



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 11:38 PM EDT

PDB ID : 6QAK  
Title : Structure of human ALDH9 in P21212 space group  
Authors : Morera, S.; Vigouroux, A.; Kopecny, D.  
Deposited on : 2018-12-19  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

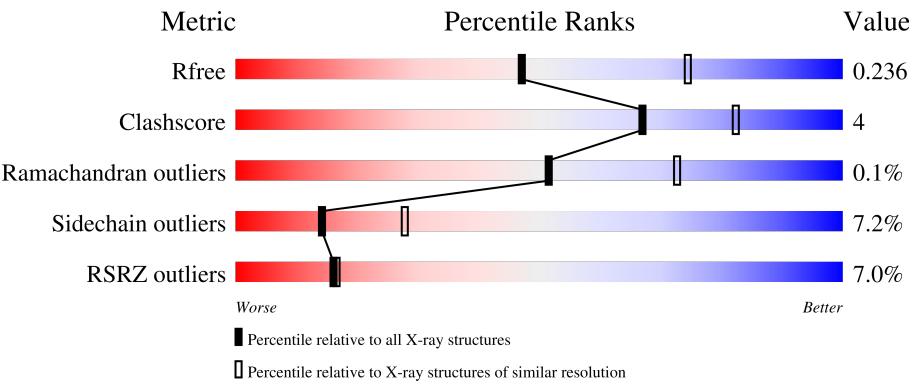
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	508	<div><div>4%</div><div></div><div>80%</div><div>12%</div><div>7%</div></div>
1	B	508	<div><div>2%</div><div></div><div>79%</div><div>13%</div><div>7%</div></div>
1	C	508	<div><div>9%</div><div></div><div>80%</div><div>13%</div><div>7%</div></div>
1	D	508	<div><div>7%</div><div></div><div>81%</div><div>12%</div><div>7%</div></div>
1	E	508	<div><div>11%</div><div></div><div>77%</div><div>15%</div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	508	<div><div></div><div>7%</div><div></div><div>78%</div><div></div><div>14%</div><div></div><div>7%</div></div>
1	G	508	<div><div></div><div>3%</div><div></div><div>80%</div><div></div><div>12%</div><div></div><div>7%</div></div>
1	H	508	<div><div></div><div>8%</div><div></div><div>79%</div><div></div><div>13%</div><div></div><div>7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28938 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 4-trimethylaminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	B	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	C	471	Total	C	N	O	S	0	2	0
			3614	2288	618	679	29			
1	D	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	E	471	Total	C	N	O	S	0	1	0
			3611	2286	618	679	28			
1	F	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	G	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	H	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P49189
A	-12	GLY	-	expression tag	UNP P49189
A	-11	SER	-	expression tag	UNP P49189
A	-10	SER	-	expression tag	UNP P49189
A	-9	HIS	-	expression tag	UNP P49189
A	-8	HIS	-	expression tag	UNP P49189
A	-7	HIS	-	expression tag	UNP P49189
A	-6	HIS	-	expression tag	UNP P49189
A	-5	HIS	-	expression tag	UNP P49189
A	-4	HIS	-	expression tag	UNP P49189
A	-3	SER	-	expression tag	UNP P49189
A	-2	GLN	-	expression tag	UNP P49189
A	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P49189
B	-13	MET	-	initiating methionine	UNP P49189
B	-12	GLY	-	expression tag	UNP P49189
B	-11	SER	-	expression tag	UNP P49189
B	-10	SER	-	expression tag	UNP P49189
B	-9	HIS	-	expression tag	UNP P49189
B	-8	HIS	-	expression tag	UNP P49189
B	-7	HIS	-	expression tag	UNP P49189
B	-6	HIS	-	expression tag	UNP P49189
B	-5	HIS	-	expression tag	UNP P49189
B	-4	HIS	-	expression tag	UNP P49189
B	-3	SER	-	expression tag	UNP P49189
B	-2	GLN	-	expression tag	UNP P49189
B	-1	ASP	-	expression tag	UNP P49189
B	0	PRO	-	expression tag	UNP P49189
C	-13	MET	-	initiating methionine	UNP P49189
C	-12	GLY	-	expression tag	UNP P49189
C	-11	SER	-	expression tag	UNP P49189
C	-10	SER	-	expression tag	UNP P49189
C	-9	HIS	-	expression tag	UNP P49189
C	-8	HIS	-	expression tag	UNP P49189
C	-7	HIS	-	expression tag	UNP P49189
C	-6	HIS	-	expression tag	UNP P49189
C	-5	HIS	-	expression tag	UNP P49189
C	-4	HIS	-	expression tag	UNP P49189
C	-3	SER	-	expression tag	UNP P49189
C	-2	GLN	-	expression tag	UNP P49189
C	-1	ASP	-	expression tag	UNP P49189
C	0	PRO	-	expression tag	UNP P49189
D	-13	MET	-	initiating methionine	UNP P49189
D	-12	GLY	-	expression tag	UNP P49189
D	-11	SER	-	expression tag	UNP P49189
D	-10	SER	-	expression tag	UNP P49189
D	-9	HIS	-	expression tag	UNP P49189
D	-8	HIS	-	expression tag	UNP P49189
D	-7	HIS	-	expression tag	UNP P49189
D	-6	HIS	-	expression tag	UNP P49189
D	-5	HIS	-	expression tag	UNP P49189
D	-4	HIS	-	expression tag	UNP P49189
D	-3	SER	-	expression tag	UNP P49189
D	-2	GLN	-	expression tag	UNP P49189
D	-1	ASP	-	expression tag	UNP P49189

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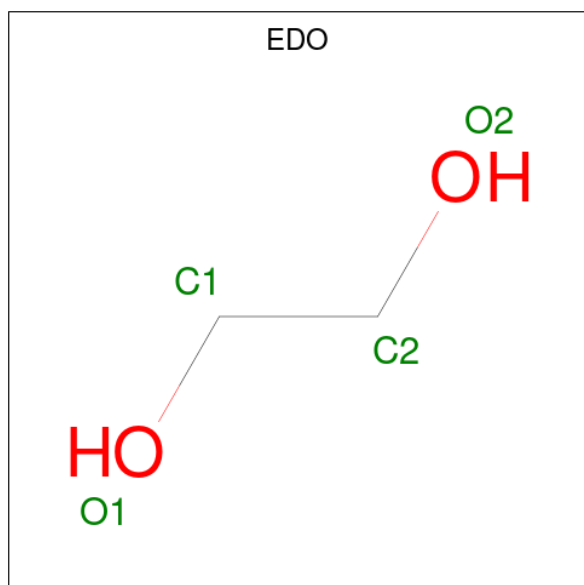
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP P49189
E	-13	MET	-	initiating methionine	UNP P49189
E	-12	GLY	-	expression tag	UNP P49189
E	-11	SER	-	expression tag	UNP P49189
E	-10	SER	-	expression tag	UNP P49189
E	-9	HIS	-	expression tag	UNP P49189
E	-8	HIS	-	expression tag	UNP P49189
E	-7	HIS	-	expression tag	UNP P49189
E	-6	HIS	-	expression tag	UNP P49189
E	-5	HIS	-	expression tag	UNP P49189
E	-4	HIS	-	expression tag	UNP P49189
E	-3	SER	-	expression tag	UNP P49189
E	-2	GLN	-	expression tag	UNP P49189
E	-1	ASP	-	expression tag	UNP P49189
E	0	PRO	-	expression tag	UNP P49189
F	-13	MET	-	initiating methionine	UNP P49189
F	-12	GLY	-	expression tag	UNP P49189
F	-11	SER	-	expression tag	UNP P49189
F	-10	SER	-	expression tag	UNP P49189
F	-9	HIS	-	expression tag	UNP P49189
F	-8	HIS	-	expression tag	UNP P49189
F	-7	HIS	-	expression tag	UNP P49189
F	-6	HIS	-	expression tag	UNP P49189
F	-5	HIS	-	expression tag	UNP P49189
F	-4	HIS	-	expression tag	UNP P49189
F	-3	SER	-	expression tag	UNP P49189
F	-2	GLN	-	expression tag	UNP P49189
F	-1	ASP	-	expression tag	UNP P49189
F	0	PRO	-	expression tag	UNP P49189
G	-13	MET	-	initiating methionine	UNP P49189
G	-12	GLY	-	expression tag	UNP P49189
G	-11	SER	-	expression tag	UNP P49189
G	-10	SER	-	expression tag	UNP P49189
G	-9	HIS	-	expression tag	UNP P49189
G	-8	HIS	-	expression tag	UNP P49189
G	-7	HIS	-	expression tag	UNP P49189
G	-6	HIS	-	expression tag	UNP P49189
G	-5	HIS	-	expression tag	UNP P49189
G	-4	HIS	-	expression tag	UNP P49189
G	-3	SER	-	expression tag	UNP P49189
G	-2	GLN	-	expression tag	UNP P49189
G	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	PRO	-	expression tag	UNP P49189
H	-13	MET	-	initiating methionine	UNP P49189
H	-12	GLY	-	expression tag	UNP P49189
H	-11	SER	-	expression tag	UNP P49189
H	-10	SER	-	expression tag	UNP P49189
H	-9	HIS	-	expression tag	UNP P49189
H	-8	HIS	-	expression tag	UNP P49189
H	-7	HIS	-	expression tag	UNP P49189
H	-6	HIS	-	expression tag	UNP P49189
H	-5	HIS	-	expression tag	UNP P49189
H	-4	HIS	-	expression tag	UNP P49189
H	-3	SER	-	expression tag	UNP P49189
H	-2	GLN	-	expression tag	UNP P49189
H	-1	ASP	-	expression tag	UNP P49189
H	0	PRO	-	expression tag	UNP P49189

