



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 08:37 PM EST

PDB ID : 5JFL  
Title : Crystal structure of Rhodopseudomonas palustris propionaldehyde dehydrogenase with bound NAD<sup>+</sup>  
Authors : Zarzycki, J.; Sutter, M.; Kerfeld, C.A.  
Deposited on : 2016-04-19  
Resolution : 2.30 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

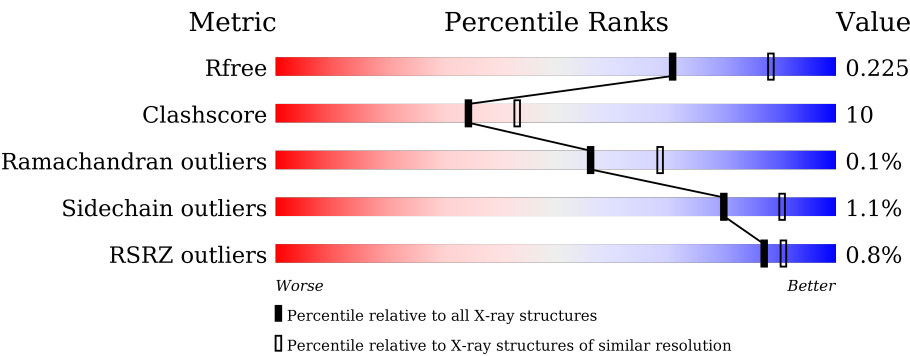
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	524	<div><div></div><div>72%12%16%</div></div>
1	B	524	<div><div></div><div>66%17%•16%</div></div>
1	C	524	<div><div>%</div><div>65%18%•16%</div></div>
1	D	524	<div><div></div><div>68%17%15%</div></div>
1	E	524	<div><div></div><div>63%21%16%</div></div>
1	F	524	<div><div>%</div><div>64%19%•16%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	524	<div><div></div><div>68%17%15%</div></div>
1	H	524	<div><div>3%</div><div>60%22%16%</div></div>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 27656 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	440	Total	C	N	O	S	0	0	0
			3291	2072	567	630	22			
1	B	439	Total	C	N	O	S	0	1	0
			3294	2077	566	629	22			
1	C	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	D	445	Total	C	N	O	S	0	0	0
			3326	2092	573	639	22			
1	E	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	F	440	Total	C	N	O	S	0	0	0
			3291	2072	567	630	22			
1	G	445	Total	C	N	O	S	0	0	0
			3326	2092	573	639	22			
1	H	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q21A49
A	2	ALA	-	expression tag	UNP Q21A49
A	3	TRP	-	expression tag	UNP Q21A49
A	4	SER	-	expression tag	UNP Q21A49
A	5	HIS	-	expression tag	UNP Q21A49
A	6	PRO	-	expression tag	UNP Q21A49
A	7	GLN	-	expression tag	UNP Q21A49
A	8	PHE	-	expression tag	UNP Q21A49
A	9	GLU	-	expression tag	UNP Q21A49
A	10	LYS	-	expression tag	UNP Q21A49
A	11	GLY	-	expression tag	UNP Q21A49
A	12	HIS	-	expression tag	UNP Q21A49
A	13	MET	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASN	-	expression tag	UNP Q21A49
A	15	ASP	-	expression tag	UNP Q21A49
A	16	ALA	-	expression tag	UNP Q21A49
A	17	ASN	-	expression tag	UNP Q21A49
A	18	ILE	-	expression tag	UNP Q21A49
A	19	ALA	-	expression tag	UNP Q21A49
A	20	ASP	-	expression tag	UNP Q21A49
A	21	VAL	-	expression tag	UNP Q21A49
A	22	VAL	-	expression tag	UNP Q21A49
A	23	THR	-	expression tag	UNP Q21A49
A	24	LYS	-	expression tag	UNP Q21A49
A	25	VAL	-	expression tag	UNP Q21A49
A	26	LEU	-	expression tag	UNP Q21A49
A	27	GLY	-	expression tag	UNP Q21A49
A	28	GLU	-	expression tag	UNP Q21A49
A	29	TYR	-	expression tag	UNP Q21A49
A	30	GLY	-	expression tag	UNP Q21A49
A	31	ALA	-	expression tag	UNP Q21A49
A	32	PRO	-	expression tag	UNP Q21A49
A	33	GLY	-	expression tag	UNP Q21A49
A	34	ALA	-	expression tag	UNP Q21A49
A	35	VAL	-	expression tag	UNP Q21A49
A	36	SER	-	expression tag	UNP Q21A49
A	37	VAL	-	expression tag	UNP Q21A49
A	38	ALA	-	expression tag	UNP Q21A49
A	39	ALA	-	expression tag	UNP Q21A49
A	40	LEU	-	expression tag	UNP Q21A49
A	41	THR	-	expression tag	UNP Q21A49
A	42	ALA	-	expression tag	UNP Q21A49
A	43	LYS	-	expression tag	UNP Q21A49
A	44	SER	-	expression tag	UNP Q21A49
A	45	PRO	-	expression tag	UNP Q21A49
A	46	ASP	-	expression tag	UNP Q21A49
A	47	GLY	-	expression tag	UNP Q21A49
A	48	LYS	-	expression tag	UNP Q21A49
A	49	SER	-	expression tag	UNP Q21A49
A	50	ASN	-	expression tag	UNP Q21A49
A	51	SER	-	expression tag	UNP Q21A49
A	52	SER	-	expression tag	UNP Q21A49
A	53	ALA	-	expression tag	UNP Q21A49
A	54	ASP	-	expression tag	UNP Q21A49
A	55	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ASP	-	expression tag	UNP Q21A49
A	57	VAL	-	expression tag	UNP Q21A49
A	58	VAL	-	expression tag	UNP Q21A49
A	59	ALA	-	expression tag	UNP Q21A49
A	60	ARG	-	expression tag	UNP Q21A49
B	1	MET	-	initiating methionine	UNP Q21A49
B	2	ALA	-	expression tag	UNP Q21A49
B	3	TRP	-	expression tag	UNP Q21A49
B	4	SER	-	expression tag	UNP Q21A49
B	5	HIS	-	expression tag	UNP Q21A49
B	6	PRO	-	expression tag	UNP Q21A49
B	7	GLN	-	expression tag	UNP Q21A49
B	8	PHE	-	expression tag	UNP Q21A49
B	9	GLU	-	expression tag	UNP Q21A49
B	10	LYS	-	expression tag	UNP Q21A49
B	11	GLY	-	expression tag	UNP Q21A49
B	12	HIS	-	expression tag	UNP Q21A49
B	13	MET	-	expression tag	UNP Q21A49
B	14	ASN	-	expression tag	UNP Q21A49
B	15	ASP	-	expression tag	UNP Q21A49
B	16	ALA	-	expression tag	UNP Q21A49
B	17	ASN	-	expression tag	UNP Q21A49
B	18	ILE	-	expression tag	UNP Q21A49
B	19	ALA	-	expression tag	UNP Q21A49
B	20	ASP	-	expression tag	UNP Q21A49
B	21	VAL	-	expression tag	UNP Q21A49
B	22	VAL	-	expression tag	UNP Q21A49
B	23	THR	-	expression tag	UNP Q21A49
B	24	LYS	-	expression tag	UNP Q21A49
B	25	VAL	-	expression tag	UNP Q21A49
B	26	LEU	-	expression tag	UNP Q21A49
B	27	GLY	-	expression tag	UNP Q21A49
B	28	GLU	-	expression tag	UNP Q21A49
B	29	TYR	-	expression tag	UNP Q21A49
B	30	GLY	-	expression tag	UNP Q21A49
B	31	ALA	-	expression tag	UNP Q21A49
B	32	PRO	-	expression tag	UNP Q21A49
B	33	GLY	-	expression tag	UNP Q21A49
B	34	ALA	-	expression tag	UNP Q21A49
B	35	VAL	-	expression tag	UNP Q21A49
B	36	SER	-	expression tag	UNP Q21A49
B	37	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	ALA	-	expression tag	UNP Q21A49
B	39	ALA	-	expression tag	UNP Q21A49
B	40	LEU	-	expression tag	UNP Q21A49
B	41	THR	-	expression tag	UNP Q21A49
B	42	ALA	-	expression tag	UNP Q21A49
B	43	LYS	-	expression tag	UNP Q21A49
B	44	SER	-	expression tag	UNP Q21A49
B	45	PRO	-	expression tag	UNP Q21A49
B	46	ASP	-	expression tag	UNP Q21A49
B	47	GLY	-	expression tag	UNP Q21A49
B	48	LYS	-	expression tag	UNP Q21A49
B	49	SER	-	expression tag	UNP Q21A49
B	50	ASN	-	expression tag	UNP Q21A49
B	51	SER	-	expression tag	UNP Q21A49
B	52	SER	-	expression tag	UNP Q21A49
B	53	ALA	-	expression tag	UNP Q21A49
B	54	ASP	-	expression tag	UNP Q21A49
B	55	ALA	-	expression tag	UNP Q21A49
B	56	ASP	-	expression tag	UNP Q21A49
B	57	VAL	-	expression tag	UNP Q21A49
B	58	VAL	-	expression tag	UNP Q21A49
B	59	ALA	-	expression tag	UNP Q21A49
B	60	ARG	-	expression tag	UNP Q21A49
C	1	MET	-	initiating methionine	UNP Q21A49
C	2	ALA	-	expression tag	UNP Q21A49
C	3	TRP	-	expression tag	UNP Q21A49
C	4	SER	-	expression tag	UNP Q21A49
C	5	HIS	-	expression tag	UNP Q21A49
C	6	PRO	-	expression tag	UNP Q21A49
C	7	GLN	-	expression tag	UNP Q21A49
C	8	PHE	-	expression tag	UNP Q21A49
C	9	GLU	-	expression tag	UNP Q21A49
C	10	LYS	-	expression tag	UNP Q21A49
C	11	GLY	-	expression tag	UNP Q21A49
C	12	HIS	-	expression tag	UNP Q21A49
C	13	MET	-	expression tag	UNP Q21A49
C	14	ASN	-	expression tag	UNP Q21A49
C	15	ASP	-	expression tag	UNP Q21A49
C	16	ALA	-	expression tag	UNP Q21A49
C	17	ASN	-	expression tag	UNP Q21A49
C	18	ILE	-	expression tag	UNP Q21A49
C	19	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ASP	-	expression tag	UNP Q21A49
C	21	VAL	-	expression tag	UNP Q21A49
C	22	VAL	-	expression tag	UNP Q21A49
C	23	THR	-	expression tag	UNP Q21A49
C	24	LYS	-	expression tag	UNP Q21A49
C	25	VAL	-	expression tag	UNP Q21A49
C	26	LEU	-	expression tag	UNP Q21A49
C	27	GLY	-	expression tag	UNP Q21A49
C	28	GLU	-	expression tag	UNP Q21A49
C	29	TYR	-	expression tag	UNP Q21A49
C	30	GLY	-	expression tag	UNP Q21A49
C	31	ALA	-	expression tag	UNP Q21A49
C	32	PRO	-	expression tag	UNP Q21A49
C	33	GLY	-	expression tag	UNP Q21A49
C	34	ALA	-	expression tag	UNP Q21A49
C	35	VAL	-	expression tag	UNP Q21A49
C	36	SER	-	expression tag	UNP Q21A49
C	37	VAL	-	expression tag	UNP Q21A49
C	38	ALA	-	expression tag	UNP Q21A49
C	39	ALA	-	expression tag	UNP Q21A49
C	40	LEU	-	expression tag	UNP Q21A49
C	41	THR	-	expression tag	UNP Q21A49
C	42	ALA	-	expression tag	UNP Q21A49
C	43	LYS	-	expression tag	UNP Q21A49
C	44	SER	-	expression tag	UNP Q21A49
C	45	PRO	-	expression tag	UNP Q21A49
C	46	ASP	-	expression tag	UNP Q21A49
C	47	GLY	-	expression tag	UNP Q21A49
C	48	LYS	-	expression tag	UNP Q21A49
C	49	SER	-	expression tag	UNP Q21A49
C	50	ASN	-	expression tag	UNP Q21A49
C	51	SER	-	expression tag	UNP Q21A49
C	52	SER	-	expression tag	UNP Q21A49
C	53	ALA	-	expression tag	UNP Q21A49
C	54	ASP	-	expression tag	UNP Q21A49
C	55	ALA	-	expression tag	UNP Q21A49
C	56	ASP	-	expression tag	UNP Q21A49
C	57	VAL	-	expression tag	UNP Q21A49
C	58	VAL	-	expression tag	UNP Q21A49
C	59	ALA	-	expression tag	UNP Q21A49
C	60	ARG	-	expression tag	UNP Q21A49
D	1	MET	-	initiating methionine	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP Q21A49
D	3	TRP	-	expression tag	UNP Q21A49
D	4	SER	-	expression tag	UNP Q21A49
D	5	HIS	-	expression tag	UNP Q21A49
D	6	PRO	-	expression tag	UNP Q21A49
D	7	GLN	-	expression tag	UNP Q21A49
D	8	PHE	-	expression tag	UNP Q21A49
D	9	GLU	-	expression tag	UNP Q21A49
D	10	LYS	-	expression tag	UNP Q21A49
D	11	GLY	-	expression tag	UNP Q21A49
D	12	HIS	-	expression tag	UNP Q21A49
D	13	MET	-	expression tag	UNP Q21A49
D	14	ASN	-	expression tag	UNP Q21A49
D	15	ASP	-	expression tag	UNP Q21A49
D	16	ALA	-	expression tag	UNP Q21A49
D	17	ASN	-	expression tag	UNP Q21A49
D	18	ILE	-	expression tag	UNP Q21A49
D	19	ALA	-	expression tag	UNP Q21A49
D	20	ASP	-	expression tag	UNP Q21A49
D	21	VAL	-	expression tag	UNP Q21A49
D	22	VAL	-	expression tag	UNP Q21A49
D	23	THR	-	expression tag	UNP Q21A49
D	24	LYS	-	expression tag	UNP Q21A49
D	25	VAL	-	expression tag	UNP Q21A49
D	26	LEU	-	expression tag	UNP Q21A49
D	27	GLY	-	expression tag	UNP Q21A49
D	28	GLU	-	expression tag	UNP Q21A49
D	29	TYR	-	expression tag	UNP Q21A49
D	30	GLY	-	expression tag	UNP Q21A49
D	31	ALA	-	expression tag	UNP Q21A49
D	32	PRO	-	expression tag	UNP Q21A49
D	33	GLY	-	expression tag	UNP Q21A49
D	34	ALA	-	expression tag	UNP Q21A49
D	35	VAL	-	expression tag	UNP Q21A49
D	36	SER	-	expression tag	UNP Q21A49
D	37	VAL	-	expression tag	UNP Q21A49
D	38	ALA	-	expression tag	UNP Q21A49
D	39	ALA	-	expression tag	UNP Q21A49
D	40	LEU	-	expression tag	UNP Q21A49
D	41	THR	-	expression tag	UNP Q21A49
D	42	ALA	-	expression tag	UNP Q21A49
D	43	LYS	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	44	SER	-	expression tag	UNP Q21A49
D	45	PRO	-	expression tag	UNP Q21A49
D	46	ASP	-	expression tag	UNP Q21A49
D	47	GLY	-	expression tag	UNP Q21A49
D	48	LYS	-	expression tag	UNP Q21A49
D	49	SER	-	expression tag	UNP Q21A49
D	50	ASN	-	expression tag	UNP Q21A49
D	51	SER	-	expression tag	UNP Q21A49
D	52	SER	-	expression tag	UNP Q21A49
D	53	ALA	-	expression tag	UNP Q21A49
D	54	ASP	-	expression tag	UNP Q21A49
D	55	ALA	-	expression tag	UNP Q21A49
D	56	ASP	-	expression tag	UNP Q21A49
D	57	VAL	-	expression tag	UNP Q21A49
D	58	VAL	-	expression tag	UNP Q21A49
D	59	ALA	-	expression tag	UNP Q21A49
D	60	ARG	-	expression tag	UNP Q21A49
E	1	MET	-	initiating methionine	UNP Q21A49
E	2	ALA	-	expression tag	UNP Q21A49
E	3	TRP	-	expression tag	UNP Q21A49
E	4	SER	-	expression tag	UNP Q21A49
E	5	HIS	-	expression tag	UNP Q21A49
E	6	PRO	-	expression tag	UNP Q21A49
E	7	GLN	-	expression tag	UNP Q21A49
E	8	PHE	-	expression tag	UNP Q21A49
E	9	GLU	-	expression tag	UNP Q21A49
E	10	LYS	-	expression tag	UNP Q21A49
E	11	GLY	-	expression tag	UNP Q21A49
E	12	HIS	-	expression tag	UNP Q21A49
E	13	MET	-	expression tag	UNP Q21A49
E	14	ASN	-	expression tag	UNP Q21A49
E	15	ASP	-	expression tag	UNP Q21A49
E	16	ALA	-	expression tag	UNP Q21A49
E	17	ASN	-	expression tag	UNP Q21A49
E	18	ILE	-	expression tag	UNP Q21A49
E	19	ALA	-	expression tag	UNP Q21A49
E	20	ASP	-	expression tag	UNP Q21A49
E	21	VAL	-	expression tag	UNP Q21A49
E	22	VAL	-	expression tag	UNP Q21A49
E	23	THR	-	expression tag	UNP Q21A49
E	24	LYS	-	expression tag	UNP Q21A49
E	25	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
E	26	LEU	-	expression tag	UNP Q21A49
E	27	GLY	-	expression tag	UNP Q21A49
E	28	GLU	-	expression tag	UNP Q21A49
E	29	TYR	-	expression tag	UNP Q21A49
E	30	GLY	-	expression tag	UNP Q21A49
E	31	ALA	-	expression tag	UNP Q21A49
E	32	PRO	-	expression tag	UNP Q21A49
E	33	GLY	-	expression tag	UNP Q21A49
E	34	ALA	-	expression tag	UNP Q21A49
E	35	VAL	-	expression tag	UNP Q21A49
E	36	SER	-	expression tag	UNP Q21A49
E	37	VAL	-	expression tag	UNP Q21A49
E	38	ALA	-	expression tag	UNP Q21A49
E	39	ALA	-	expression tag	UNP Q21A49
E	40	LEU	-	expression tag	UNP Q21A49
E	41	THR	-	expression tag	UNP Q21A49
E	42	ALA	-	expression tag	UNP Q21A49
E	43	LYS	-	expression tag	UNP Q21A49
E	44	SER	-	expression tag	UNP Q21A49
E	45	PRO	-	expression tag	UNP Q21A49
E	46	ASP	-	expression tag	UNP Q21A49
E	47	GLY	-	expression tag	UNP Q21A49
E	48	LYS	-	expression tag	UNP Q21A49
E	49	SER	-	expression tag	UNP Q21A49
E	50	ASN	-	expression tag	UNP Q21A49
E	51	SER	-	expression tag	UNP Q21A49
E	52	SER	-	expression tag	UNP Q21A49
E	53	ALA	-	expression tag	UNP Q21A49
E	54	ASP	-	expression tag	UNP Q21A49
E	55	ALA	-	expression tag	UNP Q21A49
E	56	ASP	-	expression tag	UNP Q21A49
E	57	VAL	-	expression tag	UNP Q21A49
E	58	VAL	-	expression tag	UNP Q21A49
E	59	ALA	-	expression tag	UNP Q21A49
E	60	ARG	-	expression tag	UNP Q21A49
F	1	MET	-	initiating methionine	UNP Q21A49
F	2	ALA	-	expression tag	UNP Q21A49
F	3	TRP	-	expression tag	UNP Q21A49
F	4	SER	-	expression tag	UNP Q21A49
F	5	HIS	-	expression tag	UNP Q21A49
F	6	PRO	-	expression tag	UNP Q21A49
F	7	GLN	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	PHE	-	expression tag	UNP Q21A49
F	9	GLU	-	expression tag	UNP Q21A49
F	10	LYS	-	expression tag	UNP Q21A49
F	11	GLY	-	expression tag	UNP Q21A49
F	12	HIS	-	expression tag	UNP Q21A49
F	13	MET	-	expression tag	UNP Q21A49
F	14	ASN	-	expression tag	UNP Q21A49
F	15	ASP	-	expression tag	UNP Q21A49
F	16	ALA	-	expression tag	UNP Q21A49
F	17	ASN	-	expression tag	UNP Q21A49
F	18	ILE	-	expression tag	UNP Q21A49
F	19	ALA	-	expression tag	UNP Q21A49
F	20	ASP	-	expression tag	UNP Q21A49
F	21	VAL	-	expression tag	UNP Q21A49
F	22	VAL	-	expression tag	UNP Q21A49
F	23	THR	-	expression tag	UNP Q21A49
F	24	LYS	-	expression tag	UNP Q21A49
F	25	VAL	-	expression tag	UNP Q21A49
F	26	LEU	-	expression tag	UNP Q21A49
F	27	GLY	-	expression tag	UNP Q21A49
F	28	GLU	-	expression tag	UNP Q21A49
F	29	TYR	-	expression tag	UNP Q21A49
F	30	GLY	-	expression tag	UNP Q21A49
F	31	ALA	-	expression tag	UNP Q21A49
F	32	PRO	-	expression tag	UNP Q21A49
F	33	GLY	-	expression tag	UNP Q21A49
F	34	ALA	-	expression tag	UNP Q21A49
F	35	VAL	-	expression tag	UNP Q21A49
F	36	SER	-	expression tag	UNP Q21A49
F	37	VAL	-	expression tag	UNP Q21A49
F	38	ALA	-	expression tag	UNP Q21A49
F	39	ALA	-	expression tag	UNP Q21A49
F	40	LEU	-	expression tag	UNP Q21A49
F	41	THR	-	expression tag	UNP Q21A49
F	42	ALA	-	expression tag	UNP Q21A49
F	43	LYS	-	expression tag	UNP Q21A49
F	44	SER	-	expression tag	UNP Q21A49
F	45	PRO	-	expression tag	UNP Q21A49
F	46	ASP	-	expression tag	UNP Q21A49
F	47	GLY	-	expression tag	UNP Q21A49
F	48	LYS	-	expression tag	UNP Q21A49
F	49	SER	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	50	ASN	-	expression tag	UNP Q21A49
F	51	SER	-	expression tag	UNP Q21A49
F	52	SER	-	expression tag	UNP Q21A49
F	53	ALA	-	expression tag	UNP Q21A49
F	54	ASP	-	expression tag	UNP Q21A49
F	55	ALA	-	expression tag	UNP Q21A49
F	56	ASP	-	expression tag	UNP Q21A49
F	57	VAL	-	expression tag	UNP Q21A49
F	58	VAL	-	expression tag	UNP Q21A49
F	59	ALA	-	expression tag	UNP Q21A49
F	60	ARG	-	expression tag	UNP Q21A49
G	1	MET	-	initiating methionine	UNP Q21A49
G	2	ALA	-	expression tag	UNP Q21A49
G	3	TRP	-	expression tag	UNP Q21A49
G	4	SER	-	expression tag	UNP Q21A49
G	5	HIS	-	expression tag	UNP Q21A49
G	6	PRO	-	expression tag	UNP Q21A49
G	7	GLN	-	expression tag	UNP Q21A49
G	8	PHE	-	expression tag	UNP Q21A49
G	9	GLU	-	expression tag	UNP Q21A49
G	10	LYS	-	expression tag	UNP Q21A49
G	11	GLY	-	expression tag	UNP Q21A49
G	12	HIS	-	expression tag	UNP Q21A49
G	13	MET	-	expression tag	UNP Q21A49
G	14	ASN	-	expression tag	UNP Q21A49
G	15	ASP	-	expression tag	UNP Q21A49
G	16	ALA	-	expression tag	UNP Q21A49
G	17	ASN	-	expression tag	UNP Q21A49
G	18	ILE	-	expression tag	UNP Q21A49
G	19	ALA	-	expression tag	UNP Q21A49
G	20	ASP	-	expression tag	UNP Q21A49
G	21	VAL	-	expression tag	UNP Q21A49
G	22	VAL	-	expression tag	UNP Q21A49
G	23	THR	-	expression tag	UNP Q21A49
G	24	LYS	-	expression tag	UNP Q21A49
G	25	VAL	-	expression tag	UNP Q21A49
G	26	LEU	-	expression tag	UNP Q21A49
G	27	GLY	-	expression tag	UNP Q21A49
G	28	GLU	-	expression tag	UNP Q21A49
G	29	TYR	-	expression tag	UNP Q21A49
G	30	GLY	-	expression tag	UNP Q21A49
G	31	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
G	32	PRO	-	expression tag	UNP Q21A49
G	33	GLY	-	expression tag	UNP Q21A49
G	34	ALA	-	expression tag	UNP Q21A49
G	35	VAL	-	expression tag	UNP Q21A49
G	36	SER	-	expression tag	UNP Q21A49
G	37	VAL	-	expression tag	UNP Q21A49
G	38	ALA	-	expression tag	UNP Q21A49
G	39	ALA	-	expression tag	UNP Q21A49
G	40	LEU	-	expression tag	UNP Q21A49
G	41	THR	-	expression tag	UNP Q21A49
G	42	ALA	-	expression tag	UNP Q21A49
G	43	LYS	-	expression tag	UNP Q21A49
G	44	SER	-	expression tag	UNP Q21A49
G	45	PRO	-	expression tag	UNP Q21A49
G	46	ASP	-	expression tag	UNP Q21A49
G	47	GLY	-	expression tag	UNP Q21A49
G	48	LYS	-	expression tag	UNP Q21A49
G	49	SER	-	expression tag	UNP Q21A49
G	50	ASN	-	expression tag	UNP Q21A49
G	51	SER	-	expression tag	UNP Q21A49
G	52	SER	-	expression tag	UNP Q21A49
G	53	ALA	-	expression tag	UNP Q21A49
G	54	ASP	-	expression tag	UNP Q21A49
G	55	ALA	-	expression tag	UNP Q21A49
G	56	ASP	-	expression tag	UNP Q21A49
G	57	VAL	-	expression tag	UNP Q21A49
G	58	VAL	-	expression tag	UNP Q21A49
G	59	ALA	-	expression tag	UNP Q21A49
G	60	ARG	-	expression tag	UNP Q21A49
H	1	MET	-	initiating methionine	UNP Q21A49
H	2	ALA	-	expression tag	UNP Q21A49
H	3	TRP	-	expression tag	UNP Q21A49
H	4	SER	-	expression tag	UNP Q21A49
H	5	HIS	-	expression tag	UNP Q21A49
H	6	PRO	-	expression tag	UNP Q21A49
H	7	GLN	-	expression tag	UNP Q21A49
H	8	PHE	-	expression tag	UNP Q21A49
H	9	GLU	-	expression tag	UNP Q21A49
H	10	LYS	-	expression tag	UNP Q21A49
H	11	GLY	-	expression tag	UNP Q21A49
H	12	HIS	-	expression tag	UNP Q21A49
H	13	MET	-	expression tag	UNP Q21A49

