



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2016 – 01:47 PM EDT

PDB ID : 5FHZ
Title : Human aldehyde dehydrogenase 1A3 complexed with NAD(+) and retinoic acid
Authors : Moretti, A.; Rizzi, M.; Garavaglia, S.
Deposited on : 2015-12-22
Resolution : 2.90 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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-20027939
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-20027939

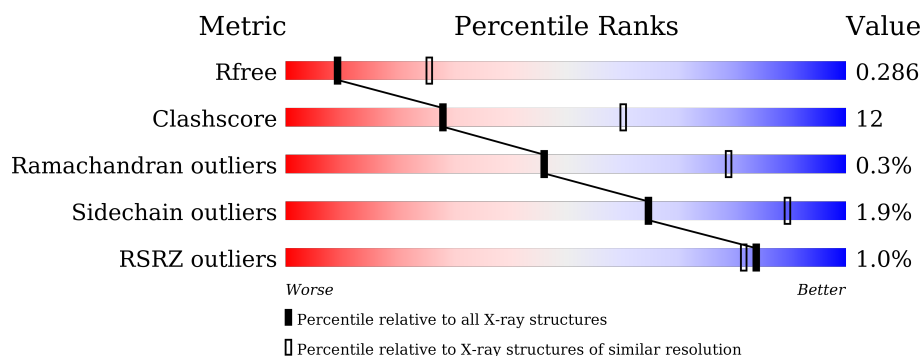
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 ≥ 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	529	<div> <div>68%</div> <div>24%</div> <div>• 8%</div> </div>
1	B	529	<div> <div>66%</div> <div>23%</div> <div>• 10%</div> </div>
1	C	529	<div> <div>68%</div> <div>23%</div> <div>• 8%</div> </div>
1	D	529	<div> <div>71%</div> <div>21%</div> <div>• 8%</div> </div>
1	E	529	<div> <div>2%</div> <div>68%</div> <div>22%</div> <div>• 10%</div> </div>
1	F	529	<div> <div>2%</div> <div>63%</div> <div>21%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	529	
1	H	529	

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	REA	A	602	-	-	X	X
3	REA	B	602	-	-	-	X
3	REA	C	602	-	-	-	X
3	REA	D	602	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 29992 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 family 1 member A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3780	2410	646	704	20			
1	B	475	Total	C	N	O	S	0	0	0
			3666	2336	628	682	20			
1	C	489	Total	C	N	O	S	0	0	0
			3779	2409	646	704	20			
1	D	488	Total	C	N	O	S	0	0	0
			3775	2407	645	703	20			
1	E	478	Total	C	N	O	S	0	0	0
			3695	2358	630	688	19			
1	F	449	Total	C	N	O	S	0	0	0
			3453	2201	586	647	19			
1	G	462	Total	C	N	O	S	0	0	0
			3570	2282	606	664	18			
1	H	488	Total	C	N	O	S	0	0	0
			3771	2403	645	703	20			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP P47895
A	-15	HIS	-	expression tag	UNP P47895
A	-14	HIS	-	expression tag	UNP P47895
A	-13	HIS	-	expression tag	UNP P47895
A	-12	HIS	-	expression tag	UNP P47895
A	-11	HIS	-	expression tag	UNP P47895
A	-10	LEU	-	expression tag	UNP P47895
A	-9	GLU	-	expression tag	UNP P47895
A	-8	SER	-	expression tag	UNP P47895
A	-7	THR	-	expression tag	UNP P47895
A	-6	SER	-	expression tag	UNP P47895
A	-5	LEU	-	expression tag	UNP P47895
A	-4	TYR	-	expression tag	UNP P47895