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		

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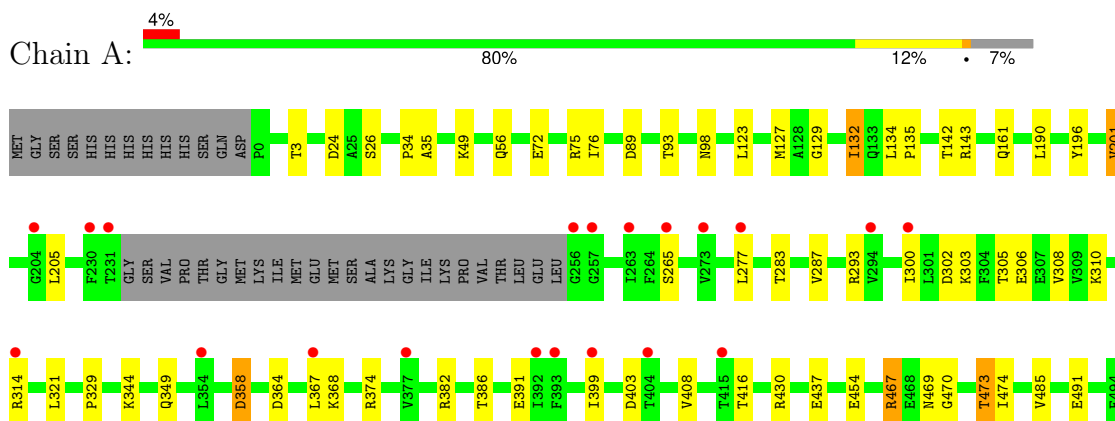
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total 16	O 16	0	0
3	C	7	Total 7	O 7	0	0
3	D	9	Total 9	O 9	0	0
3	E	5	Total 5	O 5	0	0
3	F	12	Total 12	O 12	0	0
3	G	8	Total 8	O 8	0	0
3	H	9	Total 9	O 9	0	0



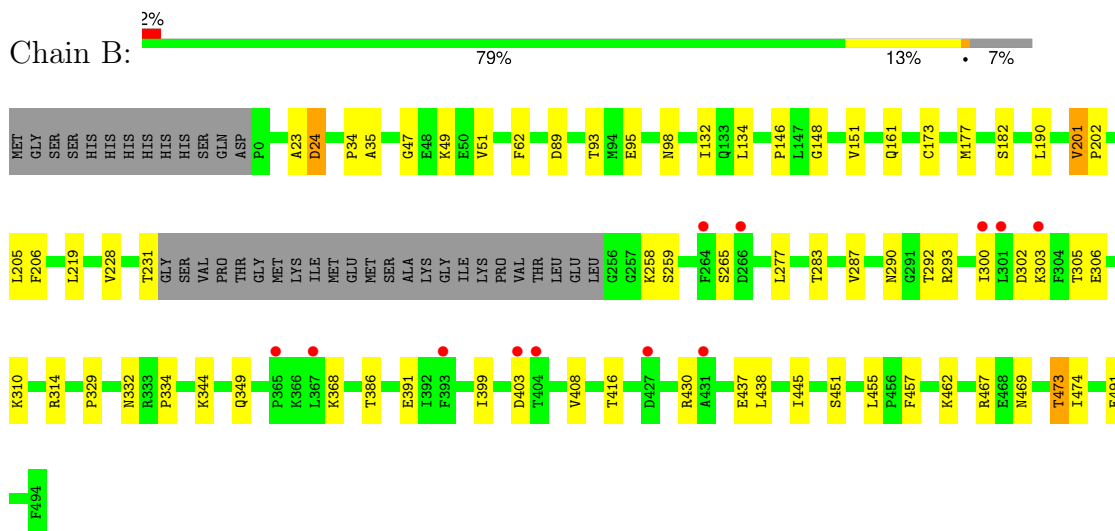
### 3 Residue-property plots [i](#)

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.

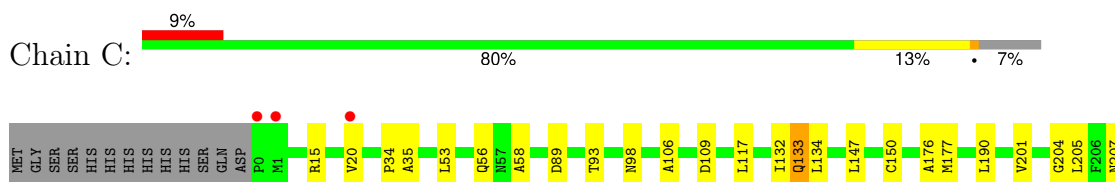
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

