



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:11 PM BST

PDB ID : 4KWF  
Title : Crystal Structure Analysis of ALDH2+ALDiB33  
Authors : Hurley, T.D.; Kimble-Hill, A.C.  
Deposited on : 2013-05-24  
Resolution : 2.31 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

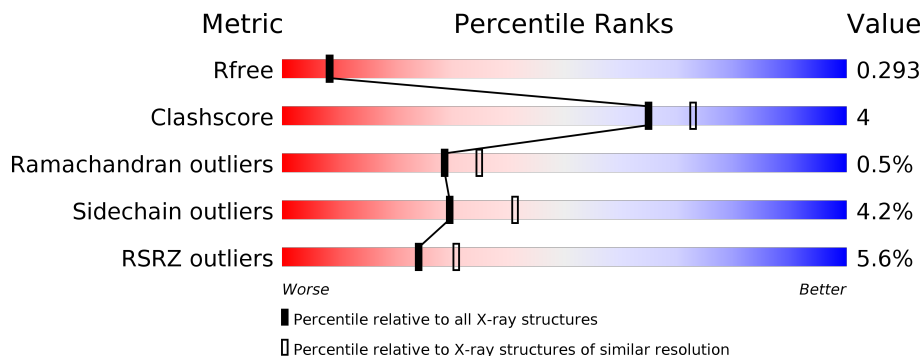
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 89% 10% .</p>
1	B	494	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">11% 85% 13% .</p>
1	C	494	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 89% 10% .</p>
1	D	494	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 89% 11%</p>
1	E	494	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 86% 14% .</p>
1	F	494	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">12% 85% 14% .</p>

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Mol	Chain	Length	Quality of chain
1	G	494	 5% 87% 12%
1	H	494	 2% 90% 9%

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
2	3AK	B	601	-	-	X	-

## 2 Entry composition [i](#)

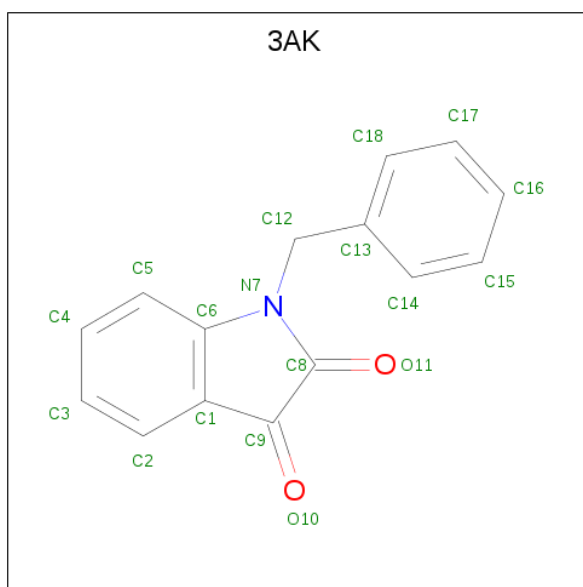
There are 6 unique types of molecules in this entry. The entry contains 30712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3798	2415	648	717	18	0	0	0
1	B	494	3798	2415	648	717	18	0	0	0
1	C	494	3798	2415	648	717	18	0	0	0
1	D	494	3798	2415	648	717	18	0	0	0
1	E	494	3798	2415	648	717	18	0	0	0
1	F	494	3798	2415	648	717	18	0	0	0
1	G	494	3798	2415	648	717	18	0	0	0
1	H	494	3798	2415	648	717	18	0	0	0

- Molecule 2 is 1-benzyl-1H-indole-2,3-dione (three-letter code: 3AK) (formula: C<sub>15</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	15	1	2		
2	B	1	Total	C	N	O	0	0
			18	15	1	2		
2	E	1	Total	C	N	O	0	0
			18	15	1	2		
2	H	1	Total	C	N	O	0	0
			18	15	1	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

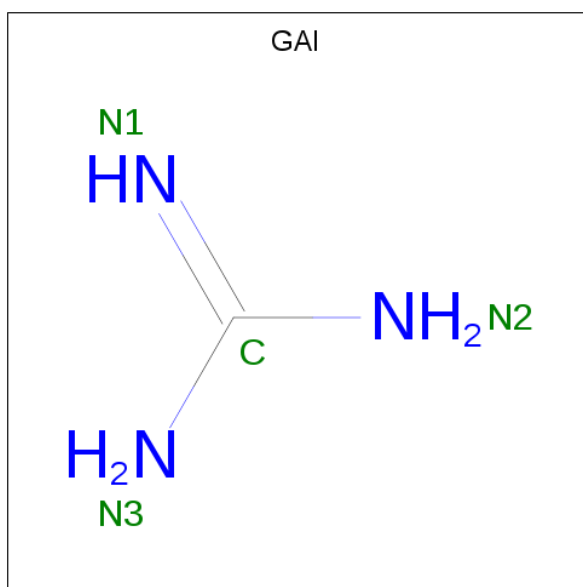
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is GUANIDINE (three-letter code: GAI) (formula: CH<sub>5</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			4	1	3		
5	B	1	Total	C	N	0	0
			4	1	3		
5	C	1	Total	C	N	0	0
			4	1	3		
5	D	1	Total	C	N	0	0
			4	1	3		
5	F	1	Total	C	N	0	0
			4	1	3		
5	G	1	Total	C	N	0	0
			4	1	3		
5	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		
6	B	15	Total	O	0	0
			15	15		
6	C	17	Total	O	0	0
			17	17		
6	D	31	Total	O	0	0
			31	31		
6	E	20	Total	O	0	0
			20	20		

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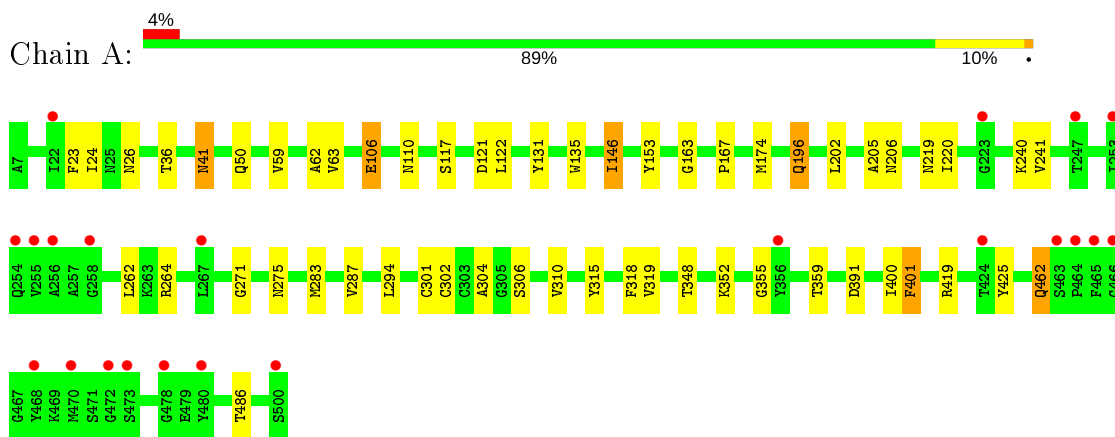
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	20	Total 20	O 20	0	0
6	G	16	Total 16	O 16	0	0
6	H	45	Total 45	O 45	0	0



