



# Full wwPDB X-ray Structure Validation Report i

Oct 5, 2021 – 12:13 PM JST

PDB ID : 7DBI  
Title : Crystal structure of the peroxisomal acyl-CoA hydrolase MpAH  
Authors : Li, S.Y.; You, C.  
Deposited on : 2020-10-20  
Resolution : 1.99 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 i symbol.

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The following versions of software and data (see [references](#) i) 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 : 2.23.2  
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) : 2.23.2

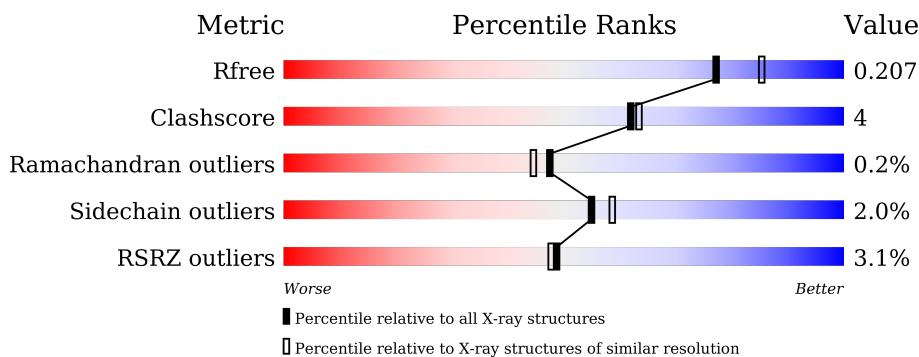
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

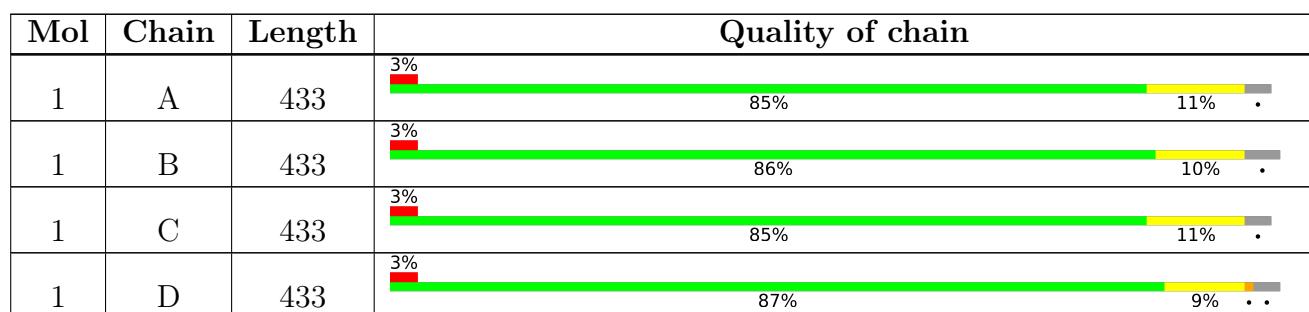
The reported resolution of this entry is 1.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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.



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14163 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 acyl-CoA hydrolase MpAH'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C 3356	N 2135	O 591	S 613	Se 5	0	0	0
1	B	417	Total	C 3332	N 2120	O 587	S 608	Se 5	0	0	0
1	C	420	Total	C 3356	N 2135	O 591	S 613	Se 5	0	0	0
1	D	418	Total	C 3343	N 2127	O 589	S 610	Se 5	0	0	0