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	LYS	-	expression tag	UNP P47895
A	-2	LYS	-	expression tag	UNP P47895
A	-1	ALA	-	expression tag	UNP P47895
A	0	GLY	-	expression tag	UNP P47895
B	-16	HIS	-	expression tag	UNP P47895
B	-15	HIS	-	expression tag	UNP P47895
B	-14	HIS	-	expression tag	UNP P47895
B	-13	HIS	-	expression tag	UNP P47895
B	-12	HIS	-	expression tag	UNP P47895
B	-11	HIS	-	expression tag	UNP P47895
B	-10	LEU	-	expression tag	UNP P47895
B	-9	GLU	-	expression tag	UNP P47895
B	-8	SER	-	expression tag	UNP P47895
B	-7	THR	-	expression tag	UNP P47895
B	-6	SER	-	expression tag	UNP P47895
B	-5	LEU	-	expression tag	UNP P47895
B	-4	TYR	-	expression tag	UNP P47895
B	-3	LYS	-	expression tag	UNP P47895
B	-2	LYS	-	expression tag	UNP P47895
B	-1	ALA	-	expression tag	UNP P47895
B	0	GLY	-	expression tag	UNP P47895
C	-16	HIS	-	expression tag	UNP P47895
C	-15	HIS	-	expression tag	UNP P47895
C	-14	HIS	-	expression tag	UNP P47895
C	-13	HIS	-	expression tag	UNP P47895
C	-12	HIS	-	expression tag	UNP P47895
C	-11	HIS	-	expression tag	UNP P47895
C	-10	LEU	-	expression tag	UNP P47895
C	-9	GLU	-	expression tag	UNP P47895
C	-8	SER	-	expression tag	UNP P47895
C	-7	THR	-	expression tag	UNP P47895
C	-6	SER	-	expression tag	UNP P47895
C	-5	LEU	-	expression tag	UNP P47895
C	-4	TYR	-	expression tag	UNP P47895
C	-3	LYS	-	expression tag	UNP P47895
C	-2	LYS	-	expression tag	UNP P47895
C	-1	ALA	-	expression tag	UNP P47895
C	0	GLY	-	expression tag	UNP P47895
D	-16	HIS	-	expression tag	UNP P47895
D	-15	HIS	-	expression tag	UNP P47895
D	-14	HIS	-	expression tag	UNP P47895
D	-13	HIS	-	expression tag	UNP P47895

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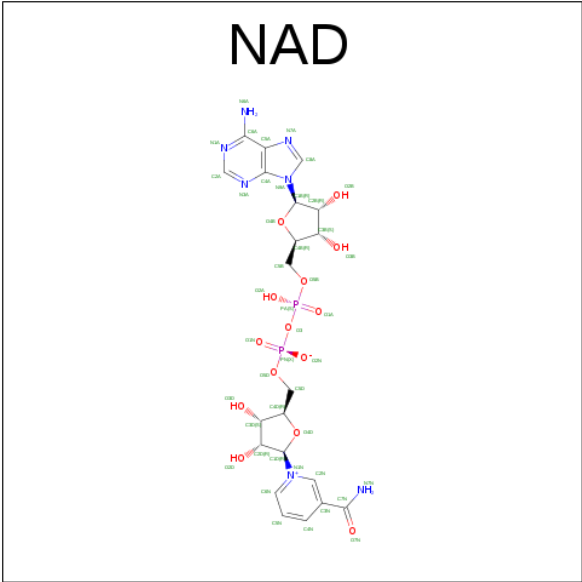
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P47895
D	-11	HIS	-	expression tag	UNP P47895
D	-10	LEU	-	expression tag	UNP P47895
D	-9	GLU	-	expression tag	UNP P47895
D	-8	SER	-	expression tag	UNP P47895
D	-7	THR	-	expression tag	UNP P47895
D	-6	SER	-	expression tag	UNP P47895
D	-5	LEU	-	expression tag	UNP P47895
D	-4	TYR	-	expression tag	UNP P47895
D	-3	LYS	-	expression tag	UNP P47895
D	-2	LYS	-	expression tag	UNP P47895
D	-1	ALA	-	expression tag	UNP P47895
D	0	GLY	-	expression tag	UNP P47895
E	-16	HIS	-	expression tag	UNP P47895
E	-15	HIS	-	expression tag	UNP P47895
E	-14	HIS	-	expression tag	UNP P47895
E	-13	HIS	-	expression tag	UNP P47895
E	-12	HIS	-	expression tag	UNP P47895
E	-11	HIS	-	expression tag	UNP P47895
E	-10	LEU	-	expression tag	UNP P47895
E	-9	GLU	-	expression tag	UNP P47895
E	-8	SER	-	expression tag	UNP P47895
E	-7	THR	-	expression tag	UNP P47895
E	-6	SER	-	expression tag	UNP P47895
E	-5	LEU	-	expression tag	UNP P47895
E	-4	TYR	-	expression tag	UNP P47895
E	-3	LYS	-	expression tag	UNP P47895
E	-2	LYS	-	expression tag	UNP P47895
E	-1	ALA	-	expression tag	UNP P47895
E	0	GLY	-	expression tag	UNP P47895
F	-16	HIS	-	expression tag	UNP P47895
F	-15	HIS	-	expression tag	UNP P47895
F	-14	HIS	-	expression tag	UNP P47895
F	-13	HIS	-	expression tag	UNP P47895
F	-12	HIS	-	expression tag	UNP P47895
F	-11	HIS	-	expression tag	UNP P47895
F	-10	LEU	-	expression tag	UNP P47895
F	-9	GLU	-	expression tag	UNP P47895
F	-8	SER	-	expression tag	UNP P47895
F	-7	THR	-	expression tag	UNP P47895
F	-6	SER	-	expression tag	UNP P47895
F	-5	LEU	-	expression tag	UNP P47895