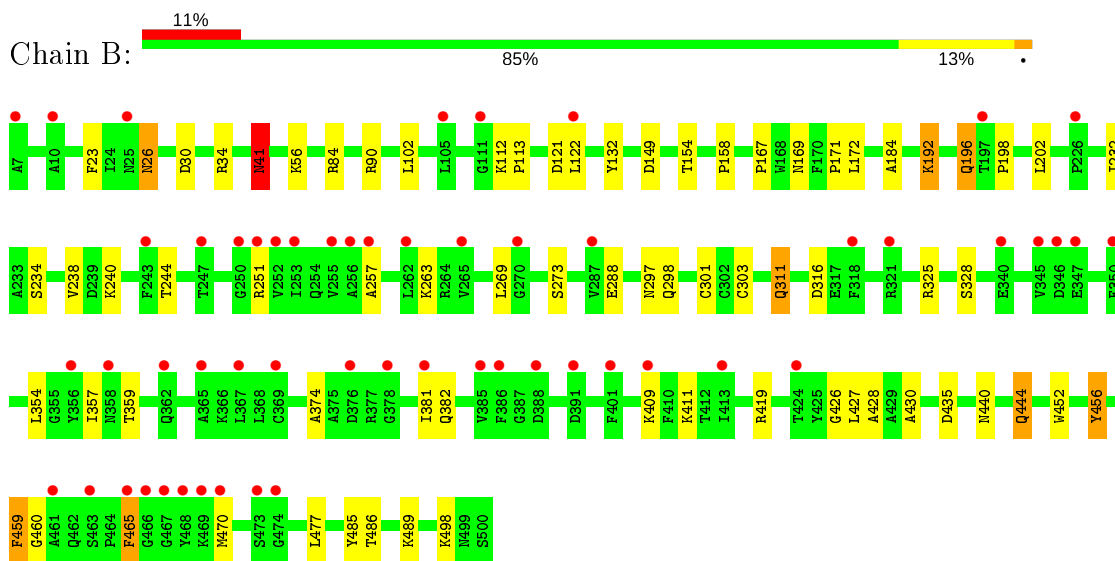
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

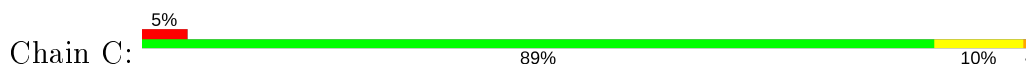
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

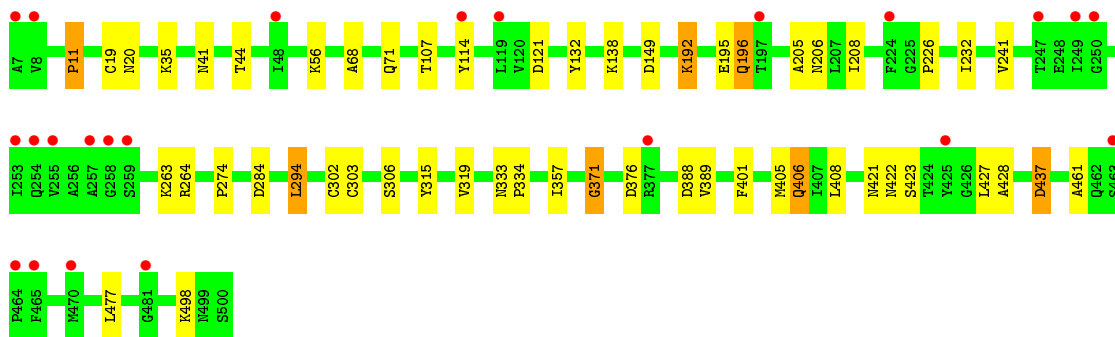


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

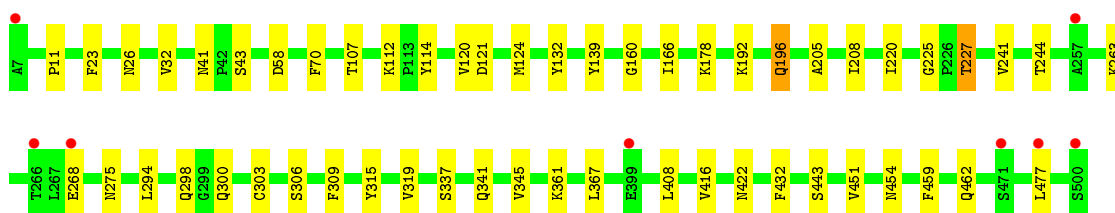
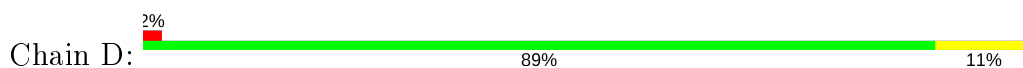


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

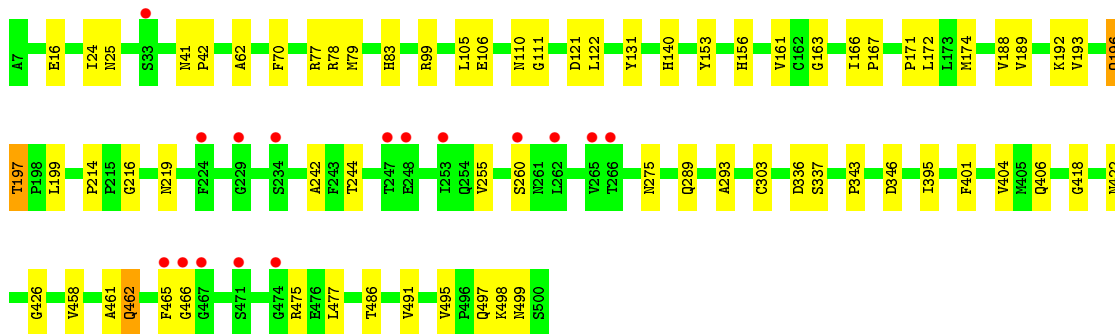
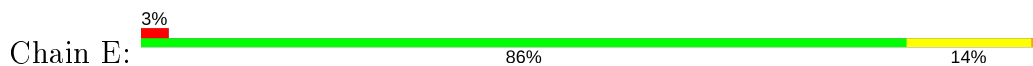




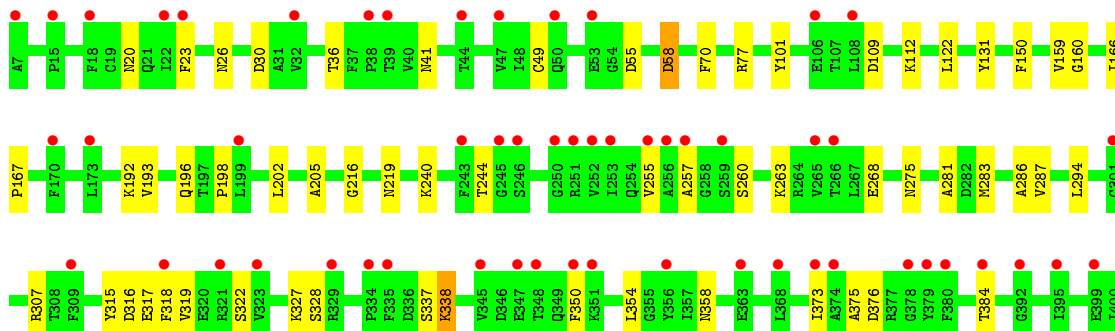
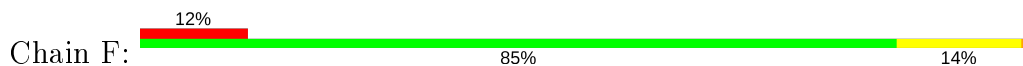
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