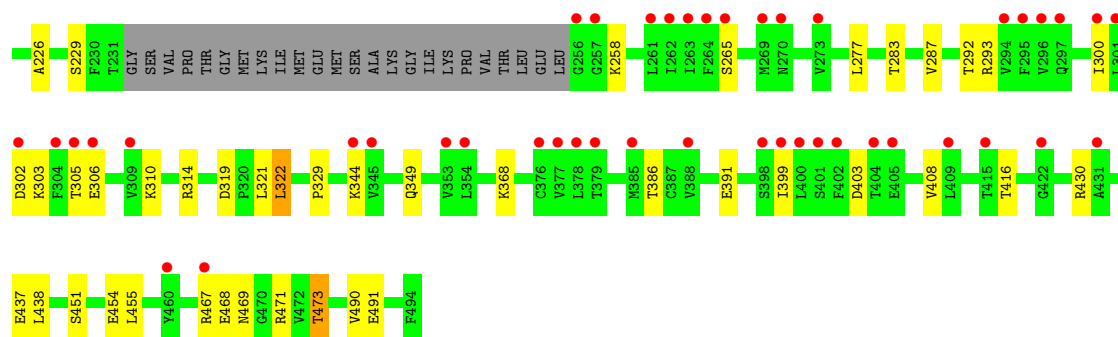


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

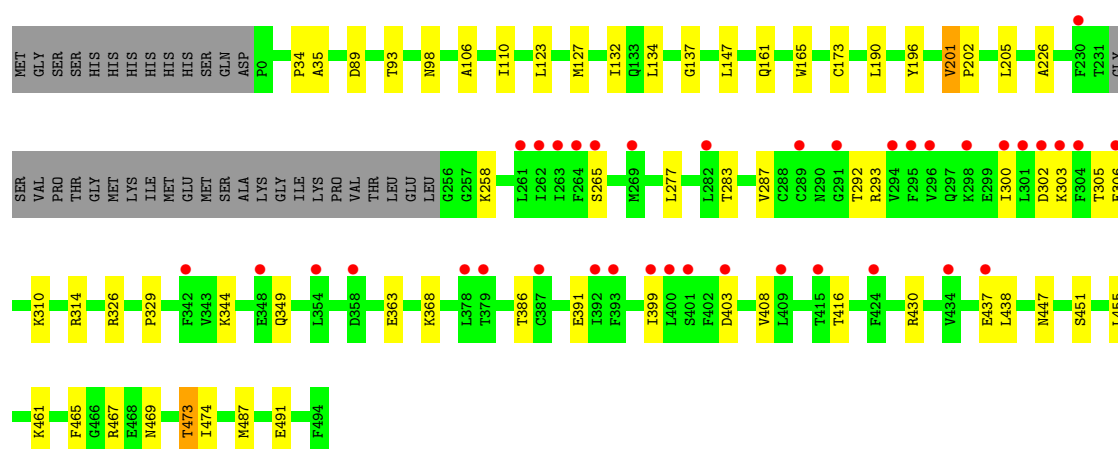
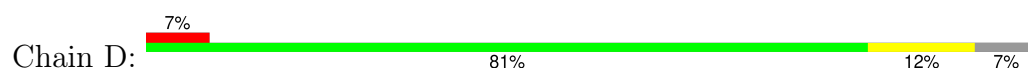


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

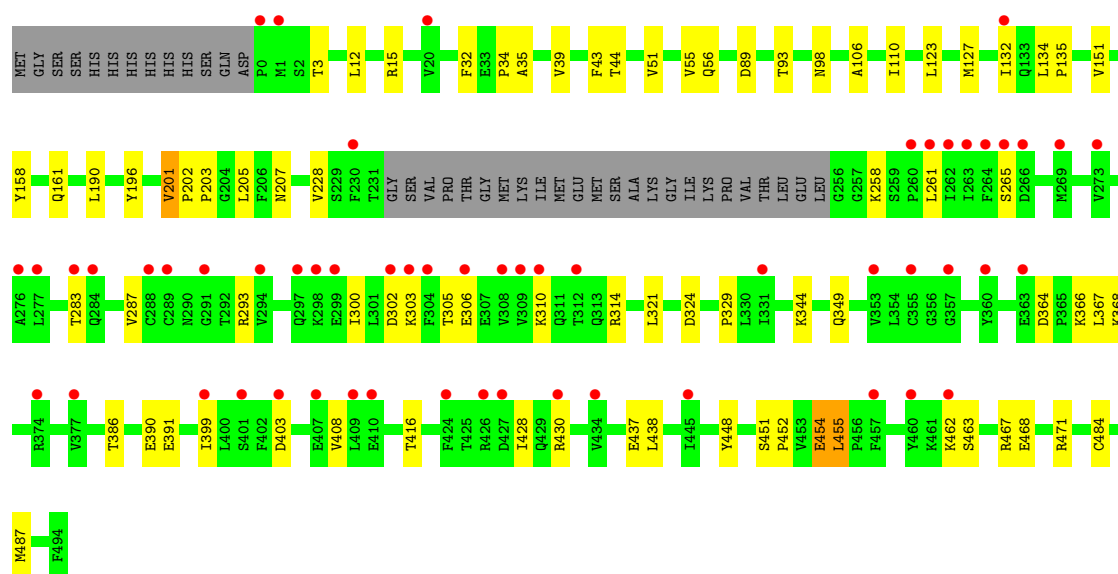
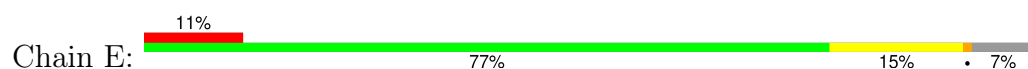





- Molecule 1: 4-trimethylaminobutylaldehyde dehydrogenase

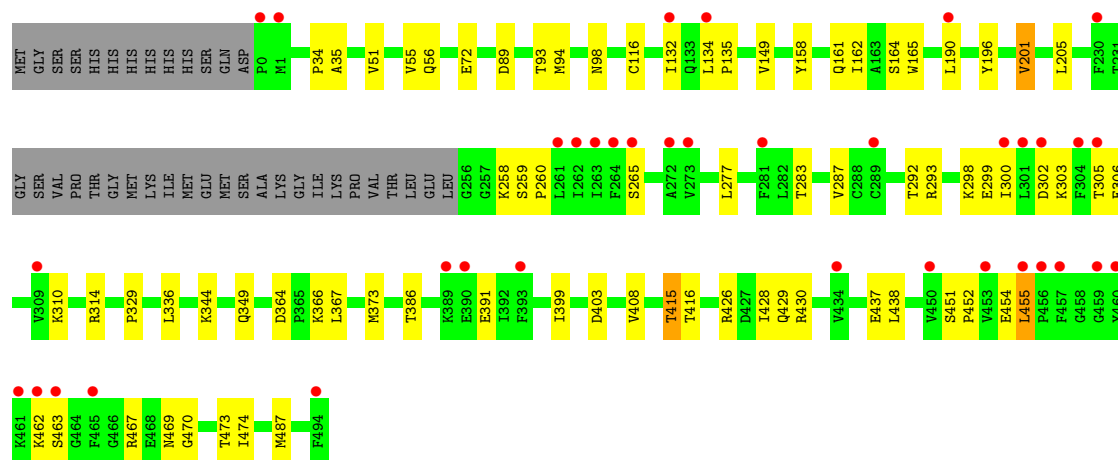


- Molecule 1: 4-trimethylaminobutylaldehyde dehydrogenase




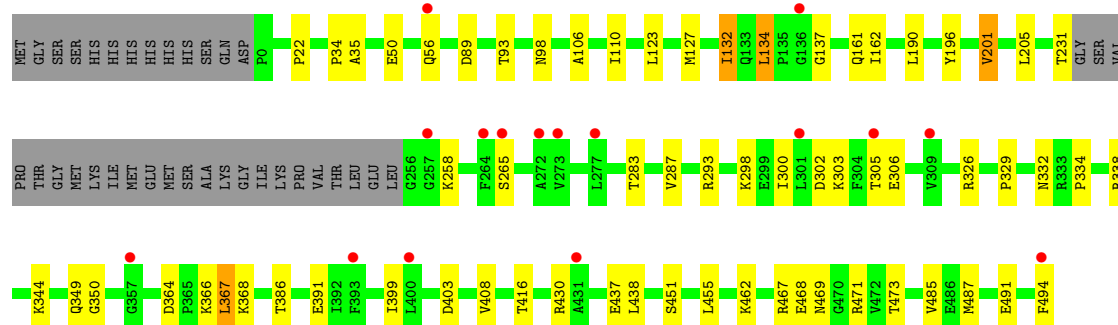
- Molecule 1: 4-trimethylaminobutylaldehyde dehydrogenase

Chain F: 




