



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 07:47 pm BST

PDB ID : 4NMJ  
Title : Thermostable aldehyde dehydrogenase from *Pyrobaculum* sp. complexed with NADP<sup>+</sup> at 2 Å resolution  
Authors : Petrova, T.; Boyko, K.M.; Bezsudnova, E.Y.; Mardanov, A.V.; Gumerov, V.M.; Ravin, N.V.; Popov, V.O.  
Deposited on : 2013-11-15  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

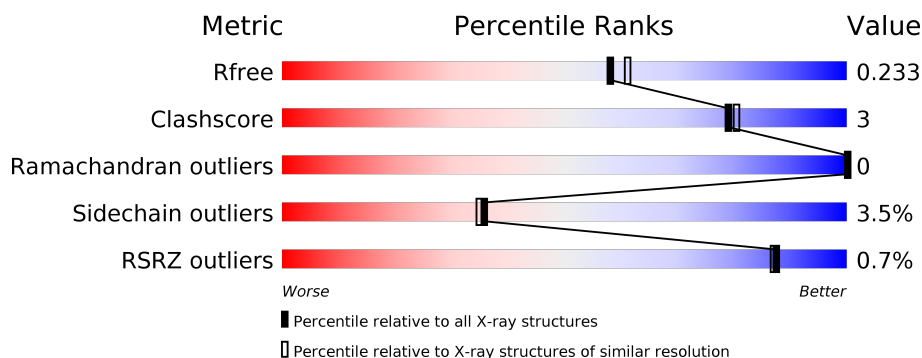
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 respectively. 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	491	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
1	B	491	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>90% 8% ..</div>
1	C	491	<div> <div style="width: 89%;"></div> <div style="width: 9%;"></div> <div style="width: 2%;"></div> </div> <div>89% 9% ..</div>
1	D	491	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div> <div>88% 10% .</div>
1	E	491	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
1	F	491	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9%</div>

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Mol	Chain	Length	Quality of chain
1	G	491	<div><div>%</div><div><div></div></div><div>90%</div><div>9%</div><div></div></div>
1	H	491	<div><div>%</div><div><div></div></div><div>90%</div><div>8%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33717 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	2	0
			3797	2421	661	703	12			
1	B	485	Total	C	N	O	S	0	2	0
			3784	2408	662	702	12			
1	C	484	Total	C	N	O	S	0	2	0
			3779	2408	659	701	11			
1	D	483	Total	C	N	O	S	0	2	0
			3767	2398	660	698	11			
1	E	485	Total	C	N	O	S	0	2	0
			3779	2408	657	702	12			
1	F	489	Total	C	N	O	S	0	2	0
			3825	2436	668	709	12			
1	G	484	Total	C	N	O	S	0	2	0
			3777	2407	657	701	12			
1	H	484	Total	C	N	O	S	0	2	0
			3771	2402	659	699	11			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	1
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	1
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	428	Total	O	0	1
			428	428		
3	B	378	Total	O	0	1
			378	378		
3	C	411	Total	O	0	2
			411	411		
3	D	357	Total	O	0	1
			357	357		

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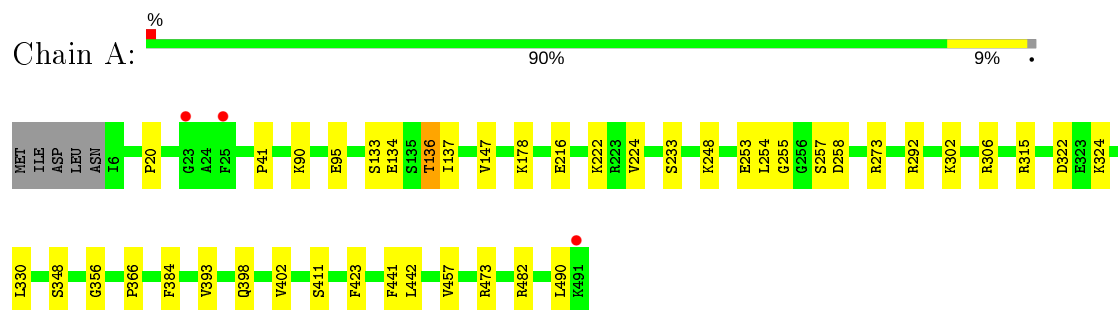
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	323	Total 323	O 323	0	1
3	F	375	Total 375	O 375	0	1
3	G	360	Total 360	O 360	0	1
3	H	422	Total 422	O 422	0	1

