10	0.62	0
2	NAD	G	300	-	41,48,48	1.88	11 (26%)	43,73,73	1.76	6 (13%)
2	NAD	H	300	-	41,48,48	2.03	9 (21%)	43,73,73	1.95	8 (18%)
3	MPD	H	301	-	7,7,7	0.36	0	9,10,10	0.85	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	300	-	-	0/22/62/62	0/5/5/5
2	NAD	B	300	-	-	0/22/62/62	0/5/5/5
3	MPD	B	301	-	1/1/2/2	0/5/5/5	0/0/0/0
2	NAD	C	300	-	-	0/22/62/62	0/5/5/5
2	NAD	D	300	-	-	0/22/62/62	0/5/5/5
3	MPD	D	302	-	-	0/5/5/5	0/0/0/0
2	NAD	E	300	-	-	0/22/62/62	0/5/5/5
3	MPD	E	302	-	1/1/2/2	0/5/5/5	0/0/0/0
2	NAD	F	300	-	-	0/22/62/62	0/5/5/5
3	MPD	F	302	-	-	0/5/5/5	0/0/0/0
2	NAD	G	300	-	-	0/22/62/62	0/5/5/5
2	NAD	H	300	-	-	0/22/62/62	0/5/5/5
3	MPD	H	301	-	-	0/5/5/5	0/0/0/0

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	300	NAD	C2D-C1D	-4.46	1.46	1.53
2	C	300	NAD	C2D-C1D	-4.25	1.46	1.53
2	B	300	NAD	C2D-C1D	-4.23	1.46	1.53
2	F	300	NAD	C2D-C1D	-4.05	1.47	1.53
2	E	300	NAD	C2D-C1D	-3.96	1.47	1.53
2	D	300	NAD	C2D-C1D	-3.69	1.47	1.53
2	C	300	NAD	C2D-C3D	-3.27	1.44	1.53
2	C	300	NAD	O7N-C7N	-3.19	1.17	1.24
2	G	300	NAD	C2D-C1D	-2.93	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	300	NAD	C2D-C3D	-2.81	1.46	1.53
2	D	300	NAD	O4B-C4B	-2.80	1.38	1.45
2	G	300	NAD	C2B-C3B	-2.64	1.46	1.53
2	B	300	NAD	O7N-C7N	-2.60	1.18	1.24
2	A	300	NAD	C2D-C3D	-2.49	1.46	1.53
2	E	300	NAD	O7N-C7N	-2.42	1.19	1.24
2	D	300	NAD	C2B-C3B	-2.09	1.47	1.53
2	E	300	NAD	O3D-C3D	-2.05	1.38	1.43
2	D	300	NAD	C2D-C3D	-2.03	1.48	1.53
2	H	300	NAD	O4D-C4D	2.02	1.49	1.45
2	A	300	NAD	C5N-C4N	2.02	1.42	1.38
2	C	300	NAD	C2A-N3A	2.04	1.35	1.32
2	E	300	NAD	C5N-C4N	2.09	1.42	1.38
2	A	300	NAD	C4A-N3A	2.12	1.38	1.35
2	F	300	NAD	C6N-C5N	2.16	1.43	1.38
2	D	300	NAD	C2N-C3N	2.18	1.42	1.39
2	C	300	NAD	C5N-C4N	2.21	1.43	1.38
2	D	300	NAD	C5N-C4N	2.21	1.43	1.38
2	E	300	NAD	C6A-N6A	2.26	1.43	1.34
2	D	300	NAD	C6A-N6A	2.33	1.43	1.34
2	C	300	NAD	C2N-C3N	2.33	1.42	1.39
2	F	300	NAD	C4A-N3A	2.33	1.39	1.35
2	G	300	NAD	O4D-C1D	2.34	1.44	1.41
2	D	300	NAD	O4D-C1D	2.35	1.44	1.41
2	B	300	NAD	C4A-N3A	2.35	1.39	1.35
2	A	300	NAD	C2A-N3A	2.37	1.36	1.32
2	F	300	NAD	C2A-N3A	2.43	1.36	1.32
2	G	300	NAD	C2N-C3N	2.46	1.42	1.39
2	B	300	NAD	C2N-C3N	2.47	1.42	1.39
2	E	300	NAD	C4N-C3N	2.57	1.43	1.39
2	F	300	NAD	C6A-N6A	2.58	1.44	1.34
2	F	300	NAD	C5N-C4N	2.60	1.43	1.38
2	E	300	NAD	C4A-N3A	2.63	1.39	1.35