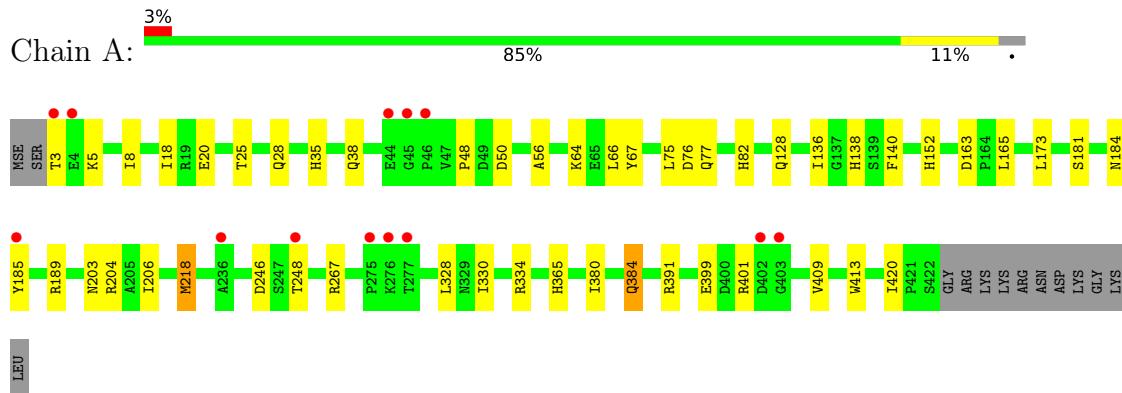
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	204	Total O 204 204	0	0
2	B	210	Total O 210 210	0	0
2	C	188	Total O 188 188	0	0
2	D	174	Total O 174 174	0	0

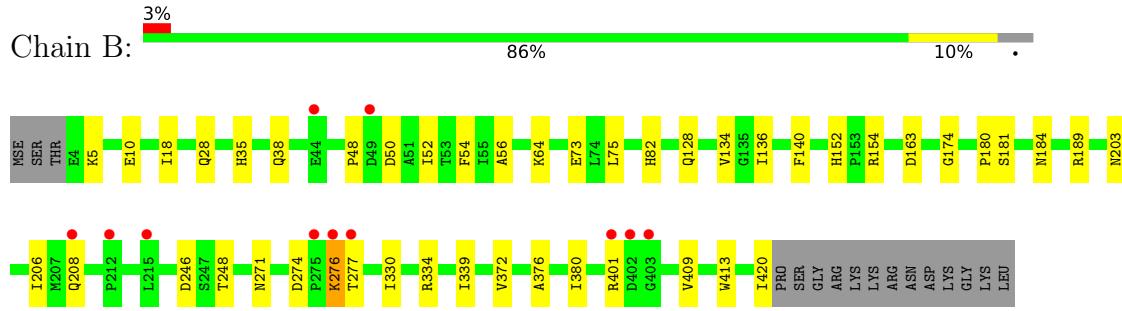
### 3 Residue-property plots

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.

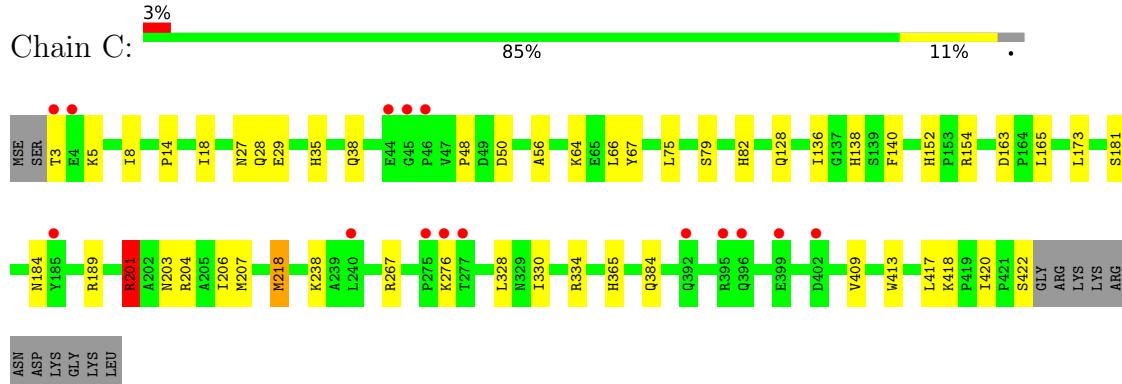
- Molecule 1: acyl-CoA hydrolase Mpah'