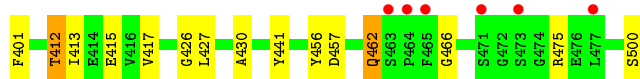


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

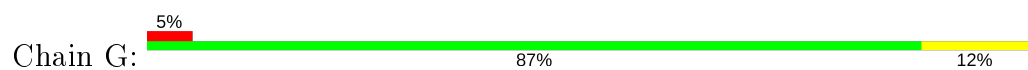


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

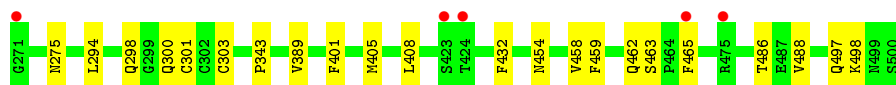
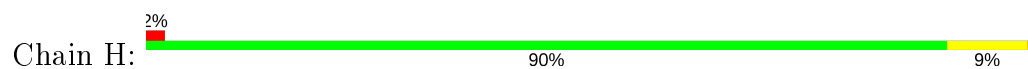




- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.29Å 177.09Å 102.55Å 90.00° 94.39° 90.00°	Depositor
Resolution (Å)	49.12 – 2.31 49.12 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.12-2.31) 98.8 (49.12-2.31)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.32Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.239 , 0.296 0.238 , 0.293	Depositor DCC
$R_{free}$ test set	8016 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 20.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	0.277 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3AK, NA, EDO, GAI

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	0.41	0/3882	0.59	0/5267
1	B	0.38	0/3882	0.56	0/5267
1	C	0.40	0/3882	0.57	0/5267
1	D	0.44	0/3882	0.59	0/5267
1	E	0.41	0/3882	0.58	0/5267
1	F	0.37	0/3882	0.56	0/5267
1	G	0.40	0/3882	0.56	0/5267
1	H	0.44	0/3882	0.60	0/5267
All	All	0.41	0/31056	0.58	0/42136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3745	32	0
1	B	3798	0	3745	40	0
1	C	3798	0	3745	24	0
1	D	3798	0	3745	28	0
1	E	3798	0	3745	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	31	0
1	G	3798	0	3745	36	0
1	H	3798	0	3745	31	0
2	A	18	0	11	3	0
2	B	18	0	11	8	0
2	E	18	0	11	4	0
2	H	18	0	11	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	2	0
4	C	8	0	12	0	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
4	H	4	0	6	0	0
5	A	4	0	4	0	0
5	B	4	0	4	1	0
5	C	4	0	4	0	0
5	D	4	0	4	0	0
5	F	4	0	4	0	0
5	G	4	0	4	0	0
5	H	4	0	4	0	0
6	A	24	0	0	0	0
6	B	15	0	0	0	0
6	C	17	0	0	0	0
6	D	31	0	0	0	0
6	E	20	0	0	0	0
6	F	20	0	0	0	0
6	G	16	0	0	0	0
6	H	45	0	0	0	0
All	All	30712	0	30080	246	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 4.