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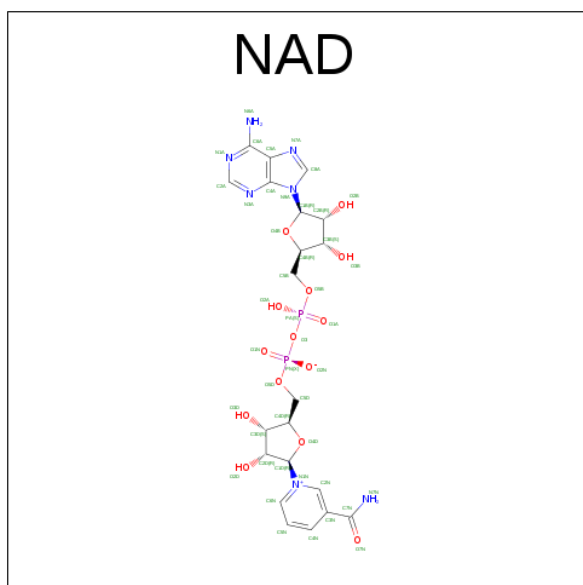
Chain	Residue	Modelled	Actual	Comment	Reference
H	14	ASN	-	expression tag	UNP Q21A49
H	15	ASP	-	expression tag	UNP Q21A49
H	16	ALA	-	expression tag	UNP Q21A49
H	17	ASN	-	expression tag	UNP Q21A49
H	18	ILE	-	expression tag	UNP Q21A49
H	19	ALA	-	expression tag	UNP Q21A49
H	20	ASP	-	expression tag	UNP Q21A49
H	21	VAL	-	expression tag	UNP Q21A49
H	22	VAL	-	expression tag	UNP Q21A49
H	23	THR	-	expression tag	UNP Q21A49
H	24	LYS	-	expression tag	UNP Q21A49
H	25	VAL	-	expression tag	UNP Q21A49
H	26	LEU	-	expression tag	UNP Q21A49
H	27	GLY	-	expression tag	UNP Q21A49
H	28	GLU	-	expression tag	UNP Q21A49
H	29	TYR	-	expression tag	UNP Q21A49
H	30	GLY	-	expression tag	UNP Q21A49
H	31	ALA	-	expression tag	UNP Q21A49
H	32	PRO	-	expression tag	UNP Q21A49
H	33	GLY	-	expression tag	UNP Q21A49
H	34	ALA	-	expression tag	UNP Q21A49
H	35	VAL	-	expression tag	UNP Q21A49
H	36	SER	-	expression tag	UNP Q21A49
H	37	VAL	-	expression tag	UNP Q21A49
H	38	ALA	-	expression tag	UNP Q21A49
H	39	ALA	-	expression tag	UNP Q21A49
H	40	LEU	-	expression tag	UNP Q21A49
H	41	THR	-	expression tag	UNP Q21A49
H	42	ALA	-	expression tag	UNP Q21A49
H	43	LYS	-	expression tag	UNP Q21A49
H	44	SER	-	expression tag	UNP Q21A49
H	45	PRO	-	expression tag	UNP Q21A49
H	46	ASP	-	expression tag	UNP Q21A49
H	47	GLY	-	expression tag	UNP Q21A49
H	48	LYS	-	expression tag	UNP Q21A49
H	49	SER	-	expression tag	UNP Q21A49
H	50	ASN	-	expression tag	UNP Q21A49
H	51	SER	-	expression tag	UNP Q21A49
H	52	SER	-	expression tag	UNP Q21A49
H	53	ALA	-	expression tag	UNP Q21A49
H	54	ASP	-	expression tag	UNP Q21A49
H	55	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
H	56	ASP	-	expression tag	UNP Q21A49
H	57	VAL	-	expression tag	UNP Q21A49
H	58	VAL	-	expression tag	UNP Q21A49
H	59	ALA	-	expression tag	UNP Q21A49
H	60	ARG	-	expression tag	UNP Q21A49