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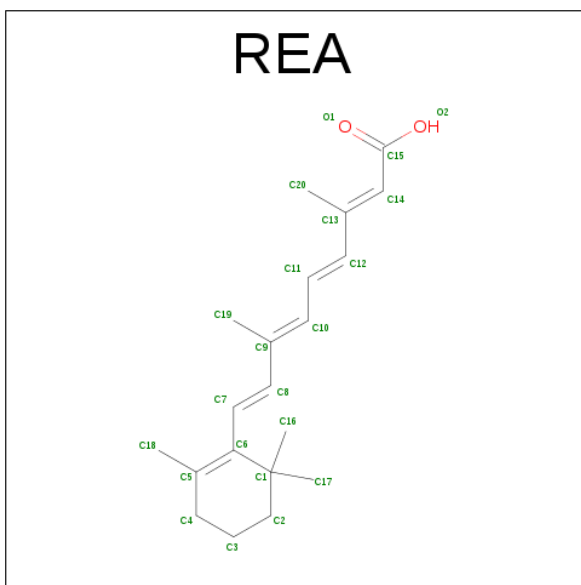
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	TYR	-	expression tag	UNP P47895
F	-3	LYS	-	expression tag	UNP P47895
F	-2	LYS	-	expression tag	UNP P47895
F	-1	ALA	-	expression tag	UNP P47895
F	0	GLY	-	expression tag	UNP P47895
G	-16	HIS	-	expression tag	UNP P47895
G	-15	HIS	-	expression tag	UNP P47895
G	-14	HIS	-	expression tag	UNP P47895
G	-13	HIS	-	expression tag	UNP P47895
G	-12	HIS	-	expression tag	UNP P47895
G	-11	HIS	-	expression tag	UNP P47895
G	-10	LEU	-	expression tag	UNP P47895
G	-9	GLU	-	expression tag	UNP P47895
G	-8	SER	-	expression tag	UNP P47895
G	-7	THR	-	expression tag	UNP P47895
G	-6	SER	-	expression tag	UNP P47895
G	-5	LEU	-	expression tag	UNP P47895
G	-4	TYR	-	expression tag	UNP P47895
G	-3	LYS	-	expression tag	UNP P47895
G	-2	LYS	-	expression tag	UNP P47895
G	-1	ALA	-	expression tag	UNP P47895
G	0	GLY	-	expression tag	UNP P47895
H	-16	HIS	-	expression tag	UNP P47895
H	-15	HIS	-	expression tag	UNP P47895
H	-14	HIS	-	expression tag	UNP P47895
H	-13	HIS	-	expression tag	UNP P47895
H	-12	HIS	-	expression tag	UNP P47895
H	-11	HIS	-	expression tag	UNP P47895
H	-10	LEU	-	expression tag	UNP P47895
H	-9	GLU	-	expression tag	UNP P47895
H	-8	SER	-	expression tag	UNP P47895
H	-7	THR	-	expression tag	UNP P47895
H	-6	SER	-	expression tag	UNP P47895
H	-5	LEU	-	expression tag	UNP P47895
H	-4	TYR	-	expression tag	UNP P47895
H	-3	LYS	-	expression tag	UNP P47895
H	-2	LYS	-	expression tag	UNP P47895
H	-1	ALA	-	expression tag	UNP P47895
H	0	GLY	-	expression tag	UNP P47895

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 RETINOIC ACID (three-letter code: REA) (formula: C₂₀H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	20	2		
3	B	1	Total	C	O	0	0
			22	20	2		
3	C	1	Total	C	O	7	0
			22	20	2		
3	D	1	Total	C	O	0	0
			22	20	2		

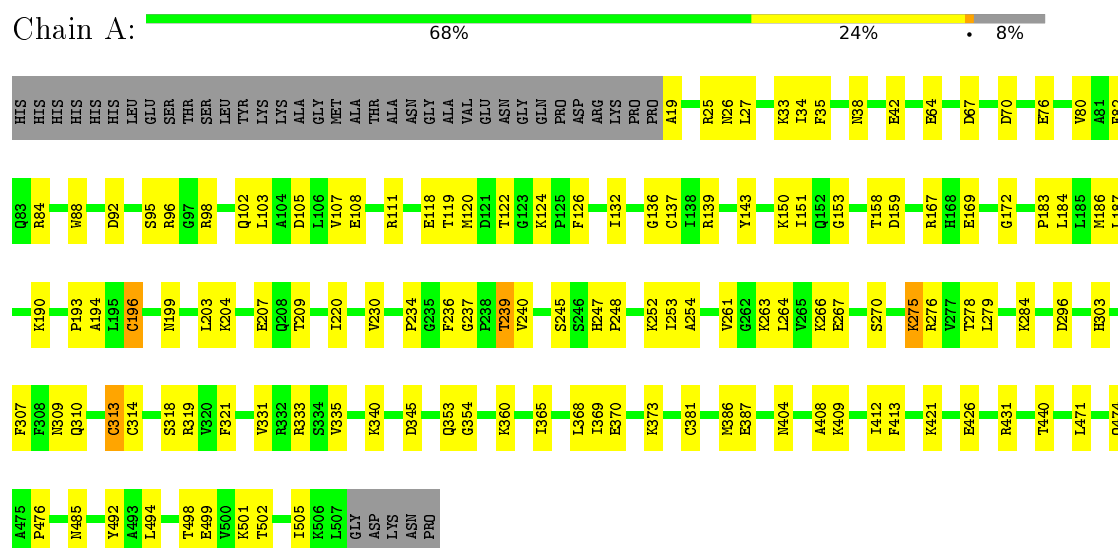
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	15	Total	O	0	0
			15	15		
4	C	9	Total	O	0	0
			9	9		
4	D	12	Total	O	0	0
			12	12		
4	E	2	Total	O	0	0
			2	2		
4	F	4	Total	O	0	0
			4	4		
4	H	2	Total	O	0	0
			2	2		