All (246) 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:B:301:CYS:SG	2:B:601:3AK:O10	2.26	0.93
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.60	0.84
1:E:303:CYS:SG	2:E:601:3AK:O10	2.43	0.77
1:G:48:ILE:HG21	1:G:108:LEU:HD21	1.69	0.75
1:E:216:GLY:HA2	1:E:219:ASN:HD21	1.54	0.71
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.71	0.71
1:G:110:ASN:HD22	1:G:197:THR:HG21	1.56	0.70
1:B:102:LEU:HD22	1:B:172:LEU:HD11	1.73	0.69
1:C:205:ALA:HA	1:C:208:ILE:HD12	1.74	0.69
1:B:196:GLN:H	1:B:196:GLN:HE21	1.39	0.69
1:D:132:TYR:OH	1:D:477:LEU:HA	1.93	0.68
1:A:294:LEU:HD12	1:A:306:SER:HA	1.75	0.68
1:B:311:GLN:NE2	1:B:411:LYS:O	2.27	0.68
1:H:196:GLN:HE21	1:H:196:GLN:H	1.39	0.68
1:C:19:CYS:SG	1:C:206:ASN:ND2	2.66	0.67
1:E:255:VAL:HG13	1:F:255:VAL:HG13	1.77	0.67
1:B:427:LEU:HD21	2:B:601:3AK:C16	2.25	0.66
1:B:427:LEU:HD21	2:B:601:3AK:C15	2.26	0.66
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.78	0.65
1:B:132:TYR:OH	1:B:477:LEU:HA	1.97	0.65
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.32	0.65
1:B:149:ASP:HA	1:B:498:LYS:HB2	1.79	0.65
1:E:465:PHE:CE2	2:E:601:3AK:H12	2.33	0.64
1:A:41:ASN:HD22	1:A:41:ASN:C	2.00	0.64
1:F:287:VAL:HG22	1:F:318:PHE:CD1	2.32	0.64
1:B:440:ASN:O	1:B:444:GLN:HB2	1.97	0.64
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.34	0.63
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.80	0.62
1:H:175:GLN:HG3	1:H:191:MET:SD	2.40	0.61
1:H:41:ASN:C	1:H:41:ASN:HD22	2.03	0.61
1:E:465:PHE:CD2	2:E:601:3AK:H12	2.36	0.61
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.82	0.61
1:A:301:CYS:HB3	2:A:601:3AK:O10	2.01	0.61
1:F:77:ARG:NE	1:G:500:SER:OG	2.32	0.61
1:C:294:LEU:HD12	1:C:306:SER:HA	1.83	0.60
1:E:106:GLU:OE1	1:E:171:PRO:HD2	2.01	0.59
1:F:315:TYR:O	1:F:319:VAL:HG23	2.03	0.59
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.36	0.59
1:D:196:GLN:H	1:D:196:GLN:HE21	1.51	0.58
1:C:315:TYR:O	1:C:319:VAL:HG23	2.02	0.58
1:E:404:VAL:HG12	1:E:406:GLN:HE22	1.68	0.58
1:G:102:LEU:HD21	1:G:203:TYR:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:SER:HA	1:D:451:VAL:HG11	1.87	0.56
1:C:132:TYR:OH	1:C:477:LEU:HA	2.06	0.56
1:B:269:LEU:HD12	1:B:470:MET:O	2.05	0.56
1:H:106:GLU:OE1	1:H:171:PRO:HD2	2.06	0.56
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.87	0.55
1:C:461:ALA:HA	1:C:477:LEU:HD22	1.88	0.55
1:D:244:THR:HG23	1:D:268:GLU:HB2	1.89	0.55
1:G:131:TYR:CE1	1:G:462:GLN:HG3	2.42	0.55
1:H:465:PHE:CE2	2:H:601:3AK:H12	2.42	0.55
1:B:112:LYS:HA	1:B:298:GLN:OE1	2.07	0.55
1:H:196:GLN:H	1:H:196:GLN:NE2	2.04	0.55
1:A:36:THR:HB	1:A:50:GLN:HG3	1.90	0.54
1:D:294:LEU:HD13	1:D:294:LEU:C	2.28	0.54
1:D:120:VAL:HG12	1:D:124:MET:CE	2.38	0.53
1:C:68:ALA:HA	1:C:71:GLN:HG2	1.89	0.53
1:B:459:PHE:CZ	2:B:601:3AK:C2	2.92	0.53
1:B:169:ASN:O	1:B:297:ASN:ND2	2.40	0.53
1:F:373:ILE:HG22	1:F:375:ALA:O	2.09	0.52
1:B:301:CYS:SG	2:B:601:3AK:C9	2.97	0.52
1:G:208:ILE:HD13	1:G:218:VAL:HG11	1.92	0.52
1:E:166:ILE:HD11	1:E:193:VAL:HG12	1.92	0.52
1:A:310:VAL:HG21	1:A:318:PHE:CD2	2.45	0.52
1:H:465:PHE:CD2	2:H:601:3AK:H12	2.44	0.52
1:B:84:ARG:NH1	1:B:184:ALA:O	2.43	0.51
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.45	0.51
1:C:196:GLN:H	1:C:196:GLN:HE21	1.59	0.51
1:F:281:ALA:HB1	1:F:286:ALA:HB2	1.93	0.51
1:D:294:LEU:HD23	1:D:306:SER:HA	1.93	0.51
1:G:110:ASN:HD22	1:G:197:THR:CG2	2.23	0.51
1:A:301:CYS:HB2	1:A:304:ALA:HB2	1.93	0.50
1:F:167:PRO:HD3	1:F:244:THR:HB	1.93	0.50
1:B:301:CYS:HG	2:B:601:3AK:C9	2.24	0.50
1:G:462:GLN:HE21	1:G:462:GLN:H	1.59	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:B:303:CYS:HB2	1:B:428:ALA:HB3	1.93	0.49
1:G:462:GLN:HB3	1:H:144:ILE:CG2	2.41	0.49
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.49
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.49
1:G:22:ILE:HD13	1:G:58:ASP:OD1	2.13	0.49
1:H:294:LEU:HD13	1:H:405:MET:HA	1.95	0.49
1:G:462:GLN:NE2	1:G:462:GLN:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HA	1:D:208:ILE:HD12	1.95	0.49
1:D:432:PHE:CD2	1:D:454:ASN:HA	2.48	0.49
1:E:111:GLY:O	1:E:343:PRO:HD2	2.13	0.48
1:E:336:ASP:OD1	1:E:337:SER:N	2.46	0.48
1:E:497:GLN:HE21	1:E:499:ASN:HD21	1.60	0.48
1:D:300:GLN:HE22	1:D:345:VAL:H	1.61	0.48
1:E:395:ILE:HD12	1:E:406:GLN:HE21	1.79	0.48
1:D:32:VAL:HG23	1:D:58:ASP:OD1	2.13	0.48
1:H:11:PRO:HB3	1:H:114:TYR:CE1	2.48	0.48
1:C:389:VAL:HB	1:C:408:LEU:HG	1.96	0.48
1:B:192:LYS:HB2	1:B:232:ILE:CD1	2.44	0.48
1:E:79:MET:HE3	1:E:83:HIS:HB3	1.96	0.48
1:C:357:ILE:HG21	1:C:371:GLY:O	2.13	0.48
1:A:41:ASN:ND2	1:A:41:ASN:C	2.65	0.47
1:G:110:ASN:ND2	1:G:197:THR:HG21	2.26	0.47
1:E:495:VAL:HG12	1:G:440:ASN:HD22	1.79	0.47
1:C:437:ASP:N	1:C:437:ASP:OD2	2.47	0.47
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.45	0.47
1:A:153:TYR:HH	4:A:603:EDO:HO1	1.61	0.47
1:F:430:ALA:HB2	1:F:456:TYR:CD1	2.50	0.47
1:F:216:GLY:O	1:F:219:ASN:ND2	2.47	0.47
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.97	0.47
1:A:205:ALA:HB2	1:A:220:ILE:CD1	2.40	0.47
1:G:36:THR:OG1	1:G:50:GLN:NE2	2.47	0.47
1:A:355:GLY:O	1:A:359:THR:HG23	2.14	0.47
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.97	0.47
1:F:281:ALA:HB1	1:F:286:ALA:CB	2.45	0.47
1:H:174:MET:HE1	2:H:601:3AK:C18	2.45	0.47
1:G:460:GLY:O	1:G:462:GLN:N	2.48	0.47
1:A:315:TYR:O	1:A:319:VAL:HG23	2.15	0.46
1:E:24:ILE:HG23	1:E:62:ALA:HA	1.96	0.46
1:D:70:PHE:CE1	1:D:160:GLY:HA2	2.50	0.46
1:A:23:PHE:O	1:A:24:ILE:HG13	2.15	0.46
1:B:167:PRO:HG3	1:B:244:THR:HG22	1.97	0.46
1:C:107:THR:OG1	1:C:114:TYR:HA	2.15	0.46
1:B:41:ASN:HD22	1:B:41:ASN:C	2.18	0.46
1:D:303:CYS:HG	1:D:459:PHE:HZ	1.64	0.46
1:F:287:VAL:HG22	1:F:318:PHE:CE1	2.51	0.46
1:E:346:ASP:OD1	1:E:346:ASP:C	2.54	0.46
1:E:41:ASN:HD22	1:E:42:PRO:HD2	1.81	0.46
1:G:26:ASN:HB3	1:G:209:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:O	1:A:205:ALA:HB3	2.15	0.46
2:A:601:3AK:O11	2:A:601:3AK:C13	2.64	0.46
1:E:465:PHE:CE2	2:E:601:3AK:C15	2.98	0.46
1:A:106:GLU:O	1:A:110:ASN:HB3	2.15	0.46