- 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		



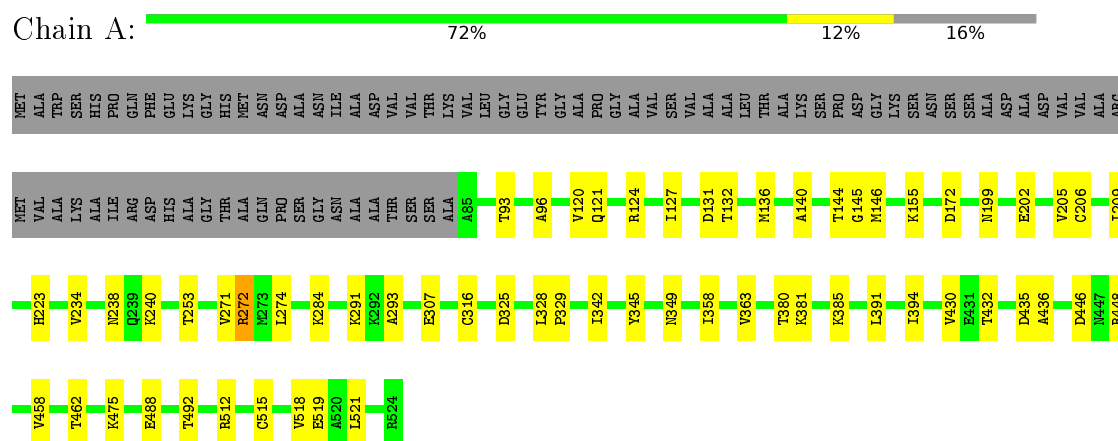
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	144	Total 144	O 144	0	0
3	C	113	Total 113	O 113	0	0
3	D	113	Total 113	O 113	0	0
3	E	131	Total 131	O 131	0	0
3	F	104	Total 104	O 104	0	0
3	G	123	Total 123	O 123	0	0
3	H	69	Total 69	O 69	0	0