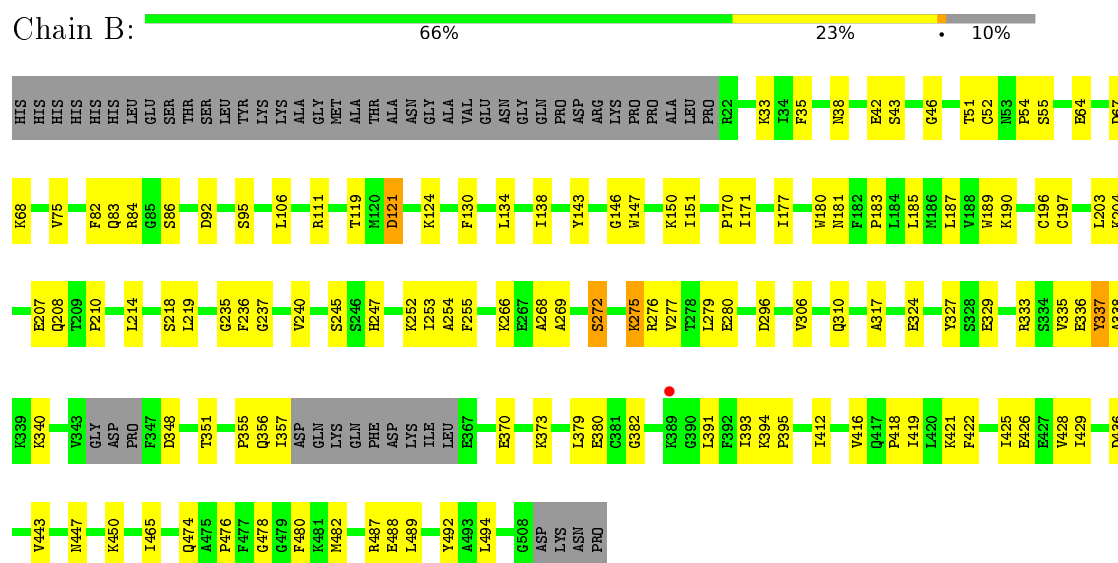
3 Residue-property plots

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 family 1 member A3



- Molecule 1: Aldehyde dehydrogenase family 1 member A3

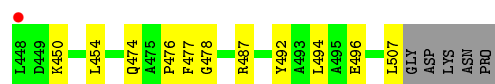


- Molecule 1: Aldehyde dehydrogenase family 1 member A3

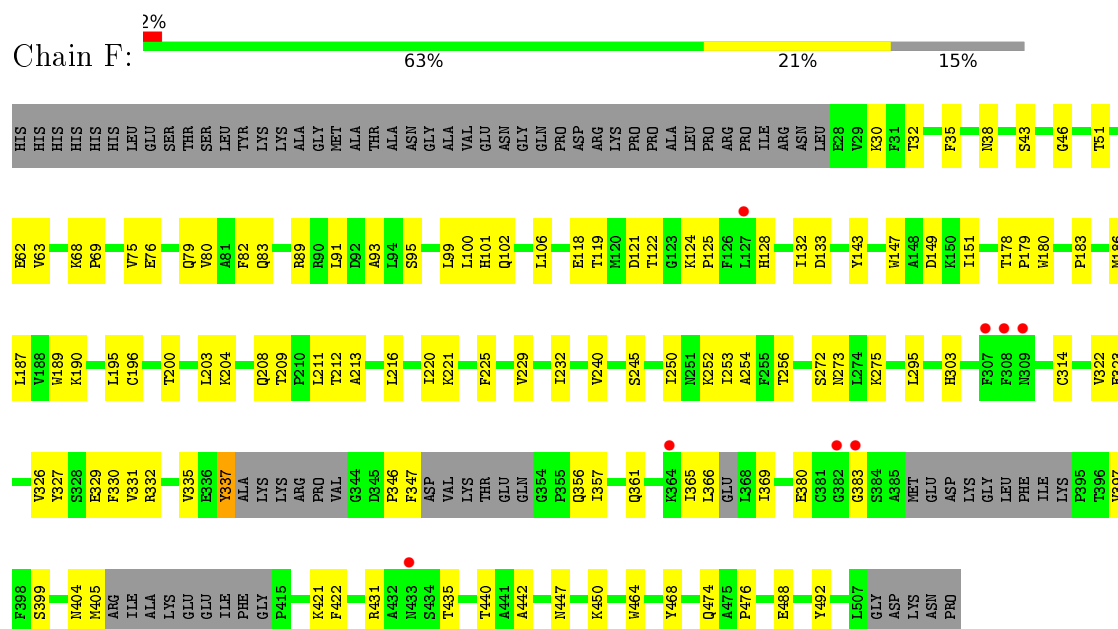
S456	K364	V230	K68	HIS
N466	I365	P234	P69	HIS
Q474	L368	P234	D70	HIS
A475	L369	V240	V71	HIS
P476	E370	G241	R89	HIS
	S371		L111	LEU
M482	K374	S245		GLU
E491	L379	I253	E118	THR
Y492	E380	I253	T119	THR
A493	C381	A268	K124	LEU
L494	G382	G382	L127	THR
T498	G383	S272	L127	LVS
			F130	LVS
I505	M386	K284		ALA
	E387	I288		GLY
G508	D388	I288	D133	ALA
ASP	K389	D294	Y143	THR
LVS	G390	L295	ASN	ALA
ASN	L391	D296	G146	ALA
PRO	K394	V299	M147	GLY
	P395		A148	ALA
	T396	Q310	D149	VAL
	N404		K150	GLU
		S318	ASN	ASN
	I407	E329	G151	GLY
	A408	F330	M161	GLN
	K409		V162	PRO
	E410		ARG	ASP
	E411	R333	L167	ARG
	E411	S334	H168	LVS
	I412	V335	E169	PRO
	F413			PRO
	G414	Y337	G172	ALA
	P415	A338		L20
	V416	K339	T178	K30
	Q417	K340	L184	
	P418	R341	L185	K33
	I419	F342		I34
	L420	V343	W189	F35
	K421	G344		
		D345	L191	N38
	I425			N39
	E426	K350	L195	N40
	E427	T351	C196	R41
	V428	E352		E42
	R431	Q353	N199	N53
			T200	P54
	D436		M201	S55
	A437	V356	V202	T56
	G438	K356	L203	S57
		T357	K204	E58
	F444	D358		
		K359	L214	E64
	K450	K360	Y215	E67
			I216	

- [illegible]