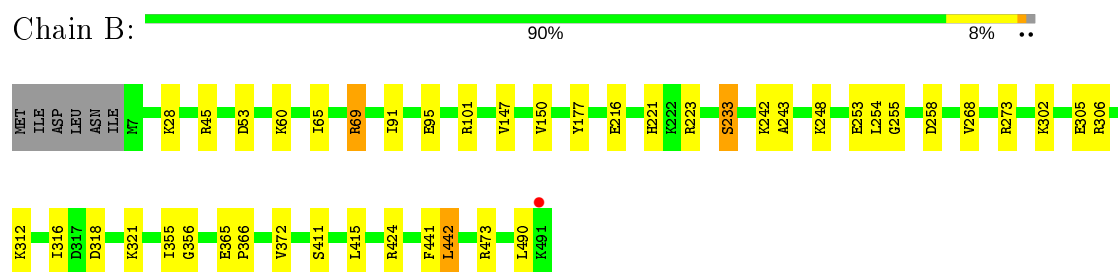
### 3 Residue-property plots [i](#)

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.

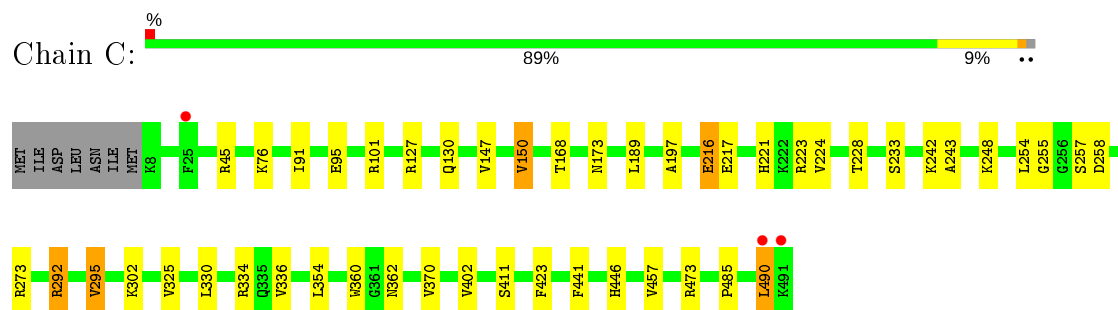
- Molecule 1: Aldehyde dehydrogenase



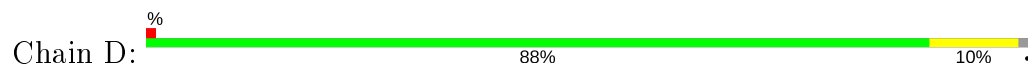
- Molecule 1: Aldehyde dehydrogenase

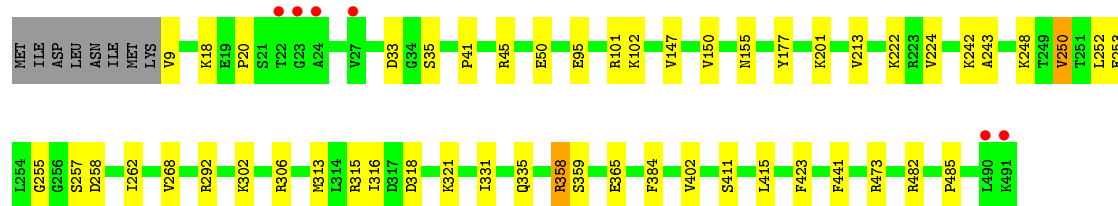


- Molecule 1: Aldehyde dehydrogenase

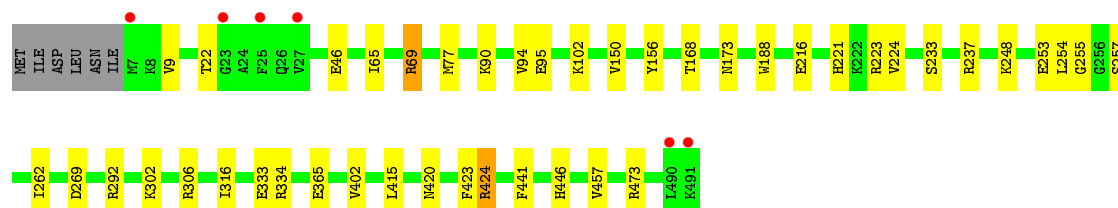
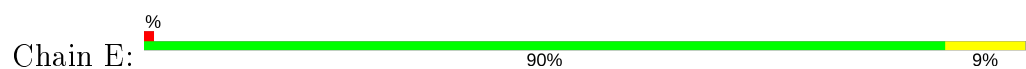