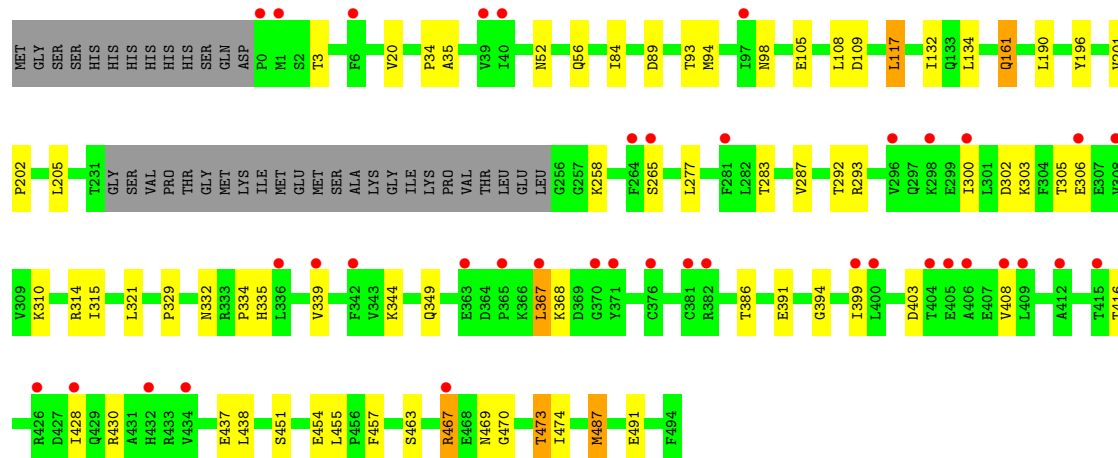
• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

Chain G: 



• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.38Å 159.59Å 160.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.90 – 2.50 48.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.90-2.50) 99.6 (48.39-2.50)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.191 , 0.220 0.206 , 0.236	Depositor DCC
$R_{free}$ test set	7140 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h 0.000 for -h,-l,-k 0.000 for k,h,-l 0.000 for l,h,k 0.000 for k,l,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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 36.70 % 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 4.8021e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0.52	0/3676	0.70	0/4971
1	B	0.53	0/3676	0.70	0/4971
1	C	0.51	0/3693	0.71	0/4994
1	D	0.50	0/3676	0.69	0/4971
1	E	0.49	0/3687	0.71	0/4986
1	F	0.51	0/3676	0.71	0/4971
1	G	0.52	0/3676	0.72	0/4971
1	H	0.52	0/3676	0.71	0/4971
All	All	0.51	0/29436	0.71	0/39806