1:H:301:CYS:HB3	2:H:601:3AK:O10	2.16	0.46
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.51	0.46
1:E:105:LEU:HD11	1:E:199:LEU:HD13	1.98	0.46
1:H:432:PHE:HA	1:H:454:ASN:OD1	2.15	0.46
1:A:135:TRP:CD1	1:C:138:LYS:HE3	2.51	0.46
1:B:374:ALA:HB2	1:B:382:GLN:N	2.31	0.45
1:B:409:LYS:O	1:B:419:ARG:NH2	2.46	0.45
1:E:163:GLY:O	1:E:242:ALA:N	2.43	0.45
1:E:167:PRO:HD3	1:E:244:THR:HB	1.98	0.45
1:G:443:SER:HA	1:G:451:VAL:HG11	1.97	0.45
1:D:309:PHE:CD2	1:D:416:VAL:HG23	2.52	0.45
1:A:294:LEU:CD1	1:A:306:SER:HA	2.43	0.45
1:D:408:LEU:N	1:D:408:LEU:HD12	2.32	0.45
1:F:70:PHE:CZ	1:F:160:GLY:HA2	2.52	0.45
1:H:238:VAL:O	1:H:263:LYS:HE3	2.17	0.45
1:B:238:VAL:O	1:B:263:LYS:HE3	2.17	0.45
1:D:107:THR:HG23	1:D:112:LYS:O	2.17	0.45
1:E:418:GLY:O	1:E:422:ASN:HB2	2.16	0.45
1:F:412:THR:OG1	1:F:415:GLU:HB2	2.16	0.45
1:A:302:CYS:HB2	2:A:601:3AK:O11	2.17	0.44
1:F:101:TYR:C	1:F:101:TYR:CD1	2.91	0.44
1:C:107:THR:HG23	1:C:334:PRO:HB2	1.98	0.44
1:E:196:GLN:H	1:E:196:GLN:HE21	1.65	0.44
1:H:298:GLN:O	1:H:300:GLN:HG3	2.18	0.44
1:A:163:GLY:O	1:A:241:VAL:HA	2.17	0.44
1:B:354:LEU:HA	1:B:357:ILE:HD12	1.99	0.44
1:F:294:LEU:HD13	1:F:294:LEU:C	2.38	0.44
1:A:196:GLN:H	1:A:196:GLN:NE2	2.16	0.44
1:D:432:PHE:CE2	1:D:454:ASN:HA	2.53	0.44
1:D:120:VAL:HG12	1:D:124:MET:HE2	2.00	0.44
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.98	0.44
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.52	0.43
1:B:459:PHE:CE1	2:B:601:3AK:C3	3.00	0.43
1:F:413:ILE:HG12	1:F:441:TYR:CE2	2.53	0.43
1:A:391:ASP:OD2	1:A:419:ARG:HD2	2.17	0.43
1:H:14:GLN:HB2	1:H:14:GLN:HE21	1.64	0.43
1:B:257:ALA:HB1	1:B:263:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PHE:CE2	2:B:601:3AK:H13	2.54	0.43
1:D:166:ILE:HG22	1:D:178:LYS:HD2	1.99	0.43
1:F:350:PHE:CZ	1:F:354:LEU:HD11	2.53	0.43
1:C:192:LYS:HB2	1:C:232:ILE:CD1	2.49	0.43
1:C:315:TYR:HH	1:C:388:ASP:H	1.64	0.43
1:G:243:PHE:CZ	1:G:249:ILE:HB	2.53	0.43
1:H:156:HIS:CD2	1:H:488:VAL:HG22	2.53	0.43
1:C:406:GLN:HE21	1:C:406:GLN:HB2	1.67	0.43
1:B:430:ALA:HA	1:B:452:TRP:O	2.19	0.43
1:D:120:VAL:HG12	1:D:124:MET:HE1	2.00	0.43
1:D:315:TYR:O	1:D:319:VAL:HG23	2.19	0.43
1:H:106:GLU:O	1:H:110:ASN:HB3	2.19	0.43
1:E:153:TYR:CZ	1:E:491:VAL:HB	2.54	0.43
1:G:300:GLN:HE22	1:G:345:VAL:HB	1.84	0.43
1:E:161:VAL:HA	1:E:188:VAL:HG23	2.01	0.43
1:B:288:GLU:OE1	1:B:325:ARG:NH2	2.52	0.42
1:A:62:ALA:O	1:A:219:ASN:ND2	2.52	0.42
1:E:461:ALA:HA	1:E:477:LEU:HD22	2.00	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.53	0.42
1:E:167:PRO:HD2	1:E:174:MET:HG3	2.01	0.42
1:G:150:PHE:CE2	1:H:458:VAL:HG21	2.54	0.42
1:B:154:THR:HA	1:B:489:LYS:O	2.19	0.42
1:B:192:LYS:HB2	1:B:232:ILE:HD11	2.01	0.42
1:C:274:PRO:HD2	1:C:428:ALA:O	2.19	0.42
1:G:144:ILE:HG23	1:H:462:GLN:HB3	2.02	0.42
1:G:177:TRP:NE1	1:G:477:LEU:HD21	2.35	0.42
1:A:167:PRO:HD2	1:A:174:MET:HG3	2.01	0.42
1:C:241:VAL:HG23	1:C:263:LYS:HD3	2.00	0.42
1:E:140:HIS:O	1:E:156:HIS:CE1	2.72	0.42
1:F:257:ALA:HB1	1:F:263:LYS:HG3	2.01	0.42
1:D:225:GLY:C	1:D:227:THR:H	2.23	0.42
1:E:110:ASN:HB2	1:E:197:THR:HG21	2.01	0.42
1:G:200:THR:O	1:G:204:VAL:HG23	2.19	0.42
1:G:331:VAL:HG12	1:G:332:GLY:N	2.35	0.42
1:H:63:VAL:HG11	1:H:235:HIS:CE1	2.54	0.42
1:B:113:PRO:HD3	1:B:298:GLN:OE1	2.20	0.42
1:H:111:GLY:O	1:H:343:PRO:HD2	2.20	0.42
1:A:271:GLY:HA2	1:A:425:TYR:HB3	2.01	0.42
1:C:302:CYS:HB3	1:C:427:LEU:CD2	2.49	0.42
1:E:70:PHE:CD1	1:E:77:ARG:HD3	2.55	0.42
1:G:70:PHE:O	1:G:70:PHE:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ASP:OD2	1:F:198:PRO:HD2	2.20	0.41
1:H:303:CYS:SG	2:H:601:3AK:O10	2.72	0.41
1:G:33:SER:O	1:G:34:ARG:HB2	2.20	0.41
1:C:421:ASN:O	1:C:423:SER:N	2.54	0.41
1:F:283:MET:O	1:F:287:VAL:HG23	2.20	0.41
1:E:289:GLN:O	1:E:293:ALA:N	2.45	0.41
1:F:131:TYR:CZ	1:F:462:GLN:HA	2.55	0.41
1:F:202:LEU:O	1:F:205:ALA:HB3	2.21	0.41
1:H:194:ALA:HB1	1:H:196:GLN:NE2	2.36	0.41
1:A:59:VAL:O	1:A:63:VAL:HG23	2.20	0.41
1:F:500:SER:OG	1:G:77:ARG:NE	2.53	0.41
1:G:247:THR:HA	1:G:269:LEU:HD13	2.01	0.41
1:B:198:PRO:O	1:B:202:LEU:HG	2.21	0.41
1:D:361:LYS:HD3	1:D:367:LEU:HD22	2.03	0.41
1:E:458:VAL:HG21	1:F:150:PHE:CE2	2.56	0.41
1:E:78:ARG:HE	1:H:497:GLN:NE2	2.19	0.41
1:G:48:ILE:CG2	1:G:108:LEU:HD21	2.46	0.41
1:F:337:SER:O	1:F:338:LYS:HB2	2.19	0.41
1:A:400:ILE:O	1:A:401:PHE:CB	2.69	0.41
1:B:381:ILE:HG22	1:B:382:GLN:O	2.21	0.41
1:D:298:GLN:HG3	1:D:341:GLN:HG3	2.02	0.41
1:A:153:TYR:OH	4:A:603:EDO:O1	2.34	0.40
1:F:244:THR:HG23	1:F:268:GLU:O	2.21	0.40
1:F:55:ASP:HB3	1:F:58:ASP:OD2	2.21	0.40
1:G:150:PHE:CZ	1:H:458:VAL:HG21	2.57	0.40
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.56	0.40
1:H:389:VAL:HB	1:H:408:LEU:HG	2.04	0.40
1:H:459:PHE:HE2	1:H:465:PHE:CE2	2.39	0.40
1:B:240:LYS:HE3	1:B:485:TYR:CE2	2.57	0.40
1:E:99:ARG:HG3	1:E:122:LEU:HD23	2.03	0.40
1:G:102:LEU:HD21	1:G:203:TYR:CD2	2.54	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.02	0.40
1:A:283:MET:O	1:A:287:VAL:HG23	2.21	0.40
1:F:456:TYR:HD2	1:F:457:ASP:OD2	2.04	0.40
1:B:158:PRO:O	5:B:603:GAI:N3	2.55	0.40
1:A:262:LEU:HD21	1:B:251:ARG:HG3	2.04	0.40
1:B:430:ALA:HB2	1:B:456:TYR:CE1	2.57	0.40
1:C:205:ALA:O	1:C:208:ILE:HB	2.21	0.40
1:G:125:VAL:HG21	1:G:172:LEU:HB3	2.04	0.40
1:G:55:ASP:O	1:G:57:GLU:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/494 (100%)	463 (94%)	29 (6%)	0	100	100
1	B	492/494 (100%)	445 (90%)	43 (9%)	4 (1%)	19	23
1	C	492/494 (100%)	457 (93%)	30 (6%)	5 (1%)	15	17
1	D	492/494 (100%)	469 (95%)	22 (4%)	1 (0%)	47	58
1	E	492/494 (100%)	468 (95%)	21 (4%)	3 (1%)	25	30
1	F	492/494 (100%)	451 (92%)	38 (8%)	3 (1%)	25	30
1	G	492/494 (100%)	456 (93%)	33 (7%)	3 (1%)	25	30
1	H	492/494 (100%)	469 (95%)	23 (5%)	0	100	100
All	All	3936/3952 (100%)	3678 (93%)	239 (6%)	19 (0%)	29	35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	LYS
1	F	307	ARG
1	F	338	LYS
1	G	56	LYS
1	B	426	GLY
1	C	422	ASN
1	E	214	PRO
1	E	260	SER
1	G	383	PRO
1	D	422	ASN
1	C	56	LYS
1	F	426	GLY
1	B	41	ASN
1	B	171	PRO
1	C	11	PRO
1	C	226	PRO
1	C	371	GLY