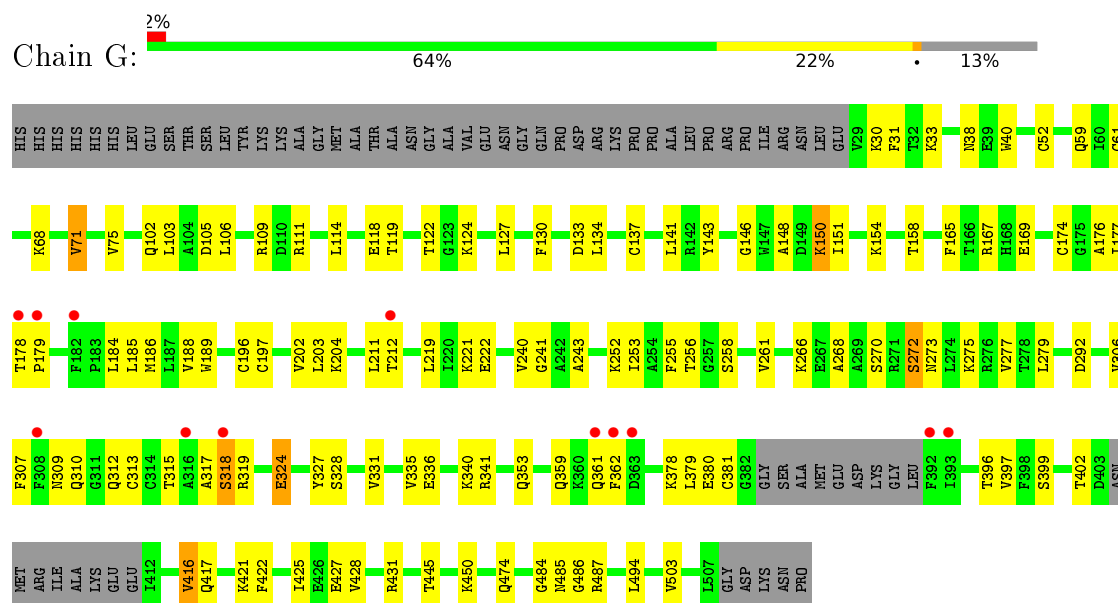
- | | | | |
|------|------|------|-----|
| V331 | L203 | Q79 | HIS |
| V335 | K204 | F82 | HIS |
| D348 | A206 | W88 | HIS |
| T351 | E207 | D92 | HIS |
| L357 | L211 | T212 | LEU |
| L365 | A213 | S95 | GLU |
| L366 | L214 | H101 | THR |
| L369 | Y215 | E108 | SPR |
| GLU | S218 | R111 | LEU |
| SER | L219 | L117 | TTR |
| GLY | V230 | E118 | LYS |
| LYS | F236 | M120 | ALA |
| L376 | G237 | K124 | GLY |
| G376 | P238 | L127 | ASN |
| C381 | T239 | L138 | ALA |
| G382 | V240 | R142 | GLY |
| G383 | H247 | Y143 | VAL |
| G384 | P248 | E135 | GLU |
| A385 | L253 | I138 | ASN |
| MET | T256 | R142 | GLN |
| GLU | V277 | L149 | PRO |
| D388 | E280 | K150 | ASP |
| F392 | L281 | I151 | ARG |
| L393 | G282 | I171 | LYS |
| K394 | G283 | G172 | PRO |
| P395 | D292 | G175 | ALA |
| E400 | A293 | P179 | LEU |
| V401 | L295 | W180 | PRO |
| M405 | D294 | M181 | ARG |
| A406 | F307 | L185 | L27 |
| A408 | F308 | M186 | F35 |
| F413 | N309 | L187 | N38 |
| K421 | Q310 | L191 | K44 |
| L425 | G311 | L195 | S45 |
| V428 | A317 | C196 | G49 |
| L429 | S318 | G198 | P49 |
| K430 | R319 | M201 | P49 |
| R431 | V326 | W202 | P49 |
| Y437 | V327 | | V75 |
| G438 | | | |
| L439 | | | |



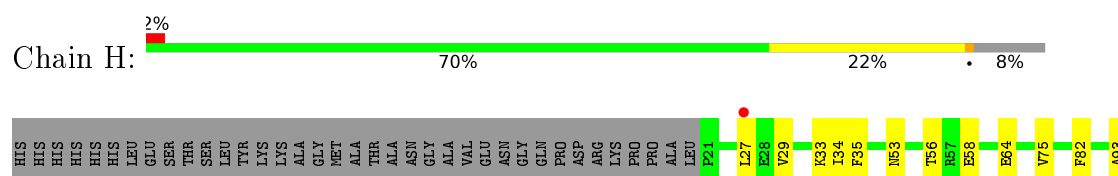
• Molecule 1: Aldehyde dehydrogenase family 1 member A3