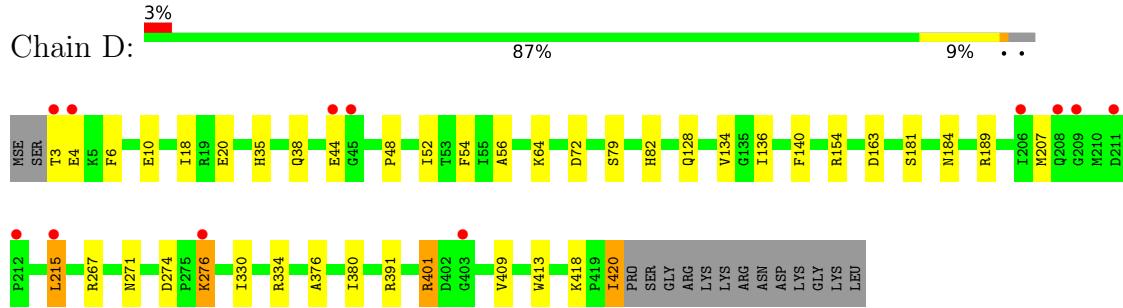
- Molecule 1: acyl-CoA hydrolase Mpah'



- Molecule 1: acyl-CoA hydrolase Mpah'



- Molecule 1: acyl-CoA hydrolase Mpah'



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.92Å    93.26Å    161.28Å 90.00°    95.12°    90.00°	Depositor
Resolution (Å)	46.63 – 1.99 46.63 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.63-1.99) 99.1 (46.63-1.99)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.86 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
$R$ , $R_{free}$	0.168 , 0.194 0.182 , 0.207	Depositor DCC
$R_{free}$ test set	6548 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14163	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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  $< |L| >$ ,  $< L^2 >$  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

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	0.70	0/3435	0.84	7/4657 (0.2%)
1	B	0.70	1/3410 (0.0%)	0.82	1/4623 (0.0%)
1	C	0.69	0/3435	0.84	5/4657 (0.1%)
1	D	0.71	1/3421 (0.0%)	0.83	5/4637 (0.1%)
All	All	0.70	2/13701 (0.0%)	0.83	18/18574 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	10	GLU	CD-OE2	-5.71	1.19	1.25
1	B	10	GLU	CD-OE2	-5.03	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	391	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	D	391	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	189	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	201	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	B	189	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	C	267	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	391	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	189	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	218	MSE	CG-SE-CE	5.46	110.91	98.90
1	D	267	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	391	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	207	MSE	CG-SE-CE	5.35	110.67	98.90
1	A	267	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	267	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	384	GLN	CB-CA-C	5.16	120.72	110.40
1	D	267	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	218	MSE	CG-SE-CE	5.08	110.09	98.90

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	3356	0	3320	32	1
1	B	3332	0	3290	36	0
1	C	3356	0	3320	33	0
1	D	3343	0	3308	29	1
2	A	204	0	0	0	0
2	B	210	0	0	4	0
2	C	188	0	0	1	0
2	D	174	0	0	2	0
All	All	14163	0	13238	117	1