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Mol	Chain	Res	Type
1	G	198	PRO
1	E	426	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	399/399 (100%)	383 (96%)	16 (4%)	31 44
1	B	399/399 (100%)	378 (95%)	21 (5%)	22 31
1	C	399/399 (100%)	381 (96%)	18 (4%)	27 38
1	D	399/399 (100%)	389 (98%)	10 (2%)	47 64
1	E	399/399 (100%)	386 (97%)	13 (3%)	38 52
1	F	399/399 (100%)	372 (93%)	27 (7%)	16 20
1	G	399/399 (100%)	383 (96%)	16 (4%)	31 44
1	H	399/399 (100%)	387 (97%)	12 (3%)	41 56
All	All	3192/3192 (100%)	3059 (96%)	133 (4%)	30 41

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	106	GLU
1	A	117	SER
1	A	121	ASP
1	A	122	LEU
1	A	146	ILE
1	A	196	GLN
1	A	206	ASN
1	A	240	LYS
1	A	264	ARG
1	A	275	ASN
1	A	348	THR
1	A	352	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	401	PHE
1	A	462	GLN
1	A	486	THR
1	B	26	ASN
1	B	30	ASP
1	B	34	ARG
1	B	41	ASN
1	B	90	ARG
1	B	121	ASP
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	234	SER
1	B	273	SER
1	B	311	GLN
1	B	316	ASP
1	B	328	SER
1	B	359	THR
1	B	435	ASP
1	B	444	GLN
1	B	456	TYR
1	B	459	PHE
1	B	465	PHE
1	B	486	THR
1	C	20	ASN
1	C	35	LYS
1	C	41	ASN
1	C	44	THR
1	C	121	ASP
1	C	192	LYS
1	C	195	GLU
1	C	196	GLN
1	C	264	ARG
1	C	284	ASP
1	C	294	LEU
1	C	303	CYS
1	C	333	ASN
1	C	376	ASP
1	C	401	PHE
1	C	405	MET
1	C	406	GLN
1	C	437	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	41	ASN
1	D	43	SER
1	D	121	ASP
1	D	139	TYR
1	D	192	LYS
1	D	196	GLN
1	D	227	THR
1	D	275	ASN
1	D	337	SER
1	D	462	GLN
1	E	16	GLU
1	E	25	ASN
1	E	121	ASP
1	E	172	LEU
1	E	189	VAL
1	E	192	LYS
1	E	196	GLN
1	E	197	THR
1	E	275	ASN
1	E	401	PHE
1	E	462	GLN
1	E	486	THR
1	E	498	LYS
1	F	20	ASN
1	F	30	ASP
1	F	36	THR
1	F	41	ASN
1	F	49	CYS
1	F	58	ASP
1	F	112	LYS
1	F	122	LEU
1	F	159	VAL
1	F	192	LYS
1	F	196	GLN
1	F	240	LYS
1	F	260	SER
1	F	275	ASN
1	F	316	ASP
1	F	317	GLU
1	F	322	SER
1	F	327	LYS
1	F	328	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	358	ASN
1	F	376	ASP
1	F	384	THR
1	F	401	PHE
1	F	412	THR
1	F	417	VAL
1	F	427	LEU
1	F	462	GLN
1	G	14	GLN
1	G	39	THR
1	G	41	ASN
1	G	112	LYS
1	G	124	MET
1	G	135	TRP
1	G	192	LYS
1	G	196	GLN
1	G	200	THR
1	G	236	GLU
1	G	240	LYS
1	G	249	ILE
1	G	275	ASN
1	G	377	ARG
1	G	401	PHE
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	41	ASN
1	H	112	LYS
1	H	174	MET
1	H	192	LYS
1	H	196	GLN
1	H	275	ASN
1	H	401	PHE
1	H	463	SER
1	H	486	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	41	ASN
1	A	196	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	362	GLN
1	A	462	GLN
1	B	41	ASN
1	B	83	HIS
1	B	175	GLN
1	B	196	GLN
1	B	289	GLN
1	B	444	GLN
1	C	13	GLN
1	C	14	GLN
1	C	20	ASN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	83	HIS
1	C	164	GLN
1	C	196	GLN
1	C	206	ASN
1	C	275	ASN
1	C	333	ASN
1	C	349	GLN
1	C	358	ASN
1	C	362	GLN
1	C	462	GLN
1	D	26	ASN
1	D	41	ASN
1	D	83	HIS
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	300	GLN
1	D	358	ASN
1	D	462	GLN
1	E	13	GLN
1	E	14	GLN
1	E	25	ASN
1	E	26	ASN
1	E	41	ASN
1	E	83	HIS
1	E	175	GLN
1	E	196	GLN
1	E	219	ASN

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Mol	Chain	Res	Type
1	E	275	ASN
1	E	406	GLN
1	E	462	GLN
1	E	497	GLN
1	F	20	ASN
1	F	26	ASN
1	F	41	ASN
1	F	175	GLN
1	F	344	GLN
1	F	462	GLN
1	G	13	GLN
1	G	20	ASN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	110	ASN
1	G	164	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	440	ASN
1	G	447	GLN
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	26	ASN
1	H	41	ASN
1	H	50	GLN
1	H	164	GLN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN
1	H	358	ASN
1	H	382	GLN
1	H	497	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