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

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	3604	0	3577	28	0
1	B	3604	0	3577	27	0
1	C	3614	0	3589	28	0
1	D	3604	0	3577	25	0
1	E	3611	0	3584	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3604	0	3577	36	0
1	G	3604	0	3577	33	0
1	H	3604	0	3577	32	0
2	B	4	0	6	0	0
3	A	19	0	0	0	0
3	B	16	0	0	0	0
3	C	7	0	0	0	0
3	D	9	0	0	0	0
3	E	5	0	0	0	0
3	F	12	0	0	0	0
3	G	8	0	0	1	0
3	H	9	0	0	0	0
All	All	28938	0	28641	222	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 (222) 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:332:ASN:HB3	1:B:334:PRO:HD2	1.63	0.80
1:F:452:PRO:HD2	1:F:455:LEU:HD11	1.62	0.80
1:A:143:ARG:HD2	1:C:133:GLN:HG3	1.69	0.71
1:E:462:LYS:HB2	1:F:135:PRO:HD3	1.73	0.71
1:E:451:SER:HB2	1:E:455:LEU:HD11	1.72	0.70
1:E:467:ARG:HE	1:G:467:ARG:HH22	1.39	0.69
1:F:428:ILE:HB	1:H:428:ILE:HB	1.74	0.68
1:A:467:ARG:HH21	1:C:467:ARG:HH12	1.42	0.68
1:A:364:ASP:HB3	1:A:367:LEU:HD12	1.76	0.67
1:E:258:LYS:HE3	1:E:390:GLU:O	1.95	0.66
1:G:162:ILE:CD1	1:G:231:THR:HG21	2.26	0.65
1:F:469:ASN:O	1:F:473:THR:HG23	1.97	0.64
1:E:452:PRO:HB2	1:E:454:GLU:OE1	1.98	0.64
1:E:428:ILE:HG22	1:H:487:MET:SD	2.38	0.63
1:A:469:ASN:O	1:A:473:THR:HG23	1.98	0.63
1:D:201:VAL:HG13	1:D:205:LEU:HB3	1.80	0.62
1:C:469:ASN:O	1:C:473:THR:HG23	2.00	0.62
1:H:105:GLU:HA	1:H:108:LEU:HD12	1.82	0.61
1:G:162:ILE:HD11	1:G:231:THR:HG21	1.82	0.61
1:H:52:ASN:O	1:H:56:GLN:HG2	2.01	0.61
1:B:469:ASN:O	1:B:473:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:ASP:HB3	1:E:367:LEU:HD22	1.81	0.60
1:D:89:ASP:O	1:D:93:THR:HG23	2.02	0.60
1:G:469:ASN:O	1:G:473:THR:HG23	2.02	0.59
1:A:89:ASP:O	1:A:93:THR:HG23	2.03	0.59
1:C:89:ASP:O	1:C:93:THR:HG23	2.02	0.59
1:F:89:ASP:O	1:F:93:THR:HG23	2.04	0.58
1:H:89:ASP:O	1:H:93:THR:HG23	2.03	0.57
1:G:364:ASP:HB3	1:G:367:LEU:HD22	1.86	0.57
1:E:34:PRO:HB2	1:E:329:PRO:HG2	1.85	0.57
1:G:332:ASN:HB3	1:G:334:PRO:HD2	1.86	0.57
1:B:173:CYS:SG	1:B:474:ILE:HD12	2.45	0.56
1:E:468:GLU:HG3	1:E:471:ARG:NH2	2.21	0.56
1:H:469:ASN:O	1:H:473:THR:HG23	2.04	0.56
1:E:89:ASP:O	1:E:93:THR:HG23	2.06	0.56
1:F:428:ILE:HG23	1:F:429:GLN:H	1.71	0.56
1:E:201:VAL:HG13	1:E:205:LEU:HB3	1.88	0.55
1:G:89:ASP:O	1:G:93:THR:HG23	2.05	0.55
1:B:89:ASP:O	1:B:93:THR:HG23	2.07	0.55
1:D:201:VAL:HG22	1:D:205:LEU:HD23	1.89	0.55
1:F:201:VAL:HG13	1:F:205:LEU:HB3	1.87	0.55
1:A:24:ASP:HB2	1:A:49:LYS:HB2	1.87	0.55
1:A:467:ARG:HH21	1:C:467:ARG:NH1	2.03	0.55
1:A:467:ARG:HE	1:C:467:ARG:HH22	1.53	0.55
1:E:462:LYS:HD2	1:F:135:PRO:HB3	1.89	0.55
1:F:452:PRO:HB2	1:F:454:GLU:OE2	2.06	0.55
1:B:34:PRO:HB2	1:B:329:PRO:HG2	1.88	0.55
1:C:34:PRO:HB2	1:C:329:PRO:HG2	1.89	0.54
1:D:34:PRO:HB2	1:D:329:PRO:HG2	1.88	0.54
1:F:34:PRO:HB2	1:F:329:PRO:HG2	1.89	0.54
1:G:494:PHE:CD1	1:H:315:ILE:HG12	2.43	0.54
1:E:467:ARG:HE	1:G:467:ARG:NH2	2.04	0.54
1:D:202:PRO:HD2	1:D:205:LEU:HD22	1.90	0.53
1:G:35:ALA:HA	1:G:329:PRO:HG3	1.90	0.53
1:B:35:ALA:HA	1:B:329:PRO:HG3	1.90	0.53
1:F:364:ASP:HB3	1:F:367:LEU:HD22	1.91	0.53
1:H:35:ALA:HA	1:H:329:PRO:HG3	1.90	0.53
1:D:469:ASN:O	1:D:473:THR:HG23	2.09	0.53
1:F:366:LYS:HG3	1:F:367:LEU:HD13	1.90	0.52
1:F:35:ALA:HA	1:F:329:PRO:HG3	1.90	0.52
1:A:35:ALA:HA	1:A:329:PRO:HG3	1.91	0.52
1:A:201:VAL:HG13	1:A:205:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ALA:HA	1:E:329:PRO:HG3	1.90	0.52
1:G:134:LEU:HD12	1:H:463:SER:HA	1.91	0.52
1:H:196:TYR:O	1:H:201:VAL:HB	2.09	0.52
1:E:467:ARG:HH21	1:G:467:ARG:HH12	1.58	0.52
1:H:3:THR:OG1	1:H:321:LEU:HD13	2.10	0.52
1:H:34:PRO:HB2	1:H:329:PRO:HG2	1.91	0.52
1:A:75:ARG:HH11	1:A:76:ILE:HD13	1.75	0.52
1:B:151:VAL:HB	1:B:228:VAL:HG22	1.91	0.52
1:C:35:ALA:HA	1:C:329:PRO:HG3	1.91	0.52
1:E:12:LEU:HD12	1:E:43:PHE:HB3	1.91	0.52
1:D:35:ALA:HA	1:D:329:PRO:HG3	1.91	0.51
1:F:165:TRP:CD1	1:F:454:GLU:HG3	2.45	0.51
1:B:451:SER:HB2	1:B:455:LEU:HD12	1.92	0.51
1:F:258:LYS:HE2	1:F:292:THR:OG1	2.10	0.51
1:E:135:PRO:HD3	1:F:462:LYS:O	2.11	0.51
1:D:258:LYS:HE2	1:D:292:THR:OG1	2.10	0.51
1:E:32:PHE:CE1	1:E:39:VAL:HG22	2.46	0.51
1:D:305:THR:HG22	1:D:399:ILE:HD13	1.93	0.50
1:A:382:ARG:NH1	1:G:350:GLY:HA3	2.25	0.50
1:G:34:PRO:HB2	1:G:329:PRO:HG2	1.93	0.50
1:H:332:ASN:HB3	1:H:334:PRO:HD2	1.92	0.50
1:C:451:SER:HB2	1:C:455:LEU:HD12	1.93	0.50
1:A:135:PRO:HG3	1:B:462:LYS:HD2	1.94	0.50
1:E:310:LYS:HE2	1:E:314:ARG:HH22	1.77	0.50
1:A:305:THR:HG22	1:A:399:ILE:HD13	1.94	0.49
1:E:202:PRO:HD2	1:E:205:LEU:HD22	1.95	0.49
1:A:265:SER:HA	1:A:300:ILE:HG12	1.95	0.49
1:B:310:LYS:HE2	1:B:314:ARG:HH22	1.77	0.49
1:D:106:ALA:O	1:D:110:ILE:HG12	2.12	0.49
1:D:310:LYS:HE2	1:D:314:ARG:HH22	1.78	0.49
1:B:349:GLN:HE22	1:B:386:THR:HG23	1.78	0.49
1:E:158:TYR:CE2	1:E:452:PRO:HG3	2.48	0.49
1:G:265:SER:HA	1:G:300:ILE:HG12	1.95	0.49
1:B:305:THR:HG22	1:B:399:ILE:HD13	1.95	0.48
1:B:23:ALA:HB1	1:B:49:LYS:HE2	1.93	0.48
1:A:358:ASP:OD1	1:A:374:ARG:HD2	2.13	0.48
1:H:451:SER:HB2	1:H:455:LEU:HD12	1.96	0.48
1:A:34:PRO:HB2	1:A:329:PRO:HG2	1.94	0.48
1:D:265:SER:HA	1:D:300:ILE:HG12	1.96	0.48
1:C:319:ASP:HB3	1:C:322:LEU:HD22	1.96	0.48
1:F:310:LYS:HE2	1:F:314:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HG13	1:B:205:LEU:HB3	1.95	0.48
1:D:137:GLY:O	1:D:487:MET:HG3	2.14	0.47
1:G:305:THR:HG22	1:G:399:ILE:HD13	1.96	0.47
1:G:485:VAL:HG12	1:G:487:MET:HE2	1.95	0.47
1:E:305:THR:HG22	1:E:399:ILE:HD13	1.95	0.47
1:F:260:PRO:HD3	1:F:415:THR:HG21	1.97	0.47
1:C:305:THR:HG22	1:C:399:ILE:HD13	1.95	0.47