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 (117) 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:271:ASN:HB2	2:B:646:HOH:O	1.79	0.82
1:C:201:ARG:NH1	1:C:204:ARG:HD3	1.96	0.80
1:C:5:LYS:HB3	1:C:75:LEU:HD23	1.63	0.79
1:B:276:LYS:HA	1:B:276:LYS:CE	2.18	0.74
1:A:28:GLN:HE22	1:D:154:ARG:HH12	1.38	0.72
1:D:52:ILE:CG2	1:D:134:VAL:HG13	2.21	0.70
1:A:246:ASP:OD1	1:A:248:THR:HG22	1.91	0.70
1:D:207:MSE:HE2	1:D:215:LEU:HG	1.74	0.70
1:D:3:THR:HG23	1:D:72:ASP:OD1	1.91	0.69
1:D:271:ASN:HB2	2:D:588:HOH:O	1.93	0.69
1:B:28:GLN:HE22	1:C:154:ARG:HH12	1.41	0.68
1:D:35:HIS:HD2	1:D:64:LYS:NZ	1.93	0.66
1:A:35:HIS:HD2	1:A:64:LYS:HZ1	1.42	0.66
1:A:35:HIS:HD2	1:A:64:LYS:NZ	1.94	0.66
1:B:52:ILE:CG2	1:B:134:VAL:HG13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:HG21	1:D:6:PHE:HD1	1.60	0.66
1:B:35:HIS:HD2	1:B:64:LYS:NZ	1.94	0.65
1:C:35:HIS:HD2	1:C:64:LYS:NZ	1.95	0.64
1:D:35:HIS:HD2	1:D:64:LYS:HZ1	1.46	0.64
1:D:3:THR:CG2	1:D:72:ASP:OD1	2.45	0.63
1:C:35:HIS:HD2	1:C:64:LYS:HZ1	1.46	0.63
1:B:276:LYS:HA	1:B:276:LYS:HE2	1.80	0.62
1:D:52:ILE:HG23	1:D:134:VAL:HG13	1.81	0.62
1:B:339:ILE:CD1	2:B:610:HOH:O	2.49	0.60
1:B:154:ARG:HH12	1:C:28:GLN:HE22	1.48	0.60
1:A:3:THR:HG22	1:A:8:ILE:HD11	1.83	0.60
1:B:52:ILE:HG23	1:B:134:VAL:HG13	1.84	0.58
1:C:3:THR:HG22	1:C:8:ILE:HD11	1.86	0.58
1:C:201:ARG:NH2	1:C:204:ARG:HG3	2.19	0.58
1:C:38:GLN:HE22	1:C:128:GLN:HE22	1.51	0.58
1:B:73:GLU:HG3	1:B:372:VAL:HG12	1.86	0.57
1:A:38:GLN:HE22	1:A:128:GLN:HE22	1.51	0.57
1:A:28:GLN:NE2	1:D:154:ARG:HH12	2.03	0.56
1:B:174:GLY:O	1:C:418:LYS:HE3	2.04	0.56
1:D:181:SER:H	1:D:184:ASN:HD22	1.54	0.55
1:B:181:SER:H	1:B:184:ASN:HD22	1.55	0.55
1:D:44:GLU:H	1:D:44:GLU:CD	2.09	0.54
1:A:35:HIS:CD2	1:A:64:LYS:HZ1	2.25	0.54
1:D:52:ILE:HG21	1:D:134:VAL:HG13	1.89	0.54
1:D:181:SER:H	1:D:184:ASN:ND2	2.06	0.54
1:B:181:SER:H	1:B:184:ASN:ND2	2.06	0.54
1:B:38:GLN:HE22	1:B:128:GLN:HE22	1.56	0.53
1:D:38:GLN:HE22	1:D:128:GLN:HE22	1.55	0.53
1:B:5:LYS:CB	1:B:75:LEU:HD23	2.39	0.53
1:A:5:LYS:CB	1:A:75:LEU:HD23	2.39	0.52
1:A:181:SER:H	1:A:184:ASN:ND2	2.08	0.52
1:A:67:TYR:OH	1:A:138:HIS:HD2	1.92	0.52
1:C:56:ALA:HA	1:C:136:ILE:O	2.10	0.52
1:C:67:TYR:OH	1:C:138:HIS:HD2	1.92	0.52
1:A:5:LYS:HB3	1:A:75:LEU:HD23	1.92	0.52
1:A:28:GLN:HE