2	B	300	NAD	C4N-C3N	2.66	1.43	1.39
2	D	300	NAD	C4A-N3A	2.68	1.39	1.35
2	H	300	NAD	C4N-C3N	2.80	1.43	1.39
2	A	300	NAD	O4D-C1D	2.83	1.45	1.41
2	E	300	NAD	C2N-C3N	2.85	1.43	1.39
2	F	300	NAD	C7N-N7N	2.89	1.38	1.33
2	A	300	NAD	C4N-C3N	2.90	1.44	1.39
2	G	300	NAD	C6N-C5N	2.92	1.45	1.38
2	D	300	NAD	C6N-C5N	2.93	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	C6N-C5N	2.96	1.45	1.38
2	F	300	NAD	C2N-C3N	2.97	1.43	1.39
2	G	300	NAD	C4A-N3A	2.98	1.39	1.35
2	D	300	NAD	C4N-C3N	3.01	1.44	1.39
2	E	300	NAD	C2A-N3A	3.09	1.37	1.32
2	C	300	NAD	C2A-N1A	3.16	1.39	1.33
2	B	300	NAD	C2A-N3A	3.19	1.37	1.32
2	G	300	NAD	O4B-C1B	3.19	1.45	1.41
2	G	300	NAD	C5N-C4N	3.23	1.45	1.38
2	C	300	NAD	C4N-C3N	3.28	1.44	1.39
2	C	300	NAD	C4A-N3A	3.29	1.40	1.35
2	B	300	NAD	C6N-C5N	3.29	1.45	1.38
2	H	300	NAD	C6N-C5N	3.34	1.46	1.38
2	B	300	NAD	C5N-C4N	3.35	1.45	1.38
2	G	300	NAD	C4N-C3N	3.50	1.45	1.39
2	E	300	NAD	C6N-C5N	3.59	1.46	1.38
2	H	300	NAD	C5N-C4N	3.62	1.45	1.38
2	B	300	NAD	O4B-C1B	3.77	1.46	1.41
2	F	300	NAD	O4B-C1B	3.94	1.46	1.41
2	B	300	NAD	C7N-N7N	3.96	1.40	1.33
2	A	300	NAD	C7N-N7N	4.02	1.40	1.33
2	A	300	NAD	C2A-N1A	4.11	1.41	1.33
2	C	300	NAD	C7N-N7N	4.18	1.41	1.33
2	F	300	NAD	C2A-N1A	4.20	1.41	1.33
2	H	300	NAD	C2A-N1A	4.20	1.41	1.33
2	F	300	NAD	C4N-C3N	4.39	1.46	1.39
2	G	300	NAD	C7N-N7N	4.48	1.41	1.33
2	C	300	NAD	O4B-C1B	4.55	1.47	1.41
2	A	300	NAD	O4B-C1B	4.62	1.47	1.41
2	D	300	NAD	C7N-N7N	4.63	1.42	1.33
2	H	300	NAD	C7N-N7N	4.70	1.42	1.33
2	B	300	NAD	C2A-N1A	4.72	1.42	1.33
2	G	300	NAD	C2A-N1A	4.80	1.42	1.33
2	E	300	NAD	C2A-N1A	4.83	1.43	1.33
2	D	300	NAD	C2A-N1A	4.90	1.43	1.33
2	H	300	NAD	O4B-C1B	5.38	1.48	1.41
2	E	300	NAD	O4B-C1B	5.43	1.48	1.41
2	E	300	NAD	C7N-N7N	5.56	1.43	1.33
2	D	300	NAD	O4B-C1B	5.81	1.49	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	NAD	N3A-C2A-N1A	-9.18	120.86	128.86
2	E	300	NAD	N3A-C2A-N1A	-8.44	121.50	128.86
2	C	300	NAD	N3A-C2A-N1A	-7.81	122.06	128.86
2	H	300	NAD	N3A-C2A-N1A	-7.41	122.40	128.86
2	D	300	NAD	C4D-O4D-C1D	-7.38	101.91	109.77
2	F	300	NAD	N3A-C2A-N1A	-6.77	122.96	128.86
2	D	300	NAD	N3A-C2A-N1A	-6.26	123.41	128.86
2	G	300	NAD	C4D-O4D-C1D	-6.06	103.32	109.77
2	G	300	NAD	N3A-C2A-N1A	-5.87	123.74	128.86
2	A	300	NAD	N3A-C2A-N1A	-4.88	124.61	128.86
2	H	300	NAD	C4D-O4D-C1D	-4.64	104.83	109.77