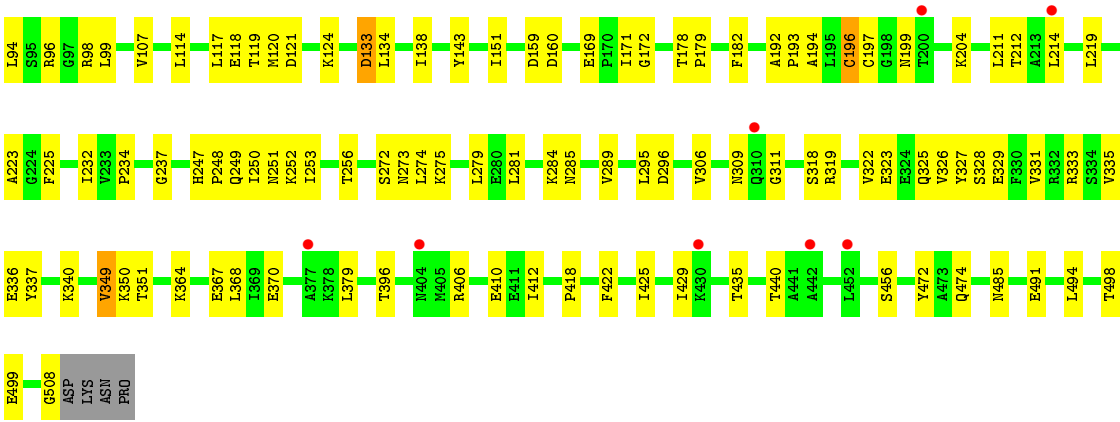


• Molecule 1: Aldehyde dehydrogenase family 1 member A3



• Molecule 1: Aldehyde dehydrogenase family 1 member A3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.66Å 159.78Å 177.65Å 90.00° 93.69° 90.00°	Depositor
Resolution (Å)	49.57 – 2.90 47.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.57-2.90) 98.3 (47.51-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.228 , 0.289 0.228 , 0.286	Depositor DCC
R_{free} test set	5047 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 16.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29992	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 36.07 % 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 5.2864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: REA, 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	0.61	0/3858	0.75	0/5221
1	B	0.61	0/3739	0.76	1/5056 (0.0%)
1	C	0.61	0/3857	0.76	0/5219
1	D	0.60	0/3853	0.75	0/5214
1	E	0.39	0/3770	0.62	0/5101
1	F	0.42	0/3521	0.61	0/4761
1	G	0.44	0/3644	0.62	0/4932
1	H	0.42	0/3849	0.62	0/5207
All	All	0.52	0/30091	0.69	1/40711 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	CB-CG-OD2	-5.95	112.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3780	0	3813	104	0
1	B	3666	0	3696	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3779	0	3811	97	0
1	D	3775	0	3808	82	0
1	E	3695	0	3721	84	0
1	F	3453	0	3457	74	0
1	G	3570	0	3593	88	0
1	H	3771	0	3801	87	0
2	A	44	0	26	1	0
2	B	44	0	26	3	0
2	C	44	0	26	4	0
2	D	44	0	26	4	0
2	E	44	0	26	4	0
2	F	44	0	26	3	0
2	G	44	0	26	5	0
2	H	44	0	26	2	0
3	A	22	0	27	18	0
3	B	22	0	27	7	0
3	C	22	0	27	7	0
3	D	22	0	27	10	0
4	A	19	0	0	2	0
4	B	15	0	0	1	0
4	C	9	0	0	0	0
4	D	12	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	0	0
4	H	2	0	0	1	0
All	All	29992	0	30016	699	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 12.

The worst 5 of 699 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:A:310:GLN:OE1	1:A:353:GLN:HG3	1.48	1.12
1:B:180:TRP:CE3	1:B:357:ILE:HD12	1.90	1.05
1:C:34:ILE:HD13	1:C:234:PRO:HD2	1.47	0.96
1:D:56:THR:O	1:D:58:GLU:N	1.98	0.96