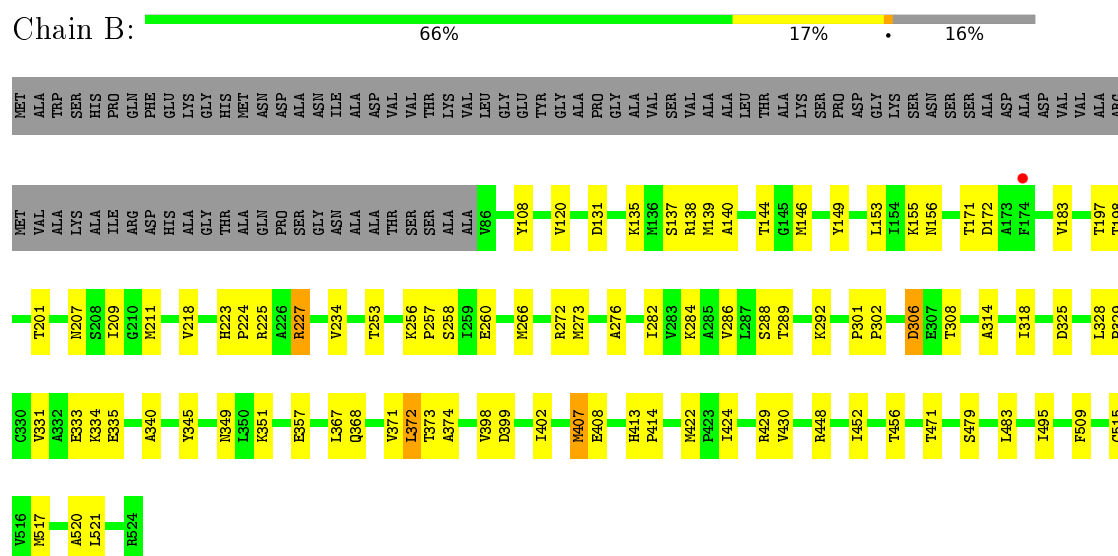
### 3 Residue-property plots

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

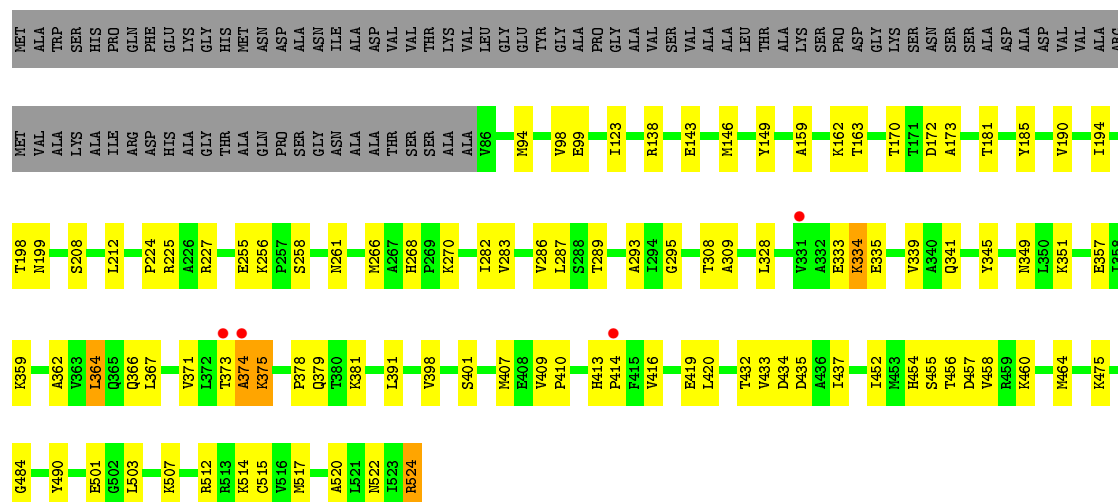


#### • Molecule 1: Aldehyde dehydrogenase

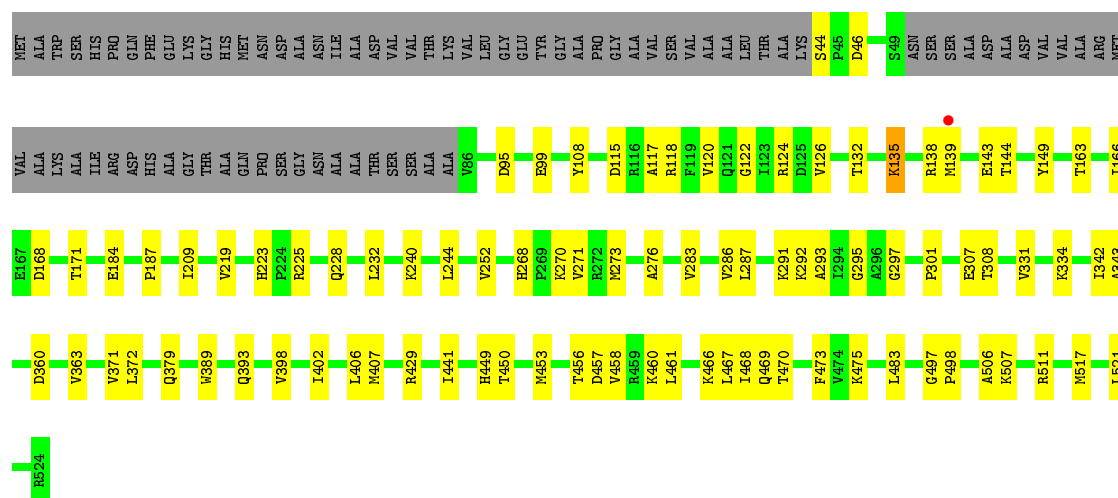


#### • Molecule 1: Aldehyde dehydrogenase

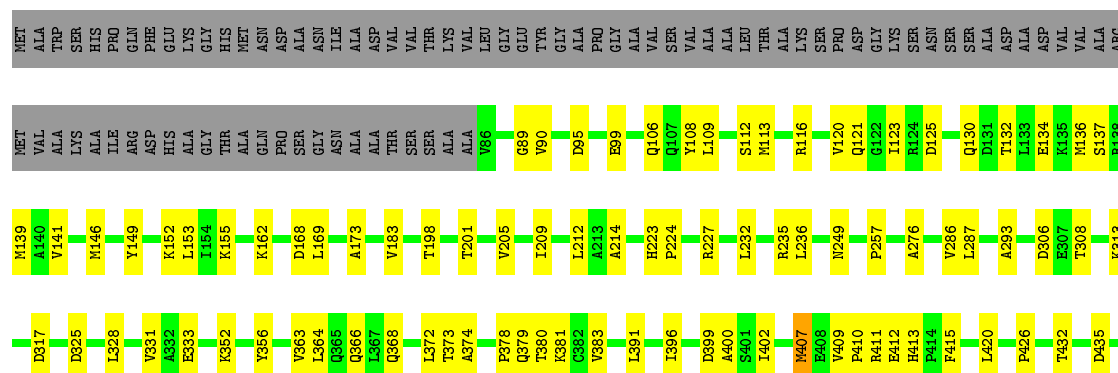


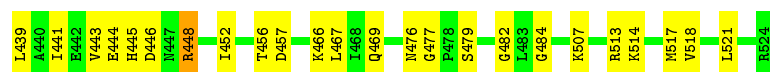


- Molecule 1: Aldehyde dehydrogenase

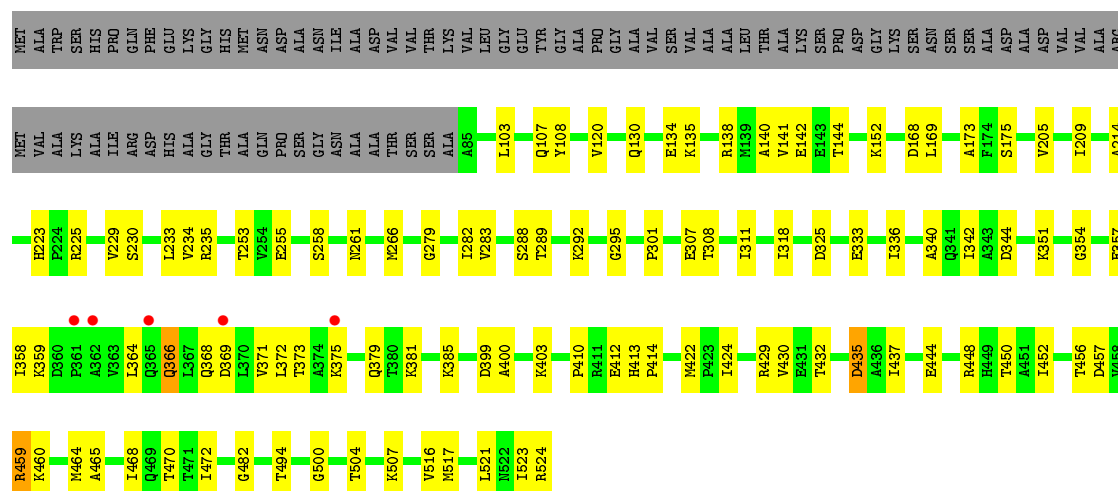


- Molecule 1: Aldehyde dehydrogenase

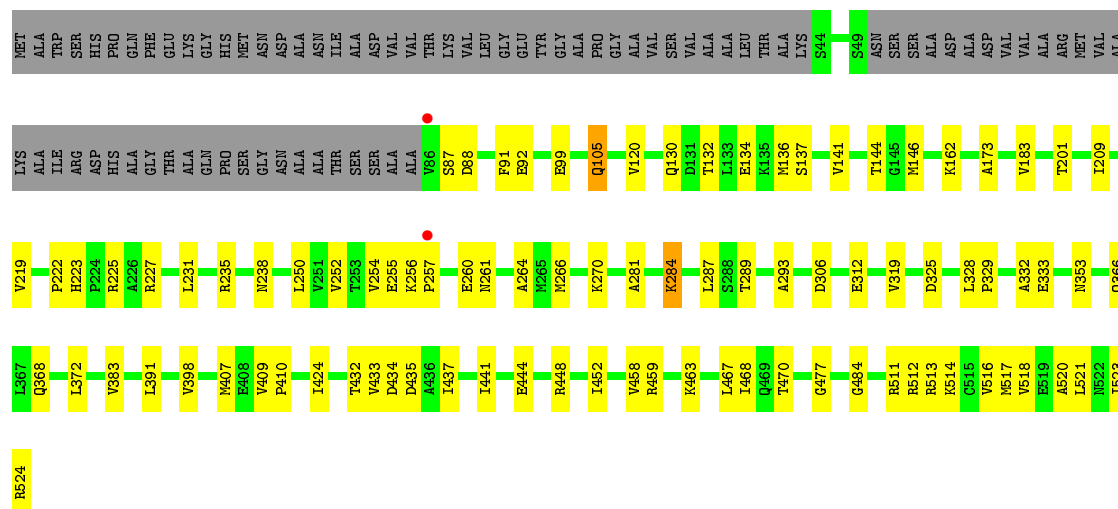




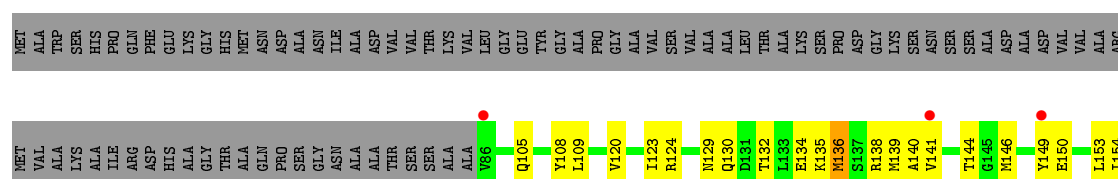
• Molecule 1: Aldehyde dehydrogenase

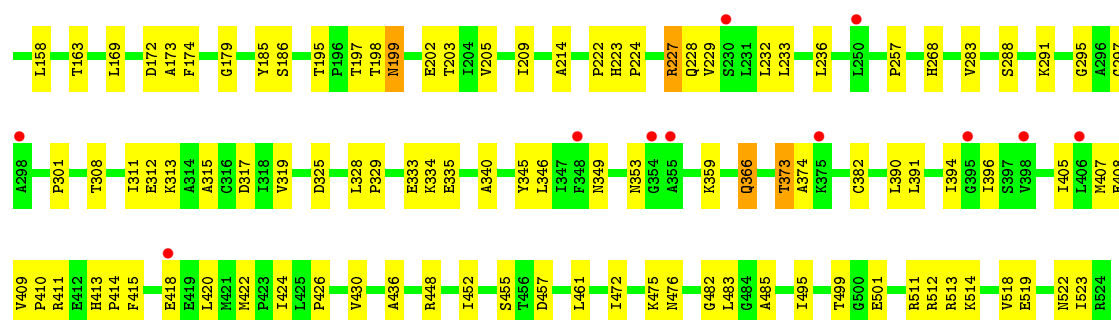


• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.39Å 154.80Å 126.59Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	33.64 – 2.30 33.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.64-2.30) 97.9 (33.64-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, $R_{free}$	0.189 , 0.228 0.184 , 0.225	Depositor DCC
$R_{free}$ test set	2007 reflections (1.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: 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	0.24	0/3338	0.45	0/4528
1	B	0.29	0/3345	0.46	0/4537
1	C	0.27	0/3333	0.47	0/4521
1	D	0.27	0/3373	0.47	2/4573 (0.0%)
1	E	0.27	0/3333	0.46	0/4521
1	F	0.26	0/3338	0.46	0/4528
1	G	0.28	0/3373	0.46	0/4573
1	H	0.30	0/3333	0.49	1/4521 (0.0%)
All	All	0.27	0/26766	0.46	3/36302 (0.0%)

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	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	LYS	CD-CE-NZ	-6.27	97.29	111.70
1	H	136	MET	CG-SD-CE	-6.23	90.23	100.20
1	D	139	MET	CB-CG-SD	-5.20	96.79	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	366	GLN	Peptide

## 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	3291	0	3382	42	0
1	B	3294	0	3386	66	0
1	C	3286	0	3377	77	0
1	D	3326	0	3413	57	0
1	E	3286	0	3377	86	0
1	F	3291	0	3382	71	0
1	G	3326	0	3413	62	0
1	H	3286	0	3377	107	0
2	A	44	0	24	2	0
2	B	44	0	24	3	0
2	C	44	0	24	3	0
2	D	44	0	24	3	0
2	E	44	0	24	0	0
2	F	44	0	24	2	0
2	G	44	0	24	2	0
2	H	44	0	24	4	0
3	A	121	0	0	7	0
3	B	144	0	0	4	0
3	C	113	0	0	5	0
3	D	113	0	0	2	0
3	E	131	0	0	5	0
3	F	104	0	0	5	0
3	G	123	0	0	3	0
3	H	69	0	0	8	0
All	All	27656	0	27299	542	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 10.