1:D:173:CYS:SG	1:D:474:ILE:HD12	2.54	0.47
1:H:305:THR:HG22	1:H:399:ILE:HD13	1.97	0.47
1:H:310:LYS:HE2	1:H:314:ARG:HH22	1.78	0.47
1:B:24:ASP:HB3	1:B:47:GLY:HA3	1.97	0.47
1:B:265:SER:HA	1:B:300:ILE:HG12	1.97	0.47
1:C:490:VAL:HG12	1:D:447:ASN:OD1	2.14	0.47
1:G:201:VAL:HG13	1:G:205:LEU:HB3	1.96	0.47
1:A:310:LYS:HE2	1:A:314:ARG:HH22	1.79	0.47
1:G:137:GLY:O	1:G:487:MET:HG3	2.15	0.47
1:C:310:LYS:HE2	1:C:314:ARG:HH22	1.80	0.46
1:H:109:ASP:HB2	1:H:161:GLN:HB2	1.96	0.46
1:B:258:LYS:HE2	1:B:292:THR:OG1	2.15	0.46
1:E:265:SER:HA	1:E:300:ILE:HG12	1.96	0.46
1:F:298:LYS:HG3	1:F:299:GLU:OE1	2.16	0.46
1:G:468:GLU:HG3	1:G:471:ARG:NH2	2.31	0.46
1:C:265:SER:HA	1:C:300:ILE:HG12	1.97	0.46
1:C:106:ALA:O	1:C:109:ASP:HB2	2.16	0.46
1:C:204:GLY:HA2	1:C:207:ASN:OD1	2.16	0.46
1:C:150:CYS:O	1:C:177:MET:HA	2.16	0.45
1:D:165:TRP:HH2	1:D:465:PHE:HE1	1.64	0.45
1:D:300:ILE:HA	1:D:303:LYS:HE2	1.98	0.45
1:E:123:LEU:O	1:E:127:MET:HG3	2.16	0.45
1:E:366:LYS:HG3	1:E:367:LEU:HD13	1.98	0.45
1:E:467:ARG:HH21	1:G:467:ARG:NH1	2.13	0.45
1:F:336:LEU:HD11	1:F:373:MET:HB3	1.98	0.45
1:F:428:ILE:HG23	1:F:429:GLN:N	2.31	0.45
1:H:300:ILE:HA	1:H:303:LYS:HE2	1.99	0.45
1:H:35:ALA:O	1:H:367:LEU:HD12	2.16	0.45
1:H:265:SER:HA	1:H:300:ILE:HG12	1.99	0.45
1:A:349:GLN:HE22	1:A:386:THR:HG23	1.81	0.45
1:F:349:GLN:HE22	1:F:386:THR:HG23	1.82	0.45
1:G:300:ILE:HA	1:G:303:LYS:HE2	1.98	0.45
1:F:158:TYR:O	1:F:162:ILE:HG22	2.17	0.45
1:H:258:LYS:HE2	1:H:292:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:ARG:O	1:H:428:ILE:HG22	2.16	0.45
1:A:300:ILE:HA	1:A:303:LYS:HE2	1.99	0.45
1:D:349:GLN:HE22	1:D:386:THR:HG23	1.82	0.45
1:F:51:VAL:O	1:F:55:VAL:HG23	2.17	0.45
1:E:106:ALA:O	1:E:110:ILE:HG12	2.17	0.44
1:C:300:ILE:HA	1:C:303:LYS:HE2	1.99	0.44
1:B:202:PRO:HD2	1:B:205:LEU:HD22	1.98	0.44
1:F:55:VAL:HG13	1:F:149:VAL:HG11	1.99	0.44
1:F:265:SER:HA	1:F:300:ILE:HG12	2.00	0.44
1:F:305:THR:HG22	1:F:399:ILE:HD13	1.98	0.44
1:A:3:THR:OG1	1:A:321:LEU:HD13	2.18	0.44
1:E:300:ILE:HA	1:E:303:LYS:HE2	2.00	0.44
1:C:147:LEU:HB3	1:C:226:ALA:HB1	1.99	0.44
1:F:300:ILE:HA	1:F:303:LYS:HE2	1.99	0.44
1:H:470:GLY:O	1:H:474:ILE:HG12	2.17	0.44
1:D:165:TRP:HH2	1:D:465:PHE:CE1	2.36	0.44
1:B:24:ASP:HB3	1:B:47:GLY:CA	2.48	0.44
1:C:201:VAL:HG13	1:C:205:LEU:HB3	2.00	0.44
1:C:15:ARG:HE	1:C:20:VAL:HG21	1.82	0.43
1:A:132:ILE:HD13	1:B:457:PHE:CZ	2.53	0.43
1:C:15:ARG:HE	1:C:15:ARG:HB2	1.65	0.43
1:F:451:SER:HB2	1:F:455:LEU:HD12	2.00	0.43
1:C:468:GLU:HG3	1:C:471:ARG:NH2	2.33	0.43
1:E:349:GLN:HE22	1:E:386:THR:HG23	1.83	0.43
1:C:349:GLN:HE22	1:C:386:THR:HG23	1.83	0.43
1:H:84:ILE:HD12	1:H:117:LEU:HD13	2.01	0.43
1:G:22:PRO:HB3	1:G:50:GLU:HG2	1.99	0.43
1:H:349:GLN:HE22	1:H:386:THR:HG23	1.84	0.43
1:D:196:TYR:O	1:D:201:VAL:HB	2.19	0.43
1:G:366:LYS:HG3	1:G:367:LEU:HD13	2.01	0.43
1:H:202:PRO:HD2	1:H:205:LEU:HD22	2.01	0.43
1:D:165:TRP:CH2	1:D:465:PHE:HE1	2.37	0.43
1:A:129:GLY:HA3	1:A:142:THR:O	2.19	0.43
1:A:123:LEU:O	1:A:127:MET:HG3	2.19	0.42
1:A:485:VAL:HG22	1:B:445:ILE:HD12	2.00	0.42
1:F:470:GLY:O	1:F:474:ILE:HG12	2.19	0.42
1:G:451:SER:HB2	1:G:455:LEU:HD12	2.01	0.42
1:A:75:ARG:NH1	1:A:76:ILE:HD13	2.34	0.42
1:B:177:MET:HE2	1:B:206:PHE:HE1	1.84	0.42
1:F:196:TYR:O	1:F:201:VAL:HB	2.19	0.42
1:H:3:THR:HG21	1:H:367:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:SER:HB2	1:D:455:LEU:HD12	2.01	0.42
1:E:202:PRO:HA	1:E:203:PRO:HD3	1.91	0.42
1:G:349:GLN:HE22	1:G:386:THR:HG23	1.83	0.42
1:H:339:VAL:HG11	1:H:394:GLY:HA3	2.00	0.42
1:B:51:VAL:HG13	1:B:219:LEU:HD23	2.01	0.42
1:C:58:ALA:HB1	1:C:176:ALA:HB1	2.01	0.42
1:E:3:THR:OG1	1:E:321:LEU:HD13	2.18	0.42
1:E:51:VAL:O	1:E:55:VAL:HG23	2.20	0.42
1:C:258:LYS:HE2	1:C:292:THR:OG1	2.19	0.42
1:G:123:LEU:O	1:G:127:MET:HG3	2.19	0.42
1:F:201:VAL:HG13	1:F:205:LEU:CB	2.50	0.42
1:B:300:ILE:HA	1:B:303:LYS:HE2	2.01	0.41
1:G:132:ILE:HD13	1:H:457:PHE:CZ	2.55	0.41
1:D:326:ARG:HD3	1:D:326:ARG:HA	1.93	0.41
1:E:15:ARG:HA	1:E:207:ASN:OD1	2.20	0.41
1:G:162:ILE:HD13	1:G:231:THR:HG21	2.02	0.41
1:A:196:TYR:O	1:A:201:VAL:HB	2.20	0.41
1:C:15:ARG:HH12	1:C:53:LEU:CD1	2.34	0.41
1:D:147:LEU:HB3	1:D:226:ALA:HB1	2.03	0.41
1:F:116:CYS:HB2	1:F:165:TRP:CZ3	2.54	0.41
1:G:326:ARG:HD3	1:G:326:ARG:HA	1.94	0.41
1:H:332:ASN:HB2	1:H:335:HIS:HB2	2.03	0.41
1:F:428:ILE:CB	1:H:428:ILE:HB	2.48	0.41
1:B:62:PHE:HE1	1:B:146:PRO:HB2	1.84	0.40
1:C:15:ARG:HH12	1:C:53:LEU:HD13	1.87	0.40
1:E:151:VAL:HB	1:E:228:VAL:HG22	2.02	0.40
1:G:106:ALA:O	1:G:110:ILE:HG12	2.21	0.40
1:B:259:SER:HB2	1:B:290:ASN:O	2.21	0.40
1:D:123:LEU:O	1:D:127:MET:HG3	2.21	0.40
1:B:62:PHE:CE1	1:B:148:GLY:HA2	2.56	0.40
1:E:261:LEU:HD13	1:E:448:TYR:CD2	2.55	0.40
1:E:467:ARG:HH22	1:H:467:ARG:NH1	2.20	0.40
1:G:196:TYR:O	1:G:201:VAL:HB	2.22	0.40
1:A:470:GLY:O	1:A:474:ILE:HG12	2.21	0.40
1:E:196:TYR:O	1:E:201:VAL:HB	2.21	0.40
1:F:366:LYS:HG3	1:F:367:LEU:CD1	2.51	0.40
1:G:34:PRO:HG3	3:G:503:HOH:O	2.21	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	467/508 (92%)	457 (98%)	10 (2%)	0	100	100
1	B	467/508 (92%)	458 (98%)	9 (2%)	0	100	100
1	C	469/508 (92%)	463 (99%)	6 (1%)	0	100	100
1	D	467/508 (92%)	461 (99%)	6 (1%)	0	100	100
1	E	468/508 (92%)	456 (97%)	11 (2%)	1 (0%)	47	68
1	F	467/508 (92%)	455 (97%)	11 (2%)	1 (0%)	47	68
1	G	467/508 (92%)	460 (98%)	6 (1%)	1 (0%)	47	68
1	H	467/508 (92%)	461 (99%)	6 (1%)	0	100	100
All	All	3739/4064 (92%)	3671 (98%)	65 (2%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	463	SER
1	F	463	SER
1	G	298	LYS