1:E:180:TRP:CE3	1:E:357:ILE:HD13	2.02	0.94

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	487/529 (92%)	464 (95%)	23 (5%)	0	100	100
1	B	469/529 (89%)	434 (92%)	35 (8%)	0	100	100
1	C	487/529 (92%)	459 (94%)	24 (5%)	4 (1%)	24	60
1	D	486/529 (92%)	462 (95%)	23 (5%)	1 (0%)	52	84
1	E	472/529 (89%)	443 (94%)	25 (5%)	4 (1%)	24	60
1	F	437/529 (83%)	419 (96%)	18 (4%)	0	100	100
1	G	456/529 (86%)	432 (95%)	22 (5%)	2 (0%)	39	74
1	H	486/529 (92%)	454 (93%)	30 (6%)	2 (0%)	39	74
All	All	3780/4232 (89%)	3567 (94%)	200 (5%)	13 (0%)	46	79

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	57	ARG
1	D	57	ARG
1	E	384	SER
1	H	349	VAL
1	C	387	GLU

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	405/437 (93%)	399 (98%)	6 (2%)	72	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	392/437 (90%)	387 (99%)	5 (1%)	76	94
1	C	405/437 (93%)	398 (98%)	7 (2%)	68	91
1	D	405/437 (93%)	397 (98%)	8 (2%)	63	88
1	E	396/437 (91%)	387 (98%)	9 (2%)	58	87
1	F	370/437 (85%)	362 (98%)	8 (2%)	60	88
1	G	383/437 (88%)	374 (98%)	9 (2%)	58	87
1	H	404/437 (92%)	396 (98%)	8 (2%)	63	88
All	All	3160/3496 (90%)	3100 (98%)	60 (2%)	65	89

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	181	ASN
1	E	413	PHE
1	H	196	CYS
1	E	292	ASP
1	F	30	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	41	HIS
1	E	79	GLN
1	G	312	GLN
1	D	79	GLN
1	G	353	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	601	-	42,48,48	1.06	2 (4%)	46,73,73	2.14	9 (19%)
3	REA	A	602	-	19,22,22	0.94	1 (5%)	26,30,30	2.19	7 (26%)
2	NAD	B	601	-	42,48,48	0.84	1 (2%)	46,73,73	1.86	7 (15%)
3	REA	B	602	-	19,22,22	0.86	0	26,30,30	2.62	9 (34%)
2	NAD	C	601	-	42,48,48	0.86	2 (4%)	46,73,73	2.02	6 (13%)
3	REA	C	602	-	19,22,22	0.93	0	26,30,30	2.29	7 (26%)
2	NAD	D	601	-	42,48,48	0.96	2 (4%)	46,73,73	2.07	9 (19%)
3	REA	D	602	-	19,22,22	1.18	2 (10%)	26,30,30	2.79	13 (50%)
2	NAD	E	601	-	42,48,48	0.92	3 (7%)	46,73,73	1.68	3 (6%)
2	NAD	F	601	-	42,48,48	0.87	3 (7%)	46,73,73	1.71	7 (15%)
2	NAD	G	601	-	42,48,48	0.92	2 (4%)	46,73,73	1.88	6 (13%)
2	NAD	H	601	-	42,48,48	0.90	2 (4%)	46,73,73	1.74	5 (10%)