2	B	300	NAD	C4D-O4D-C1D	-4.62	104.85	109.77
2	C	300	NAD	C5N-C4N-C3N	-4.36	115.22	120.35
2	H	300	NAD	C5N-C4N-C3N	-3.97	115.68	120.35
2	G	300	NAD	C5N-C4N-C3N	-3.93	115.72	120.35
2	A	300	NAD	C5N-C4N-C3N	-3.86	115.81	120.35
2	B	300	NAD	C5N-C4N-C3N	-3.74	115.95	120.35
2	C	300	NAD	C4D-O4D-C1D	-3.69	105.84	109.77
2	F	300	NAD	C4D-O4D-C1D	-3.49	106.05	109.77
2	A	300	NAD	C3N-C2N-N1N	-3.36	117.05	120.43
2	A	300	NAD	C4B-O4B-C1B	-2.95	106.63	109.77
2	E	300	NAD	C3N-C2N-N1N	-2.63	117.78	120.43
2	F	300	NAD	C5N-C4N-C3N	-2.55	117.35	120.35
2	D	300	NAD	C5N-C4N-C3N	-2.40	117.53	120.35
2	D	300	NAD	C4B-O4B-C1B	-2.12	107.52	109.77
2	A	300	NAD	O4B-C4B-C3B	2.01	109.16	105.17
2	E	300	NAD	C2A-N1A-C6A	2.04	122.35	118.77
2	H	300	NAD	C6N-C5N-C4N	2.10	122.61	119.44
2	C	300	NAD	C5D-C4D-C3D	2.18	123.60	115.29
2	H	300	NAD	O3B-C3B-C2B	2.18	118.83	111.83
2	D	300	NAD	O7N-C7N-C3N	2.20	122.19	119.62
2	E	300	NAD	N6A-C6A-N1A	2.25	123.23	118.77
2	F	300	NAD	O2B-C2B-C3B	2.30	119.21	111.83
2	F	300	NAD	C2N-C3N-C4N	2.31	120.89	118.26
2	A	300	NAD	O3B-C3B-C4B	2.49	118.37	111.09
2	C	300	NAD	O2B-C2B-C3B	2.62	120.22	111.83
2	G	300	NAD	O2B-C2B-C3B	2.64	120.27	111.83
2	C	300	NAD	O3B-C3B-C4B	2.64	118.79	111.09
2	D	300	NAD	O4B-C4B-C3B	2.64	110.42	105.17
2	B	300	NAD	O3B-C3B-C4B	2.68	118.92	111.09
2	D	300	NAD	O2B-C2B-C3B	2.74	120.62	111.83
2	E	300	NAD	O3B-C3B-C4B	2.83	119.34	111.09
2	G	300	NAD	O3B-C3B-C4B	2.83	119.37	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	NAD	O2B-C2B-C3B	2.85	120.95	111.83
2	B	300	NAD	O2B-C2B-C3B	2.92	121.19	111.83
2	D	300	NAD	O3B-C3B-C4B	2.97	119.76	111.09
2	H	300	NAD	C2N-C3N-C4N	3.07	121.76	118.26
2	A	300	NAD	O2B-C2B-C3B	3.13	121.85	111.83
2	E	300	NAD	C2N-C3N-C4N	3.21	121.92	118.26
2	G	300	NAD	C2N-C3N-C4N	3.32	122.05	118.26
2	D	300	NAD	C2N-C3N-C4N	3.45	122.20	118.26
2	B	300	NAD	C2N-C3N-C4N	3.57	122.34	118.26
2	H	300	NAD	O3B-C3B-C4B	3.68	121.82	111.09
2	C	300	NAD	C2N-C3N-C4N	3.92	122.73	118.26
2	E	300	NAD	O2B-C2B-C3B	3.94	124.44	111.83
2	A	300	NAD	C2N-C3N-C4N	5.10	124.08	118.26

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	301	MPD	C4
3	E	302	MPD	C4

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	300	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	268/278 (96%)	-0.20	8 (2%)	51	57	6, 11, 24, 45	0