- Molecule 1: Aldehyde dehydrogenase

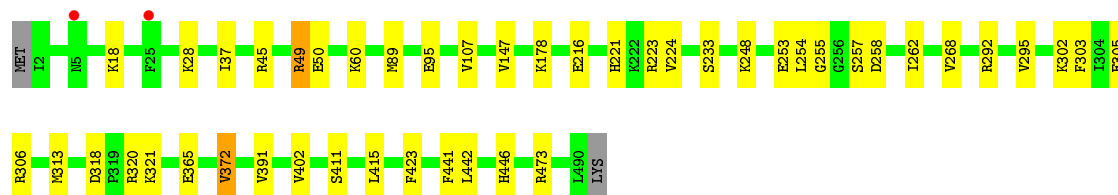




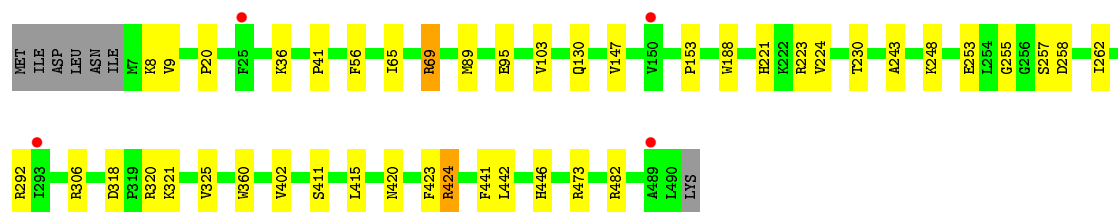
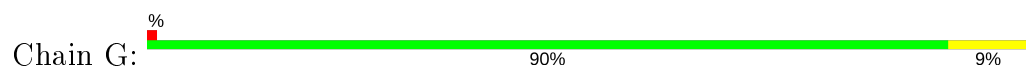
• Molecule 1: Aldehyde dehydrogenase



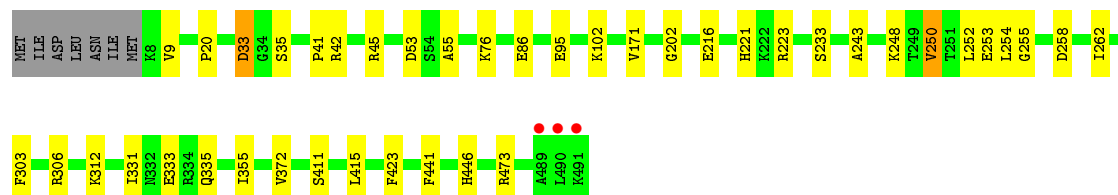
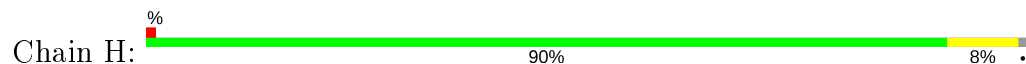
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.48Å 184.39Å 207.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.09 – 2.00 28.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.09-2.00) 99.4 (28.09-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.201 , 0.233 0.201 , 0.233	Depositor DCC
$R_{free}$ test set	21029 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3933e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NAP

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	0.39	0/3876	0.53	0/5253
1	B	0.39	0/3862	0.53	0/5235
1	C	0.39	0/3858	0.54	2/5230 (0.0%)
1	D	0.38	0/3845	0.52	0/5213
1	E	0.37	0/3858	0.52	0/5232
1	F	0.40	0/3904	0.53	0/5291
1	G	0.38	0/3856	0.52	0/5228
1	H	0.40	0/3849	0.53	0/5218
All	All	0.39	0/30908	0.53	2/41900 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	VAL	CB-CA-C	-5.94	100.12	111.40
1	C	292	ARG	NE-CZ-NH2	-5.04	117.78	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	3797	0	3801	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3784	0	3781	23	0
1	C	3779	0	3777	24	0
1	D	3767	0	3766	27	0
1	E	3779	0	3761	18	0
1	F	3825	0	3829	24	0
1	G	3777	0	3768	20	0
1	H	3771	0	3770	20	0
2	A	48	0	13	2	0
2	B	48	0	13	1	0
2	C	48	0	13	1	0
2	D	48	0	13	3	0
2	E	48	0	13	1	0
2	F	48	0	13	1	0
2	G	48	0	13	1	0
2	H	48	0	13	1	0
3	A	428	0	0	0	0
3	B	378	0	0	3	0
3	C	411	0	0	2	0
3	D	357	0	0	3	0
3	E	323	0	0	1	0
3	F	375	0	0	2	0
3	G	360	0	0	2	0
3	H	422	0	0	1	0
All	All	33717	0	30357	168	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 3.

The worst 5 of 168 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:F:255:GLY:H	2:F:500[C]:NAP:H71N	1.22	0.83
1:B:255:GLY:H	2:B:500[C]:NAP:H71N	1.26	0.80
1:B:316:ILE:HD12	1:B:365:GLU:HG2	1.64	0.79
1:A:255:GLY:H	2:A:500[C]:NAP:H71N	1.31	0.78
1:E:255:GLY:H	2:E:500[C]:NAP:H71N	1.30	0.77

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	486/491 (99%)	476 (98%)	10 (2%)	0	100	100
1	B	485/491 (99%)	474 (98%)	11 (2%)	0	100	100
1	C	484/491 (99%)	468 (97%)	16 (3%)	0	100	100
1	D	483/491 (98%)	474 (98%)	9 (2%)	0	100	100
1	E	485/491 (99%)	473 (98%)	12 (2%)	0	100	100
1	F	489/491 (100%)	479 (98%)	10 (2%)	0	100	100
1	G	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
1	H	484/491 (99%)	471 (97%)	13 (3%)	0	100	100
All	All	3880/3928 (99%)	3786 (98%)	94 (2%)	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	402/408 (98%)	385 (96%)	17 (4%)	30	27
1	B	400/408 (98%)	387 (97%)	13 (3%)	38	37
1	C	400/408 (98%)	386 (96%)	14 (4%)	36	35
1	D	398/408 (98%)	383 (96%)	15 (4%)	33	31
1	E	398/408 (98%)	382 (96%)	16 (4%)	31	29
1	F	406/408 (100%)	394 (97%)	12 (3%)	41	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	399/408 (98%)	383 (96%)	16 (4%)	31	29
1	H	398/408 (98%)	383 (96%)	15 (4%)	33	31
All	All	3201/3264 (98%)	3083 (96%)	118 (4%)	36	32

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	253[B]	GLU
1	E	253[B]	GLU
1	H	171	VAL
1	D	306	ARG
1	E	22	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	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](#)

8 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	486/491 (98%)	-0.51	3 (0%) 89 88	7, 16, 32, 59	0
1	B	485/491 (98%)	-0.44	1 (0%) 95 94	7, 17, 36, 57	0
1	C	484/491 (98%)	-0.41	3 (0%) 89 88	8, 18, 33, 68	0
1	D	483/491 (98%)	-0.38	6 (1%) 79 78	8, 19, 39, 68	0
1	E	485/491 (98%)	-0.40	6 (1%) 79 78	7, 19, 37, 59	0
1	F	489/491 (99%)	-0.46	2 (0%) 92 92	7, 17, 34, 54	0
1	G	484/491 (98%)	-0.46	4 (0%) 86 85	7, 18, 33, 46	0
1	H	484/491 (98%)	-0.38	3 (0%) 89 88	7, 16, 36, 71	0
All	All	3880/3928 (98%)	-0.43	28 (0%) 87 87	7, 17, 36, 71	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	491	LYS	7.8
1	C	491	LYS	6.7
1	D	491	LYS	6.6
1	B	491	LYS	5.7
1	E	491	LYS	4.5

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	E	500[C]	48/48	0.91	0.14	18,29,37,40	21
2	NAP	D	500[C]	48/48	0.91	0.15	16,27,33,38	21
2	NAP	B	500[C]	48/48	0.93	0.13	15,23,28,33	21
2	NAP	C	500[C]	48/48	0.94	0.11	16,23,32,36	17
2	NAP	G	500[C]	48/48	0.94	0.11	16,23,30,34	17
2	NAP	F	500[C]	48/48	0.95	0.11	16,24,30,32	17
2	NAP	A	500[C]	48/48	0.95	0.11	14,22,28,34	17
2	NAP	H	500[C]	48/48	0.95	0.11	13,23,31,37	17

## 6.5 Other polymers [i](#)

There are no such residues in this entry.