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
4	EDO	F	602	-	3,3,3	0.37	0	2,2,2	0.32	0
4	EDO	C	602	-	3,3,3	0.39	0	2,2,2	0.28	0
4	EDO	E	603	-	3,3,3	0.37	0	2,2,2	0.33	0
4	EDO	H	603	-	3,3,3	0.37	0	2,2,2	0.43	0
5	GAI	A	605	-	3,3,3	1.53	0	3,3,3	1.10	0
4	EDO	A	603	-	3,3,3	0.32	0	2,2,2	0.64	0
2	3AK	B	601	-	20,20,20	2.32	4 (20%)	28,28,28	2.48	9 (32%)
4	EDO	C	603	-	3,3,3	0.45	0	2,2,2	0.13	0
4	EDO	A	604	-	3,3,3	0.35	0	2,2,2	0.36	0
5	GAI	D	602	-	3,3,3	1.39	0	3,3,3	0.99	0
5	GAI	G	602	-	3,3,3	1.52	0	3,3,3	0.89	0
4	EDO	E	604	-	3,3,3	0.39	0	2,2,2	0.28	0
5	GAI	H	604	-	3,3,3	1.56	0	3,3,3	1.12	0
2	3AK	A	601	-	20,20,20	2.45	4 (20%)	28,28,28	2.51	7 (25%)
5	GAI	F	603	-	3,3,3	1.48	0	3,3,3	1.07	0
2	3AK	H	601	-	20,20,20	2.38	4 (20%)	28,28,28	2.50	8 (28%)
2	3AK	E	601	-	20,20,20	2.44	4 (20%)	28,28,28	2.44	9 (32%)
5	GAI	B	603	-	3,3,3	1.57	0	3,3,3	1.09	0
5	GAI	C	604	-	3,3,3	1.62	0	3,3,3	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	602	-	-	0/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	E	603	-	-	1/1/1/1	-
4	EDO	H	603	-	-	1/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
2	3AK	B	601	-	-	2/4/20/20	0/3/3/3
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-
4	EDO	E	604	-	-	0/1/1/1	-
2	3AK	A	601	-	-	2/4/20/20	0/3/3/3
2	3AK	E	601	-	-	2/4/20/20	0/3/3/3
2	3AK	H	601	-	-	2/4/20/20	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	3AK	C1-C6	7.06	1.50	1.41
2	H	601	3AK	C1-C6	6.96	1.50	1.41
2	A	601	3AK	C1-C6	6.96	1.50	1.41
2	A	601	3AK	C8-C9	-6.92	1.45	1.55
2	H	601	3AK	C8-C9	-6.63	1.45	1.55
2	B	601	3AK	C8-C9	-6.60	1.45	1.55
2	E	601	3AK	C8-C9	-6.60	1.45	1.55
2	B	601	3AK	C1-C6	6.31	1.49	1.41
2	E	601	3AK	O11-C8	3.00	1.29	1.23
2	E	601	3AK	O10-C9	2.94	1.29	1.23
2	B	601	3AK	O10-C9	2.88	1.29	1.23
2	H	601	3AK	O11-C8	2.65	1.28	1.23
2	B	601	3AK	O11-C8	2.58	1.28	1.23
2	A	601	3AK	O11-C8	2.50	1.28	1.23
2	A	601	3AK	O10-C9	2.45	1.28	1.23
2	H	601	3AK	O10-C9	2.12	1.27	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	3AK	C9-C8-N7	8.43	112.35	106.18
2	B	601	3AK	C9-C8-N7	7.92	111.98	106.18
2	H	601	3AK	C9-C8-N7	7.69	111.81	106.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	3AK	C9-C8-N7	7.68	111.80	106.18
2	H	601	3AK	C6-C1-C9	-5.54	102.91	107.71
2	A	601	3AK	C6-C1-C9	-5.26	103.15	107.71
2	A	601	3AK	O11-C8-C9	-5.26	122.24	126.54
2	B	601	3AK	O11-C8-C9	-5.17	122.32	126.54
2	H	601	3AK	C5-C6-C1	-5.10	116.15	121.97
2	E	601	3AK	O11-C8-C9	-4.92	122.52	126.54
2	E	601	3AK	C5-C6-C1	-4.78	116.52	121.97
2	B	601	3AK	C6-C1-C9	-4.62	103.71	107.71
2	E	601	3AK	C6-C1-C9	-4.58	103.74	107.71
2	A	601	3AK	C5-C6-C1	-4.28	117.09	121.97
2	B	601	3AK	C5-C6-C1	-4.24	117.13	121.97
2	H	601	3AK	O11-C8-C9	-4.20	123.11	126.54
2	H	601	3AK	C2-C1-C6	3.07	122.74	119.24
2	E	601	3AK	C13-C12-N7	-2.66	108.90	113.39
2	B	601	3AK	C12-N7-C8	2.56	127.88	123.54
2	A	601	3AK	C2-C1-C6	2.55	122.15	119.24
2	A	601	3AK	C2-C1-C9	2.53	134.70	129.84
2	B	601	3AK	C6-N7-C8	-2.53	108.67	110.74
2	B	601	3AK	O10-C9-C8	2.44	125.66	123.72
2	E	601	3AK	C2-C1-C9	2.43	134.50	129.84
2	E	601	3AK	O10-C9-C8	2.43	125.65	123.72
2	B	601	3AK	C2-C1-C9	2.39	134.42	129.84
2	H	601	3AK	C2-C1-C9	2.35	134.35	129.84
2	B	601	3AK	C2-C1-C6	2.31	121.87	119.24
2	H	601	3AK	C6-N7-C8	-2.25	108.90	110.74
2	A	601	3AK	C6-N7-C8	-2.23	108.92	110.74
2	E	601	3AK	C2-C1-C6	2.20	121.75	119.24
2	H	601	3AK	O10-C9-C8	2.18	125.45	123.72
2	E	601	3AK	C6-N7-C8	-2.11	109.02	110.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	3AK	C13-C12-N7-C8
2	B	601	3AK	C13-C12-N7-C6
2	A	601	3AK	C13-C12-N7-C6
2	H	601	3AK	C13-C12-N7-C8
2	B	601	3AK	C13-C12-N7-C8
2	H	601	3AK	C13-C12-N7-C6
2	E	601	3AK	C13-C12-N7-C8