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	601	-	-	0/22/62/62	0/5/5/5
3	REA	A	602	-	-	0/13/32/32	0/1/1/1
2	NAD	B	601	-	-	0/22/62/62	0/5/5/5
3	REA	B	602	-	-	0/13/32/32	0/1/1/1
2	NAD	C	601	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	REA	C	602	-	-	0/13/32/32	0/1/1/1
2	NAD	D	601	-	-	0/22/62/62	0/5/5/5
3	REA	D	602	-	-	0/13/32/32	0/1/1/1
2	NAD	E	601	-	-	0/22/62/62	0/5/5/5
2	NAD	F	601	-	-	0/22/62/62	0/5/5/5
2	NAD	G	601	-	-	0/22/62/62	0/5/5/5
2	NAD	H	601	-	-	0/22/62/62	0/5/5/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	C2B-C1B	-2.94	1.49	1.53
2	C	601	NAD	C5A-C4A	2.01	1.45	1.40
2	F	601	NAD	C2A-N3A	2.07	1.35	1.32
2	E	601	NAD	C2A-N3A	2.10	1.35	1.32
2	G	601	NAD	O4D-C1D	2.11	1.44	1.41

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C2A-N1A	-10.03	121.00	128.87
2	A	601	NAD	N3A-C2A-N1A	-9.40	121.49	128.87
2	B	601	NAD	N3A-C2A-N1A	-8.19	122.44	128.87
2	E	601	NAD	N3A-C2A-N1A	-8.06	122.54	128.87
2	H	601	NAD	N3A-C2A-N1A	-7.91	122.66	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
3	A	602	REA	18	0
2	B	601	NAD	3	0
3	B	602	REA	7	0
2	C	601	NAD	4	0
3	C	602	REA	7	0
2	D	601	NAD	4	0
3	D	602	REA	10	0
2	E	601	NAD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	NAD	3	0
2	G	601	NAD	5	0
2	H	601	NAD	2	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, 95th 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 ²)	Q<0.9
1	A	489/529 (92%)	-0.53	0 100 100	8, 21, 53, 82	0
1	B	475/529 (89%)	-0.48	1 (0%) 95 95	8, 19, 65, 104	0
1	C	489/529 (92%)	-0.41	2 (0%) 93 92	8, 20, 73, 108	0
1	D	488/529 (92%)	-0.56	0 100 100	8, 21, 48, 85	0
1	E	478/529 (90%)	0.01	8 (1%) 73 70	37, 61, 86, 105	0
1	F	449/529 (84%)	-0.10	8 (1%) 71 68	36, 55, 89, 111	0
1	G	462/529 (87%)	0.04	12 (2%) 59 54	39, 57, 87, 107	0
1	H	488/529 (92%)	0.00	9 (1%) 71 68	37, 59, 83, 109	0
All	All	3818/4232 (90%)	-0.26	40 (1%) 84 82	8, 47, 82, 111	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	308	PHE	4.2
1	G	392	PHE	3.8
1	G	178	THR	3.7
1	G	362	PHE	3.5
1	C	389	LYS	3.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [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, 95th 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 ²)	Q<0.9
3	REA	D	602	22/22	0.88	0.32	8.78	19,27,37,39	0
3	REA	B	602	22/22	0.90	0.31	4.49	16,35,57,64	0
3	REA	A	602	22/22	0.86	0.27	3.72	17,28,40,43	0
3	REA	C	602	22/22	0.90	0.24	3.08	12,28,75,85	7
2	NAD	A	601	44/44	0.96	0.19	0.81	17,27,76,78	0
2	NAD	D	601	44/44	0.96	0.19	0.76	18,29,89,92	0
2	NAD	E	601	44/44	0.92	0.23	0.72	56,73,103,104	0
2	NAD	B	601	44/44	0.96	0.19	0.68	11,25,84,84	0
2	NAD	H	601	44/44	0.94	0.21	0.15	43,60,92,95	0
2	NAD	C	601	44/44	0.97	0.17	0.03	14,20,64,70	0
2	NAD	F	601	44/44	0.95	0.17	-0.20	41,52,101,103	0
2	NAD	G	601	44/44	0.94	0.17	-0.58	44,53,81,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.