All (542) 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:366:GLN:HE22	1:H:394:ILE:CD1	1.20	1.50
1:H:366:GLN:NE2	1:H:394:ILE:HD12	0.95	1.28
1:H:366:GLN:CD	1:H:394:ILE:HD12	1.65	1.13
1:H:366:GLN:NE2	1:H:394:ILE:CD1	1.88	1.09
1:B:515:CYS:SG	1:D:475:LYS:NZ	2.31	1.03
1:E:444:GLU:OE1	1:E:448:ARG:HA	1.64	0.97
1:E:308:THR:HG23	1:E:456:THR:H	1.43	0.82
1:A:272:ARG:NH2	3:A:701:HOH:O	2.12	0.81
1:E:113:MET:SD	1:E:116:ARG:NH1	2.53	0.81
1:B:135:LYS:NZ	1:B:139:MET:SD	2.53	0.81
1:D:124:ARG:NH2	1:D:163:THR:O	2.13	0.81
1:E:444:GLU:OE1	1:E:448:ARG:CA	2.29	0.80
1:H:391:LEU:HD23	1:H:396:ILE:HD11	1.64	0.80
1:H:366:GLN:CD	1:H:394:ILE:CD1	2.40	0.79
1:A:462:THR:HG21	1:D:521:LEU:H	1.49	0.78
1:H:141:VAL:N	1:H:149:TYR:OH	2.16	0.78
1:C:432:THR:OG1	1:C:435:ASP:OD1	2.01	0.77
1:C:308:THR:HB	1:C:456:THR:HG22	1.65	0.77
1:C:351:LYS:NZ	1:C:357:GLU:OE1	2.18	0.77
1:F:468:ILE:HG13	1:F:470:THR:HG23	1.66	0.76
1:H:138:ARG:HA	1:H:149:TYR:CE2	2.20	0.76
1:H:366:GLN:OE1	1:H:394:ILE:CD1	2.34	0.76
1:A:271:VAL:O	1:A:291:LYS:NZ	2.18	0.75
1:H:513:ARG:NH2	3:H:702:HOH:O	2.14	0.75
1:B:301:PRO:HD2	1:B:334:LYS:HD2	1.69	0.74
1:A:518:VAL:HG12	1:A:519:GLU:HG3	1.68	0.73
1:E:399:ASP:OD2	1:E:400:ALA:N	2.21	0.73
1:H:301:PRO:HD2	1:H:334:LYS:HG3	1.70	0.73
1:A:515:CYS:SG	1:C:475:LYS:NZ	2.62	0.73
1:C:409:VAL:HG11	1:C:413:HIS:HD1	1.54	0.72
1:E:276:ALA:HB2	1:E:286:VAL:HG11	1.70	0.72
1:H:499:THR:OG1	1:H:501:GLU:OE2	2.06	0.72
1:E:223:HIS:HD2	1:E:224:PRO:HD2	1.54	0.71
1:F:412:GLU:OE1	1:F:412:GLU:N	2.23	0.71
1:B:351:LYS:CE	1:B:357:GLU:HB2	2.21	0.70
1:B:198:THR:HG23	1:B:328:LEU:HB3	1.73	0.69
1:H:345:TYR:O	1:H:349:ASN:ND2	2.24	0.69
1:B:227:ARG:HH21	1:B:256:LYS:HG2	1.56	0.69
1:F:311:ILE:HD11	1:F:342:ILE:HD12	1.75	0.68
1:H:366:GLN:OE1	1:H:394:ILE:HD13	1.93	0.68
1:H:349:ASN:O	1:H:353:ASN:ND2	2.25	0.68
1:B:227:ARG:NH2	1:B:256:LYS:HG2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLU:HG3	1:B:452:ILE:HD13	1.76	0.68
1:E:137:SER:OG	1:E:153:LEU:HD12	1.95	0.67
1:H:124:ARG:NH2	1:H:163:THR:O	2.22	0.67
1:E:391:LEU:HB3	1:E:396:ILE:HG23	1.77	0.67
1:H:405:ILE:HD12	1:H:424:ILE:HG12	1.75	0.67
1:C:364:LEU:HA	1:C:367:LEU:CD2	2.25	0.67
1:H:366:GLN:HE22	1:H:394:ILE:HD11	1.47	0.66
1:F:381:LYS:O	1:F:385:LYS:NZ	2.28	0.66
1:G:88:ASP:OD2	1:G:235:ARG:NH1	2.27	0.66
1:C:308:THR:HB	1:C:456:THR:CG2	2.26	0.66
1:E:120:VAL:HG13	1:E:209:ILE:HG23	1.77	0.66
1:G:254:VAL:HG22	1:G:255:GLU:OE1	1.94	0.66
1:C:379:GLN:OE1	1:C:381:LYS:HB2	1.96	0.66
1:G:255:GLU:OE1	1:G:255:GLU:N	2.29	0.66
1:G:183:VAL:HG11	1:G:512:ARG:HH11	1.60	0.66
1:B:155:LYS:NZ	1:B:325:ASP:OD2	2.27	0.66
1:A:380:THR:O	3:A:702:HOH:O	2.13	0.65
1:C:99:GLU:OE2	1:C:270:LYS:NZ	2.29	0.65
1:F:134:GLU:O	1:F:138:ARG:HG3	1.96	0.65
1:H:169:LEU:HD11	1:H:214:ALA:HA	1.79	0.65
1:A:124:ARG:NH1	3:A:703:HOH:O	2.30	0.65
1:B:351:LYS:HE2	1:B:357:GLU:HB2	1.79	0.65
1:F:359:LYS:NZ	3:F:712:HOH:O	2.28	0.65
1:A:155:LYS:NZ	1:A:325:ASP:OD2	2.29	0.65
1:E:513:ARG:NH2	1:F:523:ILE:O	2.29	0.65
1:G:144:THR:O	1:G:225:ARG:NH1	2.26	0.65
1:F:437:ILE:HD12	1:F:464:MET:HB2	1.78	0.64
1:G:260:GLU:N	1:G:260:GLU:OE2	2.29	0.64
1:B:331:VAL:O	1:B:479:SER:OG	2.15	0.64
1:G:281:ALA:O	1:G:284:LYS:HG3	1.98	0.63
1:A:284:LYS:NZ	3:A:713:HOH:O	2.31	0.63
1:G:162:LYS:NZ	1:G:484:GLY:O	2.31	0.63
1:B:144:THR:HG23	1:B:146:MET:H	1.64	0.63
1:H:345:TYR:OH	3:H:701:HOH:O	2.11	0.63
1:C:198:THR:HG23	1:C:328:LEU:HB3	1.80	0.62
1:D:115:ASP:OD1	1:D:118:ARG:NH2	2.32	0.62
1:F:366:GLN:OE1	1:F:369:ASP:N	2.28	0.62
1:B:483:LEU:HD21	1:B:495:ILE:HD11	1.82	0.62
1:G:368:GLN:HG3	1:G:372:LEU:HD23	1.82	0.62
1:H:135:LYS:HA	1:H:138:ARG:NH2	2.14	0.62
1:C:434:ASP:OD2	1:C:460:LYS:HE3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:MET:HG2	1:F:521:LEU:HD12	1.81	0.61
1:A:234:VAL:HG11	1:A:253:THR:HG22	1.83	0.61
1:F:368:GLN:O	1:F:372:LEU:N	2.31	0.61
1:E:446:ASP:O	1:E:448:ARG:NH1	2.32	0.61
1:A:458:VAL:O	1:A:462:THR:HG23	2.01	0.61
1:D:118:ARG:NH1	1:D:244:LEU:O	2.34	0.61
1:E:444:GLU:OE1	1:E:448:ARG:N	2.33	0.61
1:B:260:GLU:N	1:B:260:GLU:OE1	2.34	0.60
1:E:331:VAL:O	1:E:479:SER:OG	2.18	0.60
1:C:391:LEU:HD13	1:C:398:VAL:HG21	1.83	0.60
1:F:444:GLU:OE1	3:F:701:HOH:O	2.16	0.60
1:F:516:VAL:HG21	1:H:482:GLY:HA2	1.82	0.60
1:B:407:MET:HE1	1:B:424:ILE:HG23	1.82	0.60
1:H:308:THR:HG21	1:H:457:ASP:HB2	1.82	0.60
1:B:234:VAL:HG11	1:B:253:THR:HG22	1.83	0.60
1:D:44:SER:N	3:D:710:HOH:O	2.34	0.60
1:E:169:LEU:HD11	1:E:214:ALA:HA	1.84	0.60
1:A:172:ASP:OD2	1:A:512:ARG:NH1	2.35	0.59
1:C:514:LYS:O	3:C:702:HOH:O	2.17	0.59
1:A:345:TYR:O	1:A:349:ASN:ND2	2.33	0.58
1:F:399:ASP:OD1	1:F:400:ALA:N	2.36	0.58
1:H:197:THR:HG23	1:H:223:HIS:CG	2.38	0.58
1:H:359:LYS:HE2	1:H:408:GLU:HB3	1.84	0.58
1:H:518:VAL:HG12	1:H:519:GLU:HG3	1.86	0.58
1:E:466:LYS:HE3	1:H:522:ASN:O	2.03	0.58
1:F:482:GLY:O	1:H:514:LYS:NZ	2.34	0.58
1:B:325:ASP:HB3	1:B:329:PRO:HD3	1.85	0.58
1:B:131:ASP:OD2	3:B:701:HOH:O	2.17	0.58
1:D:308:THR:HG23	1:D:456:THR:H	1.69	0.58
1:E:373:THR:HG22	1:E:374:ALA:H	1.69	0.58
1:B:149:TYR:CE1	1:B:153:LEU:HD11	2.39	0.58
1:C:454:HIS:O	1:C:455:SER:OG	2.22	0.57
1:F:130:GLN:O	1:F:134:GLU:HG2	2.04	0.57
1:C:401:SER:OG	3:C:701:HOH:O	2.16	0.57
1:E:364:LEU:HD23	1:E:368:GLN:HE21	1.69	0.57
1:E:518:VAL:HG21	1:G:477:GLY:HA3	1.87	0.57
1:H:141:VAL:HB	1:H:149:TYR:CZ	2.39	0.57
1:H:136:MET:HE3	1:H:233:LEU:N	2.19	0.57
1:B:223:HIS:HD2	2:B:600:NAD:H3B	1.69	0.57
1:F:432:THR:OG1	1:F:435:ASP:OD2	2.12	0.57
1:G:130:GLN:NE2	1:G:134:GLU:OE2	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:391:LEU:HD11	1:H:405:ILE:HG12	1.86	0.57
1:C:266:MET:HB3	1:C:289:THR:HG21	1.85	0.57
1:G:409:VAL:HG22	1:G:410:PRO:HD2	1.87	0.57
1:G:432:THR:HG23	1:G:435:ASP:H	1.69	0.57
1:H:222:PRO:O	1:H:257:PRO:HB3	2.06	0.56
1:F:205:VAL:HG23	1:F:233:LEU:HD21	1.86	0.56
1:H:415:PHE:HB3	1:H:420:LEU:HD11	1.87	0.56
1:C:373:THR:HG22	1:C:374:ALA:H	1.69	0.56
1:E:317:ASP:OD1	3:E:702:HOH:O	2.18	0.56
1:C:359:LYS:NZ	3:C:713:HOH:O	2.28	0.56
1:E:249:ASN:OD1	3:E:701:HOH:O	2.17	0.56
1:F:169:LEU:HD11	1:F:214:ALA:HA	1.87	0.56
1:B:156:ASN:OD1	1:B:201:THR:OG1	2.17	0.56
1:G:173:ALA:HB2	1:H:173:ALA:HB2	1.87	0.56
1:E:155:LYS:NZ	1:E:325:ASP:OD2	2.38	0.56
1:C:138:ARG:HG3	1:C:149:TYR:CD2	2.41	0.56
1:D:360:ASP:HB3	1:D:363:VAL:HG12	1.87	0.56
1:B:345:TYR:O	1:B:349:ASN:ND2	2.39	0.56
1:E:152:LYS:NZ	3:E:706:HOH:O	2.29	0.56
1:A:93:THR:HG23	1:A:96:ALA:H	1.70	0.55
1:B:408:GLU:OE2	1:B:429:ARG:NH1	2.39	0.55
1:B:224:PRO:HG3	1:B:258:SER:HA	1.89	0.55
1:B:284:LYS:NZ	1:B:288:SER:OG	2.37	0.55
1:A:120:VAL:HG13	1:A:209:ILE:HG23	1.88	0.55
1:C:334:LYS:NZ	1:C:335:GLU:OE1	2.39	0.55
1:E:137:SER:O	1:E:141:VAL:HG23	2.06	0.55
1:F:465:ALA:O	3:H:702:HOH:O	2.18	0.55
1:E:448:ARG:HG3	1:G:511:ARG:NH2	2.21	0.55
1:E:162:LYS:NZ	1:E:484:GLY:O	2.37	0.55
1:H:198:THR:HG23	1:H:328:LEU:HB3	1.89	0.55
1:B:140:ALA:O	1:B:144:THR:HG22	2.05	0.55
1:E:89:GLY:HA2	3:E:701:HOH:O	2.06	0.55
1:F:258:SER:OG	1:F:261:ASN:OD1	2.23	0.55
1:B:172:ASP:HB2	1:B:183:VAL:HB	1.89	0.55
1:G:238:ASN:OD1	3:G:701:HOH:O	2.18	0.55
1:C:283:VAL:HG13	1:C:295:GLY:HA3	1.88	0.54
1:C:162:LYS:NZ	1:C:484:GLY:O	2.33	0.54
1:B:138:ARG:HG2	1:B:149:TYR:CD1	2.42	0.54
1:G:120:VAL:HG13	1:G:209:ILE:HG23	1.90	0.54
1:D:240:LYS:O	1:D:244:LEU:HD23	2.08	0.54
1:F:308:THR:HB	1:F:456:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:GLU:HG3	1:G:452:ILE:HD13	1.89	0.54
1:F:333:GLU:HG3	1:F:452:ILE:HD13	1.90	0.54
1:F:344:ASP:OD1	1:F:429:ARG:NH2	2.31	0.54
1:B:398:VAL:HG11	1:B:402:ILE:HD12	1.88	0.54
1:E:149:TYR:O	1:E:153:LEU:HD13	2.07	0.54
1:H:415:PHE:CG	1:H:420:LEU:HD11	2.43	0.54
1:E:113:MET:HA	1:E:116:ARG:HD2	1.88	0.54
1:C:170:THR:O	3:C:703:HOH:O	2.18	0.53
1:F:301:PRO:HB3	1:F:450:THR:HB	1.90	0.53
1:D:301:PRO:HD2	1:D:334:LYS:HG3	1.91	0.53
1:H:311:ILE:HG21	1:H:345:TYR:HE2	1.73	0.53
1:F:235:ARG:NH2	1:F:255:GLU:OE2	2.28	0.53
1:F:283:VAL:HG13	1:F:295:GLY:HA3	1.90	0.53
1:G:517:MET:HG2	1:G:521:LEU:HD12	1.90	0.53
1:D:219:VAL:HG13	1:D:252:VAL:HG23	1.90	0.53
1:H:333:GLU:HG3	1:H:452:ILE:HD13	1.90	0.53
1:B:448:ARG:O	1:B:471:THR:HG23	2.08	0.53
1:C:501:GLU:OE2	1:C:501:GLU:N	2.41	0.53
1:F:142:GLU:OE2	3:F:702:HOH:O	2.19	0.53
1:A:325:ASP:HB3	1:A:329:PRO:HD3	1.91	0.53
1:C:437:ILE:HG23	1:C:464:MET:HG3	1.91	0.53
1:F:230:SER:N	3:F:709:HOH:O	2.26	0.53
1:B:211:MET:CE	1:B:218:VAL:HG23	2.39	0.53
1:C:373:THR:OG1	1:C:379:GLN:HB2	2.09	0.53
1:E:95:ASP:O	1:E:99:GLU:HG2	2.09	0.53
1:F:457:ASP:OD2	1:F:460:LYS:HG2	2.10	0.52
1:H:140:ALA:O	1:H:144:THR:N	2.26	0.52
1:B:398:VAL:HG12	1:B:399:ASP:H	1.73	0.52
1:B:398:VAL:HG12	1:B:399:ASP:N	2.24	0.52
1:E:287:LEU:HD23	1:E:293:ALA:HB3	1.92	0.52
1:F:340:ALA:N	1:F:430:VAL:O	2.42	0.52
1:H:411:ARG:NH1	3:H:715:HOH:O	2.42	0.52
1:H:185:TYR:OH	1:H:512:ARG:NH1	2.42	0.52
1:H:186:SER:O	1:H:511:ARG:N	2.36	0.52
1:A:144:THR:HG23	1:A:146:MET:N	2.25	0.52
1:C:524:ARG:NH1	1:D:184:GLU:OE2	2.42	0.51
1:E:517:MET:HG2	1:E:521:LEU:HD12	1.92	0.51
1:D:171:THR:HG22	1:D:184:GLU:OE1	2.09	0.51
1:D:95:ASP:O	1:D:99:GLU:HG2	2.11	0.51
1:B:398:VAL:HG12	1:B:399:ASP:OD1	2.10	0.51
1:C:94:MET:O	1:C:98:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:GLN:HB3	1:E:372:LEU:HD12	1.92	0.51
1:F:168:ASP:O	1:F:507:LYS:NZ	2.34	0.51
1:A:381:LYS:O	1:A:385:LYS:NZ	2.35	0.51
1:E:168:ASP:O	1:E:507:LYS:HE2	2.11	0.51
1:G:325:ASP:HB3	1:G:329:PRO:HD3	1.93	0.51
1:H:120:VAL:O	1:H:124:ARG:HG3	2.11	0.51
1:H:312:GLU:HB2	3:H:701:HOH:O	2.09	0.51
1:B:120:VAL:HG13	1:B:209:ILE:HG23	1.91	0.51
1:D:120:VAL:HG13	1:D:209:ILE:HG23	1.93	0.51
1:G:468:ILE:HG12	1:G:470:THR:HG23	1.92	0.51
1:C:286:VAL:HG23	1:C:293:ALA:HB1	1.94	0.50
1:D:371:VAL:HG12	1:D:372:LEU:HD23	1.93	0.50
1:D:168:ASP:HB3	1:D:506:ALA:HB3	1.92	0.50
1:A:132:THR:O	1:A:136:MET:HG2	2.11	0.50
1:C:458:VAL:HG12	1:D:458:VAL:HG12	1.93	0.50
1:B:223:HIS:CD2	2:B:600:NAD:H3B	2.46	0.50
1:E:356:TYR:HB2	1:E:402:ILE:HD12	1.92	0.50
1:G:87:SER:O	3:G:702:HOH:O	2.19	0.50
2:H:600:NAD:H8A	2:H:600:NAD:O2A	2.12	0.50
1:B:308:THR:HB	1:B:456:THR:HB	1.92	0.50
1:G:441:ILE:HD11	1:G:467:LEU:HB3	1.93	0.50
1:C:159:ALA:O	1:C:163:THR:OG1	2.15	0.50
1:F:266:MET:HB3	1:F:289:THR:HG21	1.93	0.50
1:G:328:LEU:N	1:G:329:PRO:HD2	2.27	0.50
1:A:240:LYS:NZ	3:A:715:HOH:O	2.33	0.50
1:H:311:ILE:HD11	1:H:346:LEU:HB2	1.93	0.50
1:A:144:THR:HG23	1:A:146:MET:H	1.77	0.50
1:G:287:LEU:HD23	1:G:293:ALA:HB3	1.93	0.50
1:F:307:GLU:HA	1:F:342:ILE:HD13	1.94	0.49
1:A:121:GLN:OE1	3:A:703:HOH:O	2.20	0.49
1:A:432:THR:HG23	1:A:435:ASP:H	1.77	0.49
1:B:373:THR:HG22	1:B:374:ALA:H	1.77	0.49
1:C:501:GLU:OE1	3:C:704:HOH:O	2.20	0.49
1:B:171:THR:O	3:B:702:HOH:O	2.20	0.49
1:B:306:ASP:OD2	1:B:308:THR:OG1	2.28	0.49
1:C:268:HIS:CE1	1:C:270:LYS:HB2	2.48	0.49
1:H:150:GLU:HA	1:H:153:LEU:HD12	1.94	0.49
1:B:517:MET:HG2	1:B:521:LEU:HD12	1.94	0.49
1:C:123:ILE:HD11	1:C:212:LEU:HD22	1.93	0.49
1:E:477:GLY:HA3	1:G:518:VAL:HG21	1.94	0.49
1:A:199:ASN:HB3	1:A:202:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:LEU:O	1:E:236:LEU:HD12	2.12	0.49
1:H:415:PHE:CB	1:H:420:LEU:HD11	2.43	0.49
1:E:313:LYS:NZ	1:E:317:ASP:OD2	2.45	0.49
1:E:432:THR:OG1	1:E:435:ASP:OD2	2.31	0.49
1:A:234:VAL:O	1:A:238:ASN:ND2	2.35	0.48
1:C:287:LEU:HD23	1:C:293:ALA:HB3	1.95	0.48
1:E:223:HIS:CD2	1:E:224:PRO:HD2	2.43	0.48
1:H:448:ARG:NH2	3:H:710:HOH:O	2.40	0.48
1:C:364:LEU:HA	1:C:367:LEU:HD21	1.95	0.48
1:D:466:LYS:O	1:D:469:GLN:NE2	2.46	0.48
1:H:313:LYS:NZ	1:H:476:ASN:O	2.46	0.48
1:C:379:GLN:OE1	1:C:381:LYS:CB	2.62	0.48
1:C:199:ASN:ND2	2:C:600:NAD:H5N	2.28	0.48
1:C:362:ALA:O	1:C:366:GLN:HG3	2.13	0.48
1:F:366:GLN:O	1:F:366:GLN:HG3	2.13	0.48
1:H:232:LEU:HG	1:H:236:LEU:CD2	2.42	0.48
1:D:449:HIS:HD2	1:D:450:THR:OG1	1.96	0.48
1:H:268:HIS:O	1:H:291:LYS:NZ	2.46	0.48
1:H:409:VAL:HG22	1:H:410:PRO:HD2	1.96	0.48
1:B:211:MET:HE1	1:B:218:VAL:HG23	1.95	0.48
1:C:367:LEU:O	1:C:371:VAL:HG22	2.13	0.48
1:C:409:VAL:HG13	1:C:410:PRO:HD2	1.95	0.48
1:D:398:VAL:HG11	1:D:402:ILE:HG13	1.96	0.48
1:A:307:GLU:HA	1:A:342:ILE:HG12	1.95	0.48
1:B:137:SER:CB	1:B:153:LEU:HD12	2.43	0.48
1:E:169:LEU:O	1:F:524:ARG:NH1	2.47	0.48
1:E:308:THR:HG21	1:E:457:ASP:H	1.78	0.48
1:F:444:GLU:OE2	1:F:448:ARG:N	2.44	0.48
1:G:88:ASP:N	1:G:88:ASP:OD1	2.44	0.48
1:E:407:MET:CE	1:E:415:PHE:HD2	2.26	0.48
1:G:137:SER:O	1:G:141:VAL:HG23	2.14	0.48