### 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	384/416 (92%)	355 (92%)	29 (8%)	13	25
1	B	384/416 (92%)	356 (93%)	28 (7%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	386/416 (93%)	358 (93%)	28 (7%)	14	27
1	D	384/416 (92%)	358 (93%)	26 (7%)	16	30
1	E	385/416 (92%)	358 (93%)	27 (7%)	15	29
1	F	384/416 (92%)	355 (92%)	29 (8%)	13	25
1	G	384/416 (92%)	358 (93%)	26 (7%)	16	30
1	H	384/416 (92%)	355 (92%)	29 (8%)	13	25
All	All	3075/3328 (92%)	2853 (93%)	222 (7%)	14	28

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	56	GLN
1	A	72	GLU
1	A	98	ASN
1	A	132	ILE
1	A	134	LEU
1	A	161	GLN
1	A	190	LEU
1	A	201	VAL
1	A	277	LEU
1	A	283	THR
1	A	287	VAL
1	A	293	ARG
1	A	302	ASP
1	A	306	GLU
1	A	308	VAL
1	A	344	LYS
1	A	358	ASP
1	A	368	LYS
1	A	391	GLU
1	A	403	ASP
1	A	408	VAL
1	A	416	THR
1	A	430	ARG
1	A	437	GLU
1	A	454	GLU
1	A	467	ARG
1	A	473	THR
1	A	491	GLU

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Mol	Chain	Res	Type
1	B	24	ASP
1	B	95	GLU
1	B	98	ASN
1	B	132	ILE
1	B	134	LEU
1	B	161	GLN
1	B	182	SER
1	B	190	LEU
1	B	201	VAL
1	B	231	THR
1	B	277	LEU
1	B	283	THR
1	B	287	VAL
1	B	293	ARG
1	B	302	ASP
1	B	306	GLU
1	B	344	LYS
1	B	368	LYS
1	B	391	GLU
1	B	403	ASP
1	B	408	VAL
1	B	416	THR
1	B	430	ARG
1	B	437	GLU
1	B	438	LEU
1	B	467	ARG
1	B	473	THR
1	B	491	GLU
1	C	56	GLN
1	C	98	ASN
1	C	117	LEU
1	C	132	ILE
1	C	133	GLN
1	C	134	LEU
1	C	190	LEU
1	C	229	SER
1	C	277	LEU
1	C	283	THR
1	C	287	VAL
1	C	293	ARG
1	C	302	ASP
1	C	306	GLU

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Mol	Chain	Res	Type
1	C	321	LEU
1	C	322	LEU
1	C	344	LYS
1	C	368	LYS
1	C	391	GLU
1	C	403	ASP
1	C	408	VAL
1	C	416	THR
1	C	430	ARG
1	C	437	GLU
1	C	438	LEU
1	C	454	GLU
1	C	473	THR
1	C	491	GLU
1	D	98	ASN
1	D	132	ILE
1	D	134	LEU
1	D	161	GLN
1	D	190	LEU
1	D	201	VAL
1	D	277	LEU
1	D	283	THR
1	D	287	VAL
1	D	293	ARG
1	D	302	ASP
1	D	306	GLU
1	D	344	LYS
1	D	363	GLU
1	D	368	LYS
1	D	391	GLU
1	D	403	ASP
1	D	408	VAL
1	D	416	THR
1	D	430	ARG
1	D	437	GLU
1	D	438	LEU
1	D	461	LYS
1	D	467	ARG
1	D	473	THR
1	D	491	GLU
1	E	44	THR
1	E	56	GLN

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Mol	Chain	Res	Type
1	E	98	ASN
1	E	132	ILE
1	E	134	LEU
1	E	161	GLN
1	E	190	LEU
1	E	201	VAL
1	E	283	THR
1	E	287	VAL
1	E	293	ARG
1	E	302	ASP
1	E	306	GLU
1	E	324	ASP
1	E	344	LYS
1	E	368	LYS
1	E	391	GLU
1	E	403	ASP
1	E	408	VAL
1	E	416	THR
1	E	430	ARG
1	E	437	GLU
1	E	438	LEU
1	E	454	GLU
1	E	455	LEU
1	E	484	CYS
1	E	487	MET
1	F	56	GLN
1	F	72	GLU
1	F	94	MET
1	F	98	ASN
1	F	132	ILE
1	F	134	LEU
1	F	161	GLN
1	F	164	SER
1	F	190	LEU
1	F	201	VAL
1	F	259	SER
1	F	277	LEU
1	F	283	THR
1	F	287	VAL
1	F	293	ARG
1	F	302	ASP
1	F	306	GLU

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Mol	Chain	Res	Type
1	F	344	LYS
1	F	391	GLU
1	F	403	ASP
1	F	408	VAL
1	F	415	THR
1	F	416	THR
1	F	430	ARG
1	F	437	GLU
1	F	438	LEU
1	F	455	LEU
1	F	467	ARG
1	F	487	MET
1	G	56	GLN
1	G	98	ASN
1	G	132	ILE
1	G	134	LEU
1	G	161	GLN
1	G	190	LEU
1	G	201	VAL
1	G	258	LYS
1	G	283	THR
1	G	287	VAL
1	G	293	ARG
1	G	302	ASP
1	G	306	GLU
1	G	338	ARG
1	G	344	LYS
1	G	367	LEU
1	G	368	LYS
1	G	391	GLU
1	G	403	ASP
1	G	408	VAL
1	G	416	THR
1	G	430	ARG
1	G	437	GLU
1	G	438	LEU
1	G	462	LYS
1	G	491	GLU
1	H	20	VAL
1	H	94	MET
1	H	98	ASN
1	H	117	LEU

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Mol	Chain	Res	Type
1	H	132	ILE
1	H	134	LEU
1	H	161	GLN
1	H	190	LEU
1	H	277	LEU
1	H	283	THR
1	H	287	VAL
1	H	293	ARG
1	H	302	ASP
1	H	306	GLU
1	H	344	LYS
1	H	367	LEU
1	H	368	LYS
1	H	391	GLU
1	H	403	ASP
1	H	408	VAL
1	H	416	THR
1	H	430	ARG
1	H	437	GLU
1	H	438	LEU
1	H	454	GLU
1	H	467	ARG
1	H	473	THR
1	H	487	MET
1	H	491	GLU