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Mol	Chain	Res	Type	Atoms
2	E	601	3AK	C13-C12-N7-C6
4	C	603	EDO	O1-C1-C2-O2
4	E	603	EDO	O1-C1-C2-O2
4	A	604	EDO	O1-C1-C2-O2
4	C	602	EDO	O1-C1-C2-O2
4	H	603	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	EDO	2	0
2	B	601	3AK	8	0
2	A	601	3AK	3	0
2	H	601	3AK	5	0
2	E	601	3AK	4	0
5	B	603	GAI	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	494/494 (100%)	0.24	22 (4%) 33 40	29, 49, 73, 111	0
1	B	494/494 (100%)	0.65	55 (11%) 5 8	29, 63, 88, 102	0
1	C	494/494 (100%)	0.30	23 (4%) 31 38	30, 52, 74, 87	0
1	D	494/494 (100%)	0.15	8 (1%) 72 78	27, 42, 63, 79	0
1	E	494/494 (100%)	0.22	16 (3%) 47 55	29, 48, 76, 106	0
1	F	494/494 (100%)	0.73	61 (12%) 4 6	26, 63, 89, 111	0
1	G	494/494 (100%)	0.31	24 (4%) 29 37	29, 54, 76, 90	0
1	H	494/494 (100%)	0.16	12 (2%) 59 66	27, 42, 65, 88	0
All	All	3952/3952 (100%)	0.34	221 (5%) 24 31	26, 50, 82, 111	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	VAL	8.7
1	F	7	ALA	8.3
1	F	255	VAL	7.5
1	F	323	VAL	7.1
1	E	247	THR	6.7
1	F	47	VAL	6.1
1	F	259	SER	6.0
1	F	318	PHE	5.9
1	C	253	ILE	5.4
1	A	258	GLY	5.3
1	A	465	PHE	5.2
1	F	250	GLY	5.1
1	F	252	VAL	5.0
1	C	463	SER	5.0
1	C	247	THR	5.0
1	G	374	ALA	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	335	PHE	4.9
1	F	374	ALA	4.9
1	B	401	PHE	4.7
1	F	39	THR	4.6
1	C	258	GLY	4.5
1	B	356	TYR	4.4
1	F	253	ILE	4.4
1	H	250	GLY	4.4
1	B	467	GLY	4.3
1	E	474	GLY	4.3
1	G	376	ASP	4.2
1	B	287	VAL	4.1
1	F	257	ALA	4.1
1	E	248	GLU	4.1
1	H	424	THR	4.0
1	C	119	LEU	4.0
1	F	266	THR	4.0
1	F	465	PHE	4.0
1	B	111	GLY	3.9
1	B	252	VAL	3.9
1	D	257	ALA	3.9
1	A	424	THR	3.9
1	C	465	PHE	3.9
1	G	106	GLU	3.9
1	G	251	ARG	3.8
1	F	464	PRO	3.8
1	F	392	GLY	3.7
1	D	471	SER	3.7
1	G	32	VAL	3.7
1	B	466	GLY	3.7
1	A	468	TYR	3.6
1	B	247	THR	3.5
1	B	255	VAL	3.5
1	H	465	PHE	3.4
1	A	267	LEU	3.4
1	G	10	ALA	3.4
1	F	347	GLU	3.4
1	F	471	SER	3.4
1	G	477	LEU	3.4
1	F	53	GLU	3.4
1	E	33	SER	3.4
1	B	253	ILE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	7	ALA	3.3
1	E	234	SER	3.3
1	B	461	ALA	3.3
1	F	368	LEU	3.3
1	F	309	PHE	3.3
1	B	350	PHE	3.3
1	F	44	THR	3.3
1	B	378	GLY	3.3
1	B	424	THR	3.3
1	D	7	ALA	3.2
1	B	463	SER	3.2
1	B	465	PHE	3.2
1	F	380	PHE	3.2
1	A	255	VAL	3.2
1	G	255	VAL	3.2
1	A	463	SER	3.2
1	F	246	SER	3.2
1	G	353	ILE	3.2
1	B	340	GLU	3.2
1	A	500	SER	3.2
1	F	373	ILE	3.2
1	C	425	TYR	3.2
1	F	251	ARG	3.2
1	F	32	VAL	3.1
1	B	386	PHE	3.1
1	B	362	GLN	3.1
1	C	470	MET	3.0
1	F	22	ILE	3.0
1	F	399	GLU	3.0
1	F	463	SER	3.0
1	F	170	PHE	3.0
1	B	385	VAL	3.0
1	C	377	ARG	2.9
1	E	466	GLY	2.9
1	B	346	ASP	2.9
1	E	467	GLY	2.9
1	F	256	ALA	2.9
1	B	381	ILE	2.9
1	F	23	PHE	2.9
1	B	365	ALA	2.9
1	H	251	ARG	2.9
1	A	478	GLY	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	256	ALA	2.8
1	B	468	TYR	2.8
1	H	247	THR	2.8
1	H	253	ILE	2.8
1	F	321	ARG	2.8
1	F	18	PHE	2.8
1	B	391	ASP	2.8
1	B	413	ILE	2.8
1	E	260	SER	2.7
1	C	48	ILE	2.7
1	D	399	GLU	2.7
1	E	253	ILE	2.7
1	G	12	ASN	2.7
1	A	22	ILE	2.7
1	C	114	TYR	2.7
1	B	122	LEU	2.7
1	E	262	LEU	2.7
1	F	108	LEU	2.7
1	B	321	ARG	2.7
1	F	473	SER	2.7
1	F	356	TYR	2.7
1	A	470	MET	2.6
1	C	8	VAL	2.6
1	H	268	GLU	2.6
1	G	104	ALA	2.6
1	A	253	ILE	2.6
1	H	475	ARG	2.6
1	A	466	GLY	2.6
1	A	473	SER	2.6
1	F	38	PRO	2.6
1	E	471	SER	2.5
1	F	351	LYS	2.5
1	B	367	LEU	2.5
1	F	379	TYR	2.5
1	B	256	ALA	2.5
1	H	248	GLU	2.5
1	C	254	GLN	2.5
1	E	266	THR	2.5
1	F	395	ILE	2.5
1	E	465	PHE	2.5
1	F	243	PHE	2.5
1	A	472	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	266	THR	2.4
1	B	470	MET	2.4
1	G	465	PHE	2.4
1	F	15	PRO	2.4
1	F	50	GLN	2.4
1	F	378	GLY	2.4
1	G	473	SER	2.4
1	F	477	LEU	2.4
1	F	345	VAL	2.4
1	G	37	PHE	2.4
1	B	474	GLY	2.4
1	D	268	GLU	2.4
1	C	197	THR	2.4
1	H	246	SER	2.4
1	A	254	GLN	2.4
1	C	255	VAL	2.4
1	E	265	VAL	2.4
1	D	500	SER	2.4
1	G	356	TYR	2.4
1	B	25	ASN	2.3
1	F	329	ARG	2.3
1	C	481	GLY	2.3
1	C	464	PRO	2.3
1	F	199	LEU	2.3
1	A	356	TYR	2.3
1	B	473	SER	2.3
1	C	259	SER	2.3
1	E	229	GLY	2.3
1	B	265	VAL	2.3
1	B	318	PHE	2.3
1	F	350	PHE	2.3
1	F	334	PRO	2.3
1	G	350	PHE	2.3
1	C	257	ALA	2.3
1	B	250	GLY	2.2
1	B	243	PHE	2.2
1	B	409	LYS	2.2
1	F	173	LEU	2.2
1	A	480	TYR	2.2
1	A	464	PRO	2.2
1	G	17	VAL	2.2
1	B	469	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	197	THR	2.2
1	H	271	GLY	2.2
1	B	226	PRO	2.2
1	B	388	ASP	2.2
1	F	384	THR	2.2
1	B	347	GLU	2.2
1	H	423	SER	2.2
1	G	399	GLU	2.2
1	C	249	ILE	2.2
1	A	223	GLY	2.2
1	B	251	ARG	2.1
1	F	301	CYS	2.1
1	F	245	GLY	2.1
1	B	376	ASP	2.1
1	B	270	GLY	2.1
1	F	363	GLU	2.1
1	C	250	GLY	2.1
1	G	27	GLU	2.1
1	G	16	GLU	2.1
1	B	7	ALA	2.1
1	F	348	THR	2.1
1	F	265	VAL	2.1
1	D	477	LEU	2.1
1	F	106	GLU	2.1
1	B	358	ASN	2.1
1	G	471	SER	2.1
1	E	224	PHE	2.1
1	B	257	ALA	2.0
1	G	14	GLN	2.0
1	C	224	PHE	2.0
1	B	369	CYS	2.0
1	B	105	LEU	2.0
1	B	262	LEU	2.0
1	A	247	THR	2.0
1	G	463	SER	2.0
1	B	10	ALA	2.0
1	G	201	ALA	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	C	601	1/1	0.65	0.27	88,88,88,88	0
3	NA	G	601	1/1	0.73	0.21	83,83,83,83	0
3	NA	D	601	1/1	0.75	0.15	64,64,64,64	0
3	NA	E	602	1/1	0.77	0.17	73,73,73,73	0
5	GAI	B	603	4/4	0.78	0.27	93,93,94,95	0
3	NA	B	602	1/1	0.81	0.29	93,93,93,93	0
3	NA	A	602	1/1	0.82	0.22	91,91,91,91	0
4	EDO	F	602	4/4	0.83	0.17	80,82,82,83	0
5	GAI	D	602	4/4	0.83	0.15	74,77,79,79	0
3	NA	F	601	1/1	0.83	0.17	84,84,84,84	0
2	3AK	B	601	18/18	0.84	0.22	46,51,56,57	0
4	EDO	C	603	4/4	0.87	0.45	60,65,67,68	0
4	EDO	E	604	4/4	0.87	0.26	75,78,78,80	0
3	NA	H	602	1/1	0.88	0.11	65,65,65,65	0
5	GAI	F	603	4/4	0.89	0.33	73,74,74,75	0
4	EDO	C	602	4/4	0.90	0.31	63,64,64,65	0
2	3AK	A	601	18/18	0.90	0.20	42,50,59,59	0
4	EDO	A	603	4/4	0.91	0.17	68,71,72,75	0
2	3AK	E	601	18/18	0.91	0.20	43,46,49,50	0
4	EDO	H	603	4/4	0.92	0.36	71,71,72,73	0
4	EDO	A	604	4/4	0.92	0.32	65,67,67,69	0
2	3AK	H	601	18/18	0.92	0.18	47,54,63,64	0
5	GAI	C	604	4/4	0.93	0.16	74,75,75,75	0
4	EDO	E	603	4/4	0.94	0.35	81,86,88,89	0
5	GAI	A	605	4/4	0.95	0.18	69,72,73,76	0
5	GAI	H	604	4/4	0.95	0.16	70,75,75,77	0
5	GAI	G	602	4/4	0.97	0.15	66,66,69,71	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.