1:B:413:HIS:CG	1:B:414:PRO:HD2	2.48	0.48
1:D:168:ASP:O	1:D:507:LYS:HE3	2.14	0.48
1:G:227:ARG:HG3	1:G:257:PRO:HD2	1.96	0.48
1:A:199:ASN:HD22	2:A:600:NAD:H5N	1.79	0.47
1:H:414:PRO:O	1:H:418:GLU:HG3	2.14	0.47
1:C:256:LYS:O	1:C:261:ASN:ND2	2.47	0.47
1:E:132:THR:O	1:E:136:MET:HG2	2.14	0.47
1:F:141:VAL:HG23	1:F:152:LYS:HD2	1.96	0.47
1:H:315:ALA:O	1:H:319:VAL:HG23	2.14	0.47
1:E:415:PHE:HB3	1:E:426:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:ASN:HB3	1:H:132:THR:OG1	2.14	0.47
1:H:472:ILE:HD11	1:H:495:ILE:HD13	1.95	0.47
1:A:446:ASP:OD1	1:A:448:ARG:NH2	2.44	0.47
1:C:224:PRO:HG3	1:C:258:SER:HA	1.96	0.47
1:A:475:LYS:NZ	1:C:515:CYS:SG	2.63	0.47
1:F:450:THR:HG23	1:F:472:ILE:HB	1.96	0.47
1:G:132:THR:O	1:G:136:MET:HG2	2.15	0.47
1:H:139:MET:HB3	1:H:229:VAL:HG22	1.95	0.47
1:B:207:ASN:ND2	3:B:710:HOH:O	2.30	0.47
1:E:90:VAL:HG21	1:E:235:ARG:CZ	2.44	0.47
1:F:500:GLY:HA2	1:H:511:ARG:HG2	1.96	0.47
1:H:407:MET:HG3	1:H:426:PRO:HA	1.96	0.47
1:D:343:ALA:HB3	1:D:429:ARG:NH1	2.30	0.47
1:E:112:SER:O	1:E:116:ARG:HG3	2.15	0.47
1:G:261:ASN:HA	1:G:264:ALA:HB3	1.96	0.47
1:C:373:THR:O	1:C:375:LYS:N	2.47	0.47
1:D:144:THR:HA	1:D:225:ARG:HG2	1.96	0.47
1:H:130:GLN:NE2	1:H:134:GLU:OE2	2.47	0.47
1:H:158:LEU:HD11	1:H:485:ALA:HB2	1.95	0.47
1:H:311:ILE:CD1	1:H:346:LEU:HD13	2.45	0.47
1:E:130:GLN:O	1:E:134:GLU:HG3	2.14	0.47
1:E:411:ARG:HG2	1:E:439:LEU:HD11	1.97	0.47
1:B:266:MET:HB3	1:B:289:THR:HG21	1.97	0.46
1:E:201:THR:O	1:E:205:VAL:HG23	2.16	0.46
1:B:197:THR:OG1	1:B:223:HIS:CG	2.68	0.46
1:C:194:ILE:HG22	2:C:600:NAD:H4B	1.98	0.46
1:D:453:MET:HE2	1:D:473:PHE:HZ	1.79	0.46
1:B:335:GLU:OE2	3:B:703:HOH:O	2.20	0.46
1:D:297:GLY:O	2:D:600:NAD:H2N	2.15	0.46
1:A:430:VAL:HG21	1:A:436:ALA:HB2	1.98	0.46
1:C:517:MET:HG3	1:C:520:ALA:HB3	1.97	0.46
1:H:223:HIS:CD2	2:H:600:NAD:H3B	2.50	0.46
1:C:367:LEU:HD23	1:C:367:LEU:H	1.80	0.46
1:D:453:MET:HE1	1:D:461:LEU:HA	1.98	0.46
1:H:523:ILE:HG13	3:H:709:HOH:O	2.14	0.46
1:E:173:ALA:HB2	1:F:173:ALA:HB2	1.98	0.46
2:H:600:NAD:H52N	2:H:600:NAD:H6N	1.98	0.46
1:H:195:THR:HG22	1:H:203:THR:HB	1.97	0.46
1:C:333:GLU:HG3	1:C:452:ILE:HD13	1.98	0.46
1:H:483:LEU:HD23	1:H:483:LEU:O	2.16	0.46
1:B:398:VAL:CG1	1:B:402:ILE:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:VAL:HA	1:E:514:LYS:HA	1.97	0.46
1:G:255:GLU:HG2	1:G:256:LYS:HB2	1.98	0.46
1:H:461:LEU:HD22	1:H:475:LYS:HG2	1.98	0.46
1:D:138:ARG:HG2	1:D:149:TYR:CD1	2.51	0.46
1:F:288:SER:HA	1:H:288:SER:HA	1.98	0.46
1:G:524:ARG:HG3	1:H:185:TYR:O	2.16	0.46
1:D:122:GLY:O	1:D:126:VAL:HG23	2.16	0.45
1:E:409:VAL:HG22	1:E:410:PRO:HD2	1.97	0.45
1:F:457:ASP:OD1	1:F:459:ARG:HD3	2.15	0.45
1:H:334:LYS:HB2	1:H:335:GLU:OE2	2.16	0.45
1:C:334:LYS:HG3	1:C:335:GLU:OE1	2.16	0.45
1:E:448:ARG:HB2	1:E:469:GLN:O	2.16	0.45
1:E:363:VAL:O	1:E:366:GLN:HG2	2.17	0.45
1:E:413:HIS:HD1	1:E:415:PHE:HB2	1.81	0.45
1:E:443:VAL:O	1:E:445:HIS:ND1	2.46	0.45
1:F:140:ALA:O	1:F:144:THR:OG1	2.26	0.45
1:D:276:ALA:HB2	1:D:286:VAL:HG11	1.98	0.45
1:E:123:ILE:HD11	1:E:212:LEU:HD12	1.99	0.45
1:H:136:MET:CE	1:H:232:LEU:HB3	2.47	0.45
1:H:311:ILE:CG2	1:H:345:TYR:HE2	2.29	0.45
1:E:446:ASP:O	1:E:448:ARG:HD3	2.17	0.45
1:E:441:ILE:HD11	1:E:467:LEU:HB3	1.98	0.45
1:G:183:VAL:HA	1:G:513:ARG:O	2.17	0.45
1:G:91:PHE:O	1:G:255:GLU:N	2.50	0.45
1:B:276:ALA:HB2	1:B:286:VAL:HG11	1.99	0.45
1:D:379:GLN:NE2	3:D:724:HOH:O	2.49	0.45
1:D:517:MET:HG2	1:D:521:LEU:HD12	1.97	0.45
1:G:444:GLU:OE2	1:G:448:ARG:N	2.50	0.45
1:F:103:LEU:O	1:F:107:GLN:HG3	2.17	0.45
1:F:279:GLY:O	1:F:282:ILE:HG22	2.17	0.45
1:G:391:LEU:HD12	1:G:398:VAL:HG21	1.99	0.45
1:H:413:HIS:CD2	1:H:415:PHE:H	2.34	0.45
1:D:283:VAL:HG13	1:D:295:GLY:HA3	1.98	0.45
1:E:456:THR:HG23	1:F:457:ASP:OD1	2.16	0.45
1:B:273:MET:HA	1:B:292:LYS:O	2.17	0.44
1:B:314:ALA:O	1:B:318:ILE:HG13	2.17	0.44
1:C:190:VAL:HG11	1:C:270:LYS:O	2.17	0.44
1:G:136:MET:HB3	1:G:201:THR:HG21	1.99	0.44
1:G:223:HIS:CD2	2:G:600:NAD:H3B	2.53	0.44
1:H:179:GLY:O	1:H:522:ASN:HB3	2.18	0.44
1:H:150:GLU:O	1:H:154:ILE:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:HIS:HD2	1:C:414:PRO:HD2	1.83	0.44
1:C:309:ALA:HA	1:C:455:SER:HA	1.99	0.44
1:D:497:GLY:H	1:D:498:PRO:HD2	1.83	0.44
1:E:380:THR:HA	1:E:383:VAL:HG23	1.98	0.44
1:G:222:PRO:HG2	1:G:257:PRO:HG3	1.99	0.44
1:H:138:ARG:HA	1:H:149:TYR:CD2	2.51	0.44
1:H:224:PRO:HB3	1:H:257:PRO:HB2	2.00	0.44
1:H:313:LYS:NZ	1:H:317:ASP:OD2	2.40	0.44
1:A:140:ALA:O	1:A:144:THR:HG22	2.18	0.44
1:H:283:VAL:HG13	1:H:295:GLY:HA3	1.98	0.44
1:F:292:LYS:NZ	1:H:501:GLU:OE1	2.50	0.44
1:A:521:LEU:HA	1:A:521:LEU:HD23	1.90	0.44
1:C:172:ASP:OD2	1:C:512:ARG:NH2	2.44	0.44
1:C:458:VAL:CG1	1:D:458:VAL:HG12	2.47	0.44
1:D:441:ILE:HD11	1:D:467:LEU:HB3	1.99	0.44
1:E:313:LYS:NZ	1:E:476:ASN:O	2.49	0.44
1:F:366:GLN:OE1	1:F:366:GLN:HA	2.16	0.44
1:C:339:VAL:HG12	1:C:341:GLN:H	1.82	0.44
1:C:282:ILE:HD13	2:C:600:NAD:C4A	2.47	0.44
1:E:198:THR:HG22	1:E:328:LEU:HD22	1.98	0.44
1:F:225:ARG:HE	1:F:225:ARG:HB2	1.46	0.44
1:H:136:MET:HE3	1:H:232:LEU:HB3	1.99	0.44
1:A:488:GLU:O	3:A:705:HOH:O	2.21	0.44
1:E:306:ASP:OD1	1:E:308:THR:HG22	2.18	0.44
1:E:407:MET:SD	1:E:407:MET:N	2.91	0.44
1:C:345:TYR:O	1:C:349:ASN:ND2	2.43	0.44
1:E:168:ASP:OD2	1:E:507:LYS:HG3	2.18	0.44
1:F:144:THR:HG22	1:F:225:ARG:HG2	2.00	0.44
1:F:494:THR:HB	1:F:504:THR:OG1	2.18	0.44
1:G:306:ASP:HB2	1:G:433:VAL:HG22	1.99	0.44
1:B:340:ALA:N	1:B:430:VAL:O	2.51	0.43
1:E:121:GLN:NE2	1:E:125:ASP:OD1	2.50	0.43
1:E:232:LEU:HG	1:E:236:LEU:HD11	2.00	0.43
1:F:229:VAL:HG12	3:F:709:HOH:O	2.17	0.43
1:D:143:GLU:OE1	1:D:228:GLN:HB2	2.18	0.43
1:D:287:LEU:HD23	1:D:293:ALA:HB3	1.99	0.43
1:E:106:GLN:HA	1:E:109:LEU:HD12	2.00	0.43
1:H:297:GLY:O	2:H:600:NAD:H2N	2.18	0.43
1:C:334:LYS:NZ	1:C:416:VAL:O	2.51	0.43
1:D:273:MET:HG3	1:D:292:LYS:HG3	2.00	0.43
1:D:223:HIS:HD2	2:D:600:NAD:H3B	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:LEU:HD11	1:E:415:PHE:HE1	1.84	0.43
1:G:366:GLN:OE1	3:G:703:HOH:O	2.21	0.43
1:G:517:MET:HG3	1:G:520:ALA:HB3	2.00	0.43
1:C:146:MET:HB3	1:C:328:LEU:HD11	2.00	0.43
1:F:413:HIS:CG	1:F:414:PRO:HD2	2.53	0.43
1:H:198:THR:HG22	1:H:199:ASN:ND2	2.33	0.43
1:H:227:ARG:HG2	1:H:228:GLN:N	2.31	0.43
1:H:373:THR:OG1	1:H:374:ALA:N	2.48	0.43
1:C:433:VAL:HG13	1:C:460:LYS:HE2	1.99	0.43
1:F:403:LYS:HA	1:F:403:LYS:HD3	1.85	0.43
1:G:434:ASP:OD1	1:G:463:LYS:NZ	2.35	0.43
1:H:340:ALA:N	1:H:430:VAL:O	2.51	0.43
1:C:123:ILE:HD13	1:C:208:SER:HB3	2.01	0.43
1:C:143:GLU:HG2	1:C:225:ARG:O	2.19	0.43
1:C:433:VAL:CG1	1:C:460:LYS:HE2	2.48	0.43
1:C:435:ASP:OD1	1:C:435:ASP:N	2.50	0.43
1:H:325:ASP:HB3	1:H:329:PRO:HD3	2.00	0.43
1:E:412:GLU:H	1:E:412:GLU:CD	2.22	0.43
1:E:482:GLY:O	1:G:514:LYS:NZ	2.41	0.43
1:G:407:MET:HE1	1:G:424:ILE:HG23	2.00	0.43
1:C:457:ASP:OD2	1:C:460:LYS:N	2.49	0.43
1:C:173:ALA:HA	1:C:181:THR:O	2.19	0.43
1:C:456:THR:OG1	1:D:457:ASP:HA	2.18	0.43
1:D:268:HIS:CE1	1:D:270:LYS:HB2	2.54	0.43
2:D:600:NAD:H8A	2:D:600:NAD:H2B	1.92	0.43
1:H:511:ARG:HE	1:H:511:ARG:HB3	1.41	0.43
1:A:358:ILE:HG23	1:A:363:VAL:HG13	1.99	0.42
1:G:523:ILE:HD12	1:H:513:ARG:HH12	1.84	0.42
1:A:127:ILE:HG21	1:A:205:VAL:HG11	2.00	0.42
1:D:126:VAL:O	1:D:132:THR:HG21	2.19	0.42
1:D:135:LYS:HZ1	1:D:232:LEU:HD13	1.83	0.42
1:F:371:VAL:HG13	1:F:422:MET:SD	2.60	0.42
1:G:227:ARG:O	1:G:231:LEU:HG	2.19	0.42
1:E:149:TYR:CE1	1:E:153:LEU:HD11	2.54	0.42
1:G:433:VAL:O	1:G:437:ILE:HG13	2.19	0.42
1:A:206:CYS:SG	1:A:492:THR:HA	2.59	0.42
1:D:307:GLU:HA	1:D:342:ILE:HG12	2.01	0.42
1:G:458:VAL:HG13	1:G:459:ARG:HG3	2.01	0.42
1:E:333:GLU:HG3	1:E:452:ILE:HD13	2.01	0.42
1:H:522:ASN:ND2	1:H:522:ASN:O	2.53	0.42
1:A:223:HIS:CD2	2:A:600:NAD:H3B	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:GLU:OE1	1:H:202:GLU:N	2.37	0.42
1:H:455:SER:O	1:H:461:LEU:HD11	2.19	0.42
1:A:145:GLY:O	1:A:385:LYS:HE3	2.20	0.42
1:B:282:ILE:HD13	2:B:600:NAD:N3A	2.34	0.42
1:C:490:TYR:OH	1:C:503:LEU:O	2.23	0.42
1:F:152:LYS:HG3	1:F:325:ASP:OD1	2.20	0.42
1:G:219:VAL:HG13	1:G:252:VAL:HG23	2.01	0.42
1:G:99:GLU:OE2	1:G:270:LYS:NZ	2.29	0.42
1:H:146:MET:HB3	1:H:328:LEU:HD11	2.02	0.42
1:H:511:ARG:HH21	1:H:513:ARG:HG2	1.85	0.42
1:C:190:VAL:CG1	1:C:270:LYS:O	2.68	0.42
1:C:227:ARG:NH1	1:C:255:GLU:OE2	2.52	0.42
1:C:185:TYR:CE2	1:C:507:LYS:HD2	2.55	0.42
1:E:411:ARG:NH1	3:E:718:HOH:O	2.39	0.42
1:F:234:VAL:HG11	1:F:253:THR:HG22	2.01	0.42
1:B:144:THR:HG23	1:B:146:MET:N	2.32	0.42
1:B:197:THR:HG21	1:B:225:ARG:HD2	2.02	0.42
1:B:227:ARG:HH21	1:B:256:LYS:HA	1.85	0.42
1:D:406:LEU:HD12	1:D:407:MET:N	2.35	0.42
1:G:105:GLN:HB3	1:G:105:GLN:HE21	1.71	0.42
1:B:368:GLN:HA	1:B:372:LEU:HD12	2.02	0.41
1:H:105:GLN:HE22	1:H:109:LEU:HD21	1.85	0.41
1:H:333:GLU:OE2	3:H:703:HOH:O	2.22	0.41
1:D:271:VAL:O	1:D:291:LYS:NZ	2.37	0.41
1:E:137:SER:CB	1:E:153:LEU:HD12	2.50	0.41
1:F:351:LYS:HE3	1:F:357:GLU:OE2	2.20	0.41
1:C:522:ASN:N	1:C:522:ASN:OD1	2.50	0.41
1:D:117:ALA:HB2	1:D:166:ILE:HD13	2.02	0.41
1:E:139:MET:HE2	1:E:139:MET:HB2	1.89	0.41
1:G:329:PRO:HG2	1:G:332:ALA:HB2	2.02	0.41
1:H:205:VAL:O	1:H:209:ILE:HG13	2.20	0.41
1:E:378:PRO:HB3	1:E:420:LEU:HA	2.02	0.41
1:E:457:ASP:OD1	1:F:456:THR:HG23	2.20	0.41
1:F:464:MET:O	1:F:468:ILE:HG22	2.19	0.41
1:H:123:ILE:CG2	1:H:209:ILE:HG12	2.51	0.41
1:A:146:MET:HB3	1:A:328:LEU:HD11	2.02	0.41
1:A:462:THR:HG21	1:D:521:LEU:N	2.25	0.41
1:B:301:PRO:HA	1:B:302:PRO:HD3	1.94	0.41
1:C:364:LEU:HD11	1:C:407:MET:HG3	2.03	0.41
1:E:139:MET:HE1	1:E:232:LEU:HD22	2.03	0.41
1:E:482:GLY:HA2	1:G:516:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:MET:HB3	1:G:289:THR:HG21	2.03	0.41
1:G:319:VAL:HG11	1:G:353:ASN:HB3	2.01	0.41
2:G:600:NAD:PA	2:G:600:NAD:H8A	2.61	0.41
1:H:430:VAL:HG21	1:H:436:ALA:HB2	2.02	0.41
1:D:453:MET:CE	1:D:461:LEU:HA	2.50	0.41
1:E:146:MET:HB3	1:E:328:LEU:HD11	2.01	0.41
1:H:223:HIS:ND1	1:H:224:PRO:HD2	2.36	0.41
1:H:413:HIS:ND1	1:H:414:PRO:HD2	2.35	0.41
1:B:367:LEU:O	1:B:371:VAL:HG22	2.20	0.41
1:D:389:TRP:O	1:D:393:GLN:HG2	2.21	0.41
1:E:372:LEU:HD11	1:E:415:PHE:CE1	2.56	0.41
1:B:227:ARG:CG	1:B:257:PRO:HD2	2.51	0.41
1:C:409:VAL:HG11	1:C:413:HIS:ND1	2.30	0.41
1:D:468:ILE:HG23	1:D:470:THR:HG23	2.03	0.41
1:F:358:ILE:HG21	1:F:364:LEU:HB2	2.02	0.41
1:A:391:LEU:HD23	1:A:394:ILE:HD11	2.02	0.41
1:B:227:ARG:HE	1:B:257:PRO:HD2	1.86	0.41
1:B:517:MET:HG3	1:B:520:ALA:HB3	2.03	0.41
1:H:197:THR:HG23	1:H:223:HIS:CD2	2.55	0.41
1:H:382:CYS:HB3	1:H:390:LEU:CD2	2.51	0.41
1:C:378:PRO:HG3	1:C:420:LEU:HD23	2.03	0.41
1:F:379:GLN:HB3	1:F:381:LYS:HG2	2.02	0.41
1:G:250:LEU:HD12	1:G:250:LEU:HA	1.93	0.41
1:A:274:LEU:O	1:A:293:ALA:HA	2.20	0.40
1:D:331:VAL:HG21	1:D:483:LEU:HD21	2.03	0.40
1:F:223:HIS:HD2	2:F:600:NAD:H3B	1.86	0.40
1:G:92:GLU:HA	1:G:255:GLU:HB3	2.03	0.40
1:G:146:MET:HG2	1:G:383:VAL:O	2.22	0.40
1:G:183:VAL:CG1	1:G:512:ARG:HD3	2.51	0.40
1:H:422:MET:C	1:H:424:ILE:H	2.24	0.40
1:D:457:ASP:OD2	1:D:460:LYS:HG2	2.21	0.40
1:F:120:VAL:HG13	1:F:209:ILE:HG23	2.03	0.40
1:H:172:ASP:HB3	1:H:174:PHE:CZ	2.57	0.40
1:B:422:MET:C	1:B:424:ILE:H	2.24	0.40
1:F:175:SER:O	1:F:524:ARG:NH2	2.54	0.40
1:F:318:ILE:HG21	1:F:336:ILE:HD11	2.04	0.40
1:F:373:THR:HG22	1:F:375:LYS:H	1.86	0.40
1:F:292:LYS:HD3	1:H:499:THR:HB	2.02	0.40
1:B:273:MET:HE1	1:B:509:PHE:HD1	1.85	0.40
1:C:173:ALA:HB3	1:D:171:THR:OG1	2.21	0.40
1:D:187:PRO:O	1:D:511:ARG:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PRO:HD2	1:D:334:LYS:CG	2.51	0.40
1:E:227:ARG:HD2	1:E:257:PRO:HD2	2.04	0.40
1:E:364:LEU:O	1:E:368:GLN:HG3	2.21	0.40
1:F:422:MET:C	1:F:424:ILE:H	2.24	0.40
1:G:284:LYS:C	1:G:284:LYS:HD2	2.42	0.40
1:H:366:GLN:HE21	1:H:366:GLN:HB3	1.72	0.40
1:B:146:MET:HB3	1:B:328:LEU:HD11	2.03	0.40
1:F:282:ILE:HG21	2:F:600:NAD:H52A	2.04	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	438/524 (84%)	425 (97%)	13 (3%)	0	100	100
1	B	438/524 (84%)	420 (96%)	18 (4%)	0	100	100
1	C	437/524 (83%)	423 (97%)	12 (3%)	2 (0%)	34	41
1	D	441/524 (84%)	432 (98%)	9 (2%)	0	100	100
1	E	437/524 (83%)	417 (95%)	20 (5%)	0	100	100
1	F	438/524 (84%)	421 (96%)	15 (3%)	2 (0%)	34	41
1	G	441/524 (84%)	426 (97%)	15 (3%)	0	100	100
1	H	437/524 (83%)	417 (95%)	19 (4%)	1 (0%)	52	64
All	All	3507/4192 (84%)	3381 (96%)	121 (4%)	5 (0%)	56	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	ALA
1	F	410	PRO