1	B	257/278 (92%)	-0.09	11 (4%)	36	41	6, 14, 27, 48	0
1	C	257/278 (92%)	-0.16	7 (2%)	55	61	7, 13, 23, 42	0
1	D	269/278 (96%)	-0.18	8 (2%)	51	57	6, 13, 26, 47	0
1	E	256/278 (92%)	0.02	10 (3%)	40	45	7, 18, 32, 46	0
1	F	274/278 (98%)	-0.19	10 (3%)	43	49	7, 12, 23, 45	0
1	G	267/278 (96%)	-0.23	7 (2%)	56	62	6, 11, 24, 40	0
1	H	249/278 (89%)	-0.23	2 (0%)	86	88	7, 15, 25, 41	0
All	All	2097/2224 (94%)	-0.16	63 (3%)	51	57	6, 13, 27, 48	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	LEU	8.0
1	E	219	TRP	6.6
1	B	234	GLY	6.5
1	C	220	LEU	6.4
1	B	219	TRP	6.3
1	F	229	THR	6.2
1	F	228	ASP	5.9
1	F	230	PRO	5.6
1	D	228	ASP	5.6
1	C	219	TRP	5.5
1	G	232	ALA	5.5
1	A	228	ASP	5.3
1	G	231	GLY	5.0
1	E	234	GLY	4.9
1	A	231	GLY	4.8
1	G	226	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	4	SER	4.5
1	A	232	ALA	4.3
1	C	234	GLY	4.2
1	G	227	THR	3.9
1	F	3	ARG	3.9
1	A	226	ALA	3.8
1	E	238	PRO	3.8
1	G	219	TRP	3.8
1	D	229	THR	3.6
1	H	219	TRP	3.6
1	D	232	ALA	3.5
1	E	236	ALA	3.5
1	F	232	ALA	3.5
1	F	5	SER	3.5
1	F	231	GLY	3.4
1	B	238	PRO	3.3
1	H	240	GLU	3.3
1	A	233	MET	3.3
1	B	239	VAL	3.2
1	F	226	ALA	3.1
1	D	231	GLY	3.0
1	D	227	THR	2.9
1	F	227	THR	2.8
1	E	217	ARG	2.8
1	D	225	ALA	2.7
1	E	8	PRO	2.7
1	C	218	GLU	2.7
1	E	239	VAL	2.6
1	B	276	LYS	2.6
1	G	233	MET	2.6
1	E	276	LYS	2.6
1	A	219	TRP	2.5
1	E	212	ASN	2.5
1	G	224	ALA	2.4
1	D	10	THR	2.4
1	B	235	ASN	2.3
1	C	238	PRO	2.2
1	C	236	ALA	2.2
1	A	227	THR	2.1
1	E	216	THR	2.1
1	B	241	VAL	2.1
1	B	236	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	226	ALA	2.1
1	B	240	GLU	2.1
1	B	217	ARG	2.0
1	A	215	PHE	2.0
1	C	239	VAL	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
3	MPD	H	301	8/8	0.94	0.10	3.10	19,25,26,27	0
3	MPD	B	301	8/8	0.93	0.10	2.15	18,24,27,27	0
3	MPD	D	302	8/8	0.93	0.10	1.86	13,16,17,19	0
3	MPD	E	302	8/8	0.83	0.14	1.41	15,23,25,27	0
3	MPD	F	302	8/8	0.93	0.09	1.07	14,15,17,19	0
2	NAD	H	300	44/44	0.98	0.07	-0.35	7,10,12,14	0
2	NAD	B	300	44/44	0.99	0.07	-0.37	7,10,12,12	0
2	NAD	A	300	44/44	0.99	0.06	-0.67	5,7,8,10	0
2	NAD	E	300	44/44	0.98	0.06	-0.72	12,14,18,20	0
2	NAD	G	300	44/44	0.98	0.06	-0.82	6,8,9,9	0
2	NAD	F	300	44/44	0.98	0.06	-0.92	5,7,9,9	0
2	NAD	C	300	44/44	0.99	0.06	-1.21	8,9,12,13	0
2	NAD	D	300	44/44	0.99	0.06	-1.24	6,9,11,12	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.