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

Mol	Chain	Res	Type
1	F	432	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	EDO	B	501	-	3,3,3	0.69	0	2,2,2	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	471/508 (92%)	0.36	20 (4%)	36	39	44, 71, 106, 128	0
1	B	471/508 (92%)	0.25	12 (2%)	57	61	46, 69, 102, 125	0
1	C	471/508 (92%)	0.64	47 (9%)	7	6	51, 77, 126, 146	0
1	D	471/508 (92%)	0.48	38 (8%)	12	12	50, 76, 125, 146	0
1	E	471/508 (92%)	0.71	56 (11%)	4	4	48, 86, 139, 164	0
1	F	471/508 (92%)	0.51	37 (7%)	12	12	51, 77, 121, 143	0
1	G	471/508 (92%)	0.28	16 (3%)	45	48	44, 68, 105, 125	0
1	H	471/508 (92%)	0.57	39 (8%)	11	11	45, 84, 126, 148	0
All	All	3768/4064 (92%)	0.47	265 (7%)	16	16	44, 75, 123, 164	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	VAL	7.4
1	C	263	ILE	6.6
1	H	409	LEU	6.1
1	H	296	VAL	5.8
1	F	263	ILE	5.7
1	E	403	ASP	5.7
1	C	400	LEU	5.6
1	D	263	ILE	5.5
1	C	261	LEU	5.4
1	H	298	LYS	5.2
1	C	399	ILE	5.0
1	C	301	LEU	5.0
1	E	434	VAL	5.0
1	C	273	VAL	4.8
1	E	264	PHE	4.8
1	C	409	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	426	ARG	4.5
1	H	415	THR	4.4
1	C	309	VAL	4.3
1	H	365	PRO	4.3
1	E	291	GLY	4.3
1	F	460	TYR	4.2
1	E	309	VAL	4.2
1	F	309	VAL	4.2
1	E	299	GLU	4.2
1	E	277	LEU	4.1
1	E	262	ILE	4.1
1	A	354	LEU	4.1
1	E	401	SER	4.0
1	E	266	ASP	4.0
1	F	494	PHE	4.0
1	G	273	VAL	4.0
1	E	374	ARG	3.9
1	D	393	PHE	3.9
1	D	303	LYS	3.9
1	E	260	PRO	3.8
1	E	261	LEU	3.8
1	F	450	VAL	3.8
1	F	264	PHE	3.8
1	A	399	ILE	3.8
1	C	304	PHE	3.7
1	H	399	ILE	3.7
1	F	462	LYS	3.7
1	E	0	PRO	3.7
1	A	404	THR	3.7
1	D	415	THR	3.7
1	E	462	LYS	3.6
1	F	457	PHE	3.6
1	A	230	PHE	3.6
1	C	401	SER	3.6
1	E	460	TYR	3.6
1	C	388	VAL	3.6
1	G	431	ALA	3.6
1	C	305	THR	3.6
1	H	0	PRO	3.5
1	D	348	GLU	3.5
1	F	1	MET	3.5
1	F	289	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	304	PHE	3.5
1	G	494	PHE	3.5
1	A	204	GLY	3.5
1	D	379	THR	3.5
1	D	392	ILE	3.5
1	H	428	ILE	3.5
1	D	301	LEU	3.5
1	E	353	VAL	3.4
1	E	457	PHE	3.4
1	H	300	ILE	3.4
1	B	264	PHE	3.4
1	B	300	ILE	3.4
1	H	342	PHE	3.4
1	H	381	CYS	3.4
1	H	97	ILE	3.4
1	H	363	GLU	3.3
1	E	265	SER	3.3
1	D	300	ILE	3.2
1	D	304	PHE	3.2
1	D	306	GLU	3.2
1	F	393	PHE	3.2
1	C	294	VAL	3.2
1	C	354	LEU	3.2
1	H	426	ARG	3.2
1	H	371	TYR	3.2
1	D	437	GLU	3.2
1	F	453	VAL	3.2
1	C	405	GLU	3.1
1	F	304	PHE	3.1
1	D	261	LEU	3.1
1	D	291	GLY	3.1
1	D	378	LEU	3.0
1	D	409	LEU	3.0
1	E	297	GLN	3.0
1	E	407	GLU	3.0
1	F	305	THR	3.0
1	F	465	PHE	3.0
1	C	20	VAL	3.0
1	A	392	ILE	3.0
1	C	270	ASN	3.0
1	E	288	CYS	3.0
1	C	256	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	295	PHE	3.0
1	E	263	ILE	3.0
1	H	370	GLY	3.0
1	C	295	PHE	3.0
1	D	262	ILE	3.0
1	C	377	VAL	2.9
1	C	415	THR	2.9
1	H	404	THR	2.9
1	E	306	GLU	2.9
1	F	230	PHE	2.9
1	G	136	GLY	2.9
1	C	398	SER	2.9
1	D	354	LEU	2.9
1	E	410	GLU	2.9
1	H	432	HIS	2.9
1	E	269	MET	2.8
1	D	230	PHE	2.8
1	E	276	ALA	2.8
1	E	289	CYS	2.8
1	H	412	ALA	2.8
1	C	378	LEU	2.8
1	C	431	ALA	2.8
1	C	404	THR	2.8
1	F	261	LEU	2.8
1	E	294	VAL	2.8
1	D	296	VAL	2.7
1	F	0	PRO	2.7
1	H	6	PHE	2.7
1	C	306	GLU	2.7
1	F	272	ALA	2.7
1	D	282	LEU	2.7
1	C	376	CYS	2.7
1	C	402	PHE	2.7
1	F	134	LEU	2.7
1	G	393	PHE	2.7
1	F	459	GLY	2.7
1	B	301	LEU	2.7
1	E	409	LEU	2.7
1	A	265	SER	2.6
1	A	263	ILE	2.6
1	F	301	LEU	2.6
1	G	257	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	300	ILE	2.6
1	E	377	VAL	2.6
1	D	424	PHE	2.6
1	E	230	PHE	2.6
1	E	445	ILE	2.6
1	G	264	PHE	2.6
1	H	306	GLU	2.6
1	C	297	GLN	2.6
1	G	305	THR	2.6
1	A	300	ILE	2.6
1	H	281	PHE	2.6
1	A	256	GLY	2.6
1	D	294	VAL	2.5
1	E	273	VAL	2.5
1	B	303	LYS	2.5
1	D	264	PHE	2.5
1	H	40	ILE	2.5
1	C	422	GLY	2.5
1	F	190	LEU	2.5
1	H	408	VAL	2.5
1	H	467	ARG	2.5
1	F	132	ILE	2.5
1	F	463	SER	2.5
1	E	360	TYR	2.5
1	C	353	VAL	2.5
1	E	427	ASP	2.5
1	E	298	LYS	2.5
1	C	345	VAL	2.5
1	E	308	VAL	2.5
1	A	393	PHE	2.5
1	D	298	LYS	2.5
1	H	367	LEU	2.5
1	D	265	SER	2.5
1	D	342	PHE	2.5
1	H	1	MET	2.5
1	D	302	ASP	2.5
1	D	434	VAL	2.4
1	B	393	PHE	2.4
1	C	300	ILE	2.4
1	G	277	LEU	2.4
1	C	264	PHE	2.4
1	E	357	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	301	LEU	2.4
1	E	132	ILE	2.4
1	F	390	GLU	2.4
1	D	401	SER	2.4
1	F	302	ASP	2.4
1	A	377	VAL	2.4
1	G	56	GLN	2.4
1	H	265	SER	2.4
1	A	367	LEU	2.4
1	A	273	VAL	2.3
1	E	430	ARG	2.3
1	H	382	ARG	2.3
1	A	314	ARG	2.3
1	F	265	SER	2.3
1	D	358	ASP	2.3
1	H	376	CYS	2.3
1	C	262	ILE	2.3
1	F	262	ILE	2.3
1	E	302	ASP	2.3
1	F	434	VAL	2.3
1	C	269	MET	2.3
1	C	385	MET	2.3
1	E	355	CYS	2.3
1	E	363	GLU	2.3
1	A	277	LEU	2.3
1	G	400	LEU	2.3
1	E	310	LYS	2.3
1	F	389	LYS	2.3
1	G	265	SER	2.3
1	B	365	PRO	2.2
1	H	434	VAL	2.2
1	H	264	PHE	2.2
1	C	0	PRO	2.2
1	B	403	ASP	2.2
1	E	399	ILE	2.2
1	H	400	LEU	2.2
1	D	403	ASP	2.2
1	E	20	VAL	2.2
1	C	467	ARG	2.2
1	E	283	THR	2.2
1	E	312	THR	2.2
1	B	367	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	269	MET	2.2
1	E	303	LYS	2.2
1	F	456	PRO	2.2
1	F	273	VAL	2.2
1	B	431	ALA	2.2
1	C	344	LYS	2.2
1	B	266	ASP	2.2
1	E	424	PHE	2.2
1	H	39	VAL	2.2
1	C	302	ASP	2.2
1	F	455	LEU	2.2
1	H	336	LEU	2.2
1	F	461	LYS	2.1
1	C	1	MET	2.1
1	H	308	VAL	2.1
1	E	1	MET	2.1
1	D	289	CYS	2.1
1	H	339	VAL	2.1
1	A	231	THR	2.1
1	C	460	TYR	2.1
1	D	387	CYS	2.1
1	E	331	ILE	2.1
1	G	272	ALA	2.1
1	D	399	ILE	2.1
1	G	357	GLY	2.1
1	G	309	VAL	2.1
1	F	281	PHE	2.1
1	D	400	LEU	2.0
1	C	257	GLY	2.0
1	H	406	ALA	2.0
1	A	415	THR	2.0
1	B	404	THR	2.0
1	C	265	SER	2.0
1	A	257	GLY	2.0
1	B	427	ASP	2.0
1	H	405	GLU	2.0
1	C	379	THR	2.0
1	A	294	VAL	2.0
1	E	284	GLN	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 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( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	501	4/4	0.82	0.21	79,81,81,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.