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Mol	Chain	Res	Type
1	C	419	GLU
1	H	373	THR
1	F	354	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	358/417 (86%)	355 (99%)	3 (1%)	86	94
1	B	359/417 (86%)	353 (98%)	6 (2%)	68	83
1	C	358/417 (86%)	354 (99%)	4 (1%)	80	90
1	D	363/417 (87%)	361 (99%)	2 (1%)	90	96
1	E	358/417 (86%)	352 (98%)	6 (2%)	68	83
1	F	358/417 (86%)	354 (99%)	4 (1%)	80	90
1	G	363/417 (87%)	360 (99%)	3 (1%)	86	94
1	H	358/417 (86%)	354 (99%)	4 (1%)	80	90
All	All	2875/3336 (86%)	2843 (99%)	32 (1%)	80	90

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	A	272	ARG
1	A	316	CYS
1	B	108	TYR
1	B	227	ARG
1	B	272	ARG
1	B	306	ASP
1	B	372	LEU
1	B	407	MET
1	C	334	LYS
1	C	364	LEU
1	C	375	LYS

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Mol	Chain	Res	Type
1	C	524	ARG
1	D	46	ASP
1	D	108	TYR
1	E	108	TYR
1	E	352	LYS
1	E	379	GLN
1	E	381	LYS
1	E	407	MET
1	E	448	ARG
1	F	108	TYR
1	F	135	LYS
1	F	435	ASP
1	F	459	ARG
1	G	105	GLN
1	G	284	LYS
1	G	312	GLU
1	H	108	TYR
1	H	199	ASN
1	H	227	ARG
1	H	366	GLN

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

Mol	Chain	Res	Type
1	B	199	ASN
1	B	228	GLN
1	D	449	HIS
1	E	106	GLN
1	E	368	GLN
1	E	393	GLN
1	G	105	GLN
1	G	261	ASN
1	H	105	GLN
1	H	199	ASN
1	H	366	GLN
1	H	368	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	600	-	42,48,48	5.09	16 (38%)	46,73,73	2.04	6 (13%)
2	NAD	B	600	-	42,48,48	5.08	16 (38%)	46,73,73	1.89	4 (8%)
2	NAD	C	600	-	42,48,48	5.08	16 (38%)	46,73,73	1.93	3 (6%)
2	NAD	D	600	-	42,48,48	5.09	16 (38%)	46,73,73	1.99	7 (15%)
2	NAD	E	600	-	42,48,48	5.07	16 (38%)	46,73,73	1.86	2 (4%)
2	NAD	F	600	-	42,48,48	5.09	16 (38%)	46,73,73	1.99	5 (10%)
2	NAD	G	600	-	42,48,48	5.09	16 (38%)	46,73,73	1.89	3 (6%)
2	NAD	H	600	-	42,48,48	5.09	16 (38%)	46,73,73	1.91	3 (6%)

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	600	-	-	0/22/62/62	0/5/5/5
2	NAD	B	600	-	-	0/22/62/62	0/5/5/5
2	NAD	C	600	-	-	0/22/62/62	0/5/5/5
2	NAD	D	600	-	-	0/22/62/62	0/5/5/5
2	NAD	E	600	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	600	-	-	0/22/62/62	0/5/5/5
2	NAD	G	600	-	-	0/22/62/62	0/5/5/5
2	NAD	H	600	-	-	0/22/62/62	0/5/5/5

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	NAD	C2B-C1B	-15.54	1.28	1.53
2	A	600	NAD	C2B-C1B	-15.46	1.29	1.53
2	A	600	NAD	C2D-C1D	-15.38	1.29	1.53
2	H	600	NAD	C2B-C1B	-15.36	1.29	1.53
2	G	600	NAD	C2B-C1B	-15.36	1.29	1.53
2	B	600	NAD	C2B-C1B	-15.35	1.29	1.53
2	B	600	NAD	C2D-C1D	-15.35	1.29	1.53
2	C	600	NAD	C2D-C1D	-15.35	1.29	1.53
2	D	600	NAD	C2D-C1D	-15.34	1.29	1.53
2	F	600	NAD	C2B-C1B	-15.31	1.29	1.53
2	D	600	NAD	C2B-C1B	-15.30	1.29	1.53
2	F	600	NAD	C2D-C1D	-15.29	1.29	1.53
2	E	600	NAD	C2B-C1B	-15.29	1.29	1.53
2	G	600	NAD	C2D-C1D	-15.24	1.29	1.53
2	E	600	NAD	C2D-C1D	-15.19	1.29	1.53
2	H	600	NAD	C2D-C1D	-15.03	1.29	1.53
2	F	600	NAD	O4B-C4B	-6.37	1.30	1.45
2	D	600	NAD	O4B-C4B	-6.37	1.30	1.45
2	C	600	NAD	O4B-C4B	-6.31	1.30	1.45
2	E	600	NAD	O4B-C4B	-6.29	1.30	1.45
2	G	600	NAD	O4B-C4B	-6.28	1.30	1.45
2	H	600	NAD	O4B-C4B	-6.27	1.30	1.45
2	A	600	NAD	O4B-C4B	-6.26	1.30	1.45
2	B	600	NAD	O4B-C4B	-6.20	1.30	1.45
2	H	600	NAD	O4D-C4D	-5.92	1.31	1.45
2	F	600	NAD	O4D-C4D	-5.88	1.31	1.45
2	B	600	NAD	O4D-C4D	-5.87	1.31	1.45
2	G	600	NAD	O4D-C4D	-5.86	1.31	1.45
2	C	600	NAD	O4D-C4D	-5.85	1.31	1.45
2	E	600	NAD	O4D-C4D	-5.84	1.31	1.45
2	D	600	NAD	O4D-C4D	-5.80	1.31	1.45
2	A	600	NAD	O4D-C4D	-5.77	1.31	1.45
2	E	600	NAD	O3D-C3D	-3.27	1.35	1.43
2	G	600	NAD	O3D-C3D	-3.24	1.35	1.43
2	F	600	NAD	O3D-C3D	-3.23	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NAD	O3D-C3D	-3.23	1.35	1.43
2	B	600	NAD	O3D-C3D	-3.23	1.35	1.43
2	C	600	NAD	O3D-C3D	-3.20	1.35	1.43
2	H	600	NAD	O3D-C3D	-3.19	1.35	1.43
2	D	600	NAD	O3D-C3D	-3.17	1.35	1.43
2	H	600	NAD	O3B-C3B	-3.06	1.35	1.43
2	D	600	NAD	O3B-C3B	-3.03	1.35	1.43
2	F	600	NAD	O3B-C3B	-3.02	1.35	1.43
2	E	600	NAD	O3B-C3B	-3.01	1.35	1.43
2	C	600	NAD	O3B-C3B	-3.01	1.35	1.43
2	A	600	NAD	O3B-C3B	-3.01	1.35	1.43
2	G	600	NAD	O3B-C3B	-2.99	1.35	1.43
2	B	600	NAD	O3B-C3B	-2.96	1.36	1.43
2	F	600	NAD	C5A-C4A	-2.37	1.35	1.40
2	D	600	NAD	C5A-C4A	-2.36	1.35	1.40
2	C	600	NAD	C5A-C4A	-2.36	1.35	1.40
2	B	600	NAD	C5A-C4A	-2.34	1.35	1.40
2	H	600	NAD	C5A-C4A	-2.32	1.35	1.40
2	G	600	NAD	C5A-C4A	-2.31	1.35	1.40
2	A	600	NAD	C5A-C4A	-2.29	1.35	1.40
2	E	600	NAD	C5A-C4A	-2.29	1.35	1.40
2	C	600	NAD	C2N-N1N	2.26	1.38	1.35
2	B	600	NAD	C2N-N1N	2.27	1.38	1.35
2	B	600	NAD	C6A-N6A	2.34	1.43	1.34
2	F	600	NAD	C2N-N1N	2.34	1.38	1.35
2	A	600	NAD	C6A-N6A	2.35	1.43	1.34
2	E	600	NAD	C6A-N6A	2.35	1.43	1.34
2	D	600	NAD	C6A-N6A	2.35	1.43	1.34
2	G	600	NAD	C6A-N6A	2.36	1.43	1.34
2	D	600	NAD	O2D-C2D	2.36	1.48	1.43
2	F	600	NAD	C6A-N6A	2.36	1.43	1.34
2	C	600	NAD	C6A-N6A	2.36	1.43	1.34
2	H	600	NAD	C6A-N6A	2.37	1.43	1.34
2	E	600	NAD	C2N-N1N	2.37	1.38	1.35
2	G	600	NAD	O2D-C2D	2.38	1.48	1.43
2	C	600	NAD	O2D-C2D	2.39	1.48	1.43
2	E	600	NAD	O2D-C2D	2.40	1.48	1.43
2	A	600	NAD	O2D-C2D	2.40	1.48	1.43
2	A	600	NAD	C2N-N1N	2.40	1.38	1.35
2	D	600	NAD	C2N-N1N	2.41	1.38	1.35
2	F	600	NAD	O2D-C2D	2.42	1.48	1.43
2	F	600	NAD	C2A-N3A	2.42	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	600	NAD	O2D-C2D	2.42	1.48	1.43
2	C	600	NAD	C2A-N3A	2.42	1.36	1.32
2	D	600	NAD	C2A-N3A	2.43	1.36	1.32
2	H	600	NAD	C2N-N1N	2.45	1.38	1.35
2	B	600	NAD	O2D-C2D	2.46	1.48	1.43
2	G	600	NAD	C2A-N3A	2.46	1.36	1.32
2	G	600	NAD	C2N-N1N	2.48	1.38	1.35
2	H	600	NAD	C2A-N3A	2.48	1.36	1.32
2	B	600	NAD	C2A-N3A	2.49	1.36	1.32
2	A	600	NAD	C2A-N3A	2.49	1.36	1.32
2	E	600	NAD	C2A-N3A	2.53	1.36	1.32
2	F	600	NAD	O2B-C2B	2.77	1.49	1.43
2	H	600	NAD	O2B-C2B	2.78	1.49	1.43
2	A	600	NAD	O2B-C2B	2.80	1.49	1.43
2	C	600	NAD	O2B-C2B	2.80	1.49	1.43
2	B	600	NAD	O2B-C2B	2.80	1.49	1.43
2	G	600	NAD	O2B-C2B	2.81	1.49	1.43
2	D	600	NAD	O2B-C2B	2.82	1.49	1.43
2	E	600	NAD	O2B-C2B	2.84	1.49	1.43
2	D	600	NAD	C3N-C7N	3.29	1.55	1.50
2	A	600	NAD	C3N-C7N	3.35	1.55	1.50
2	F	600	NAD	C3N-C7N	3.36	1.55	1.50
2	C	600	NAD	C3N-C7N	3.38	1.55	1.50
2	H	600	NAD	C3N-C7N	3.38	1.55	1.50
2	B	600	NAD	C3N-C7N	3.38	1.55	1.50
2	E	600	NAD	C3N-C7N	3.38	1.55	1.50
2	G	600	NAD	C3N-C7N	3.41	1.55	1.50
2	G	600	NAD	C7N-N7N	5.79	1.44	1.33
2	A	600	NAD	C7N-N7N	5.83	1.44	1.33
2	E	600	NAD	C7N-N7N	5.84	1.44	1.33
2	F	600	NAD	C7N-N7N	5.85	1.44	1.33
2	D	600	NAD	C7N-N7N	5.86	1.44	1.33
2	C	600	NAD	C7N-N7N	5.86	1.44	1.33
2	B	600	NAD	C7N-N7N	5.90	1.44	1.33
2	H	600	NAD	C7N-N7N	5.90	1.44	1.33
2	B	600	NAD	O4D-C1D	14.24	1.61	1.41
2	A	600	NAD	O4D-C1D	14.29	1.61	1.41
2	D	600	NAD	O4D-C1D	14.35	1.61	1.41
2	F	600	NAD	O4D-C1D	14.37	1.61	1.41
2	C	600	NAD	O4D-C1D	14.39	1.61	1.41
2	E	600	NAD	O4D-C1D	14.41	1.61	1.41
2	G	600	NAD	O4D-C1D	14.51	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	NAD	O4B-C1B	14.51	1.62	1.41
2	H	600	NAD	O4D-C1D	14.63	1.62	1.41
2	E	600	NAD	O4B-C1B	14.76	1.62	1.41
2	G	600	NAD	O4B-C1B	14.77	1.62	1.41
2	A	600	NAD	O4B-C1B	14.80	1.62	1.41
2	H	600	NAD	O4B-C1B	14.86	1.62	1.41
2	F	600	NAD	O4B-C1B	14.86	1.62	1.41
2	B	600	NAD	O4B-C1B	14.89	1.62	1.41
2	D	600	NAD	O4B-C1B	14.96	1.62	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	NAD	N3A-C2A-N1A	-11.44	119.88	128.87
2	G	600	NAD	N3A-C2A-N1A	-11.30	120.00	128.87
2	D	600	NAD	N3A-C2A-N1A	-11.24	120.04	128.87
2	C	600	NAD	N3A-C2A-N1A	-11.22	120.06	128.87
2	H	600	NAD	N3A-C2A-N1A	-11.21	120.06	128.87
2	B	600	NAD	N3A-C2A-N1A	-11.20	120.07	128.87
2	A	600	NAD	N3A-C2A-N1A	-11.16	120.11	128.87
2	E	600	NAD	N3A-C2A-N1A	-11.10	120.15	128.87
2	A	600	NAD	C4D-O4D-C1D	-3.81	105.61	109.64
2	F	600	NAD	C1B-N9A-C4A	-2.85	123.63	126.81
2	D	600	NAD	C1B-N9A-C4A	-2.65	123.84	126.81
2	H	600	NAD	C1B-N9A-C4A	-2.65	123.85	126.81
2	D	600	NAD	C4D-O4D-C1D	-2.59	106.90	109.64
2	D	600	NAD	C4B-O4B-C1B	-2.56	106.93	109.64
2	F	600	NAD	C4D-O4D-C1D	-2.52	106.97	109.64
2	H	600	NAD	N6A-C6A-N1A	-2.45	114.40	118.52
2	B	600	NAD	N6A-C6A-N1A	-2.41	114.47	118.52
2	F	600	NAD	N6A-C6A-N1A	-2.37	114.54	118.52
2	E	600	NAD	N6A-C6A-N1A	-2.33	114.61	118.52
2	G	600	NAD	N6A-C6A-N1A	-2.32	114.63	118.52
2	C	600	NAD	N6A-C6A-N1A	-2.32	114.63	118.52
2	F	600	NAD	C4B-O4B-C1B	-2.31	107.19	109.64
2	C	600	NAD	C1B-N9A-C4A	-2.27	124.27	126.81
2	A	600	NAD	N6A-C6A-N1A	-2.27	114.70	118.52
2	A	600	NAD	C2D-C1D-N1N	-2.27	109.08	113.53
2	A	600	NAD	C1B-N9A-C4A	-2.24	124.30	126.81
2	D	600	NAD	N6A-C6A-N1A	-2.22	114.79	118.52
2	B	600	NAD	C4D-O4D-C1D	-2.19	107.32	109.64
2	B	600	NAD	C1B-N9A-C4A	-2.05	124.52	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	NAD	C2D-C1D-N1N	-2.01	109.60	113.53
2	G	600	NAD	C1B-N9A-C4A	-2.00	124.57	126.81
2	D	600	NAD	O4D-C1D-N1N	2.50	110.80	108.10
2	A	600	NAD	O4D-C1D-N1N	3.81	112.22	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAD	2	0
2	B	600	NAD	3	0
2	C	600	NAD	3	0
2	D	600	NAD	3	0
2	F	600	NAD	2	0
2	G	600	NAD	2	0
2	H	600	NAD	4	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	440/524 (83%)	-0.20	0 100 100	23, 34, 47, 61	0
1	B	439/524 (83%)	-0.19	1 (0%) 95 97	22, 33, 49, 62	0
1	C	439/524 (83%)	-0.05	4 (0%) 85 89	24, 40, 54, 73	0
1	D	445/524 (84%)	-0.13	1 (0%) 95 97	22, 36, 49, 57	0
1	E	439/524 (83%)	-0.19	0 100 100	24, 34, 49, 61	0
1	F	440/524 (83%)	-0.01	5 (1%) 82 86	24, 37, 64, 85	0
1	G	445/524 (84%)	-0.15	2 (0%) 93 95	24, 37, 51, 66	0
1	H	439/524 (83%)	0.24	14 (3%) 51 60	25, 50, 74, 90	0
All	All	3526/4192 (84%)	-0.08	27 (0%) 87 90	22, 36, 58, 90	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	375	LYS	3.6
1	H	398	VAL	3.6
1	H	149	TYR	3.6
1	F	361	PRO	3.0
1	F	362	ALA	3.0
1	H	375	LYS	2.9
1	H	406	LEU	2.8
1	F	365	GLN	2.7
1	H	298	ALA	2.6
1	C	373	THR	2.5
1	C	374	ALA	2.5
1	H	355	ALA	2.4
1	H	348	PHE	2.4
1	H	354	GLY	2.3
1	H	395	GLY	2.2
1	H	230	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	369	ASP	2.2
1	C	414	PRO	2.2
1	D	139	MET	2.1
1	G	86	VAL	2.1
1	H	418	GLU	2.1
1	C	331	VAL	2.1
1	H	250	LEU	2.1
1	H	86	VAL	2.1
1	H	141	VAL	2.0
1	B	174[A]	PHE	2.0
1	G	257	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	C	600	44/44	0.91	0.18	1.92	39,47,59,62	44
2	NAD	H	600	44/44	0.87	0.20	1.49	43,62,67,68	44
2	NAD	E	600	44/44	0.93	0.15	1.18	30,38,45,48	44
2	NAD	B	600	44/44	0.95	0.13	0.36	31,44,49,52	0
2	NAD	G	600	44/44	0.93	0.13	0.08	31,41,44,49	44
2	NAD	F	600	44/44	0.94	0.14	-0.10	38,44,48,50	44
2	NAD	A	600	44/44	0.94	0.12	-0.21	32,43,47,50	0
2	NAD	D	600	44/44	0.95	0.12	-0.26	29,42,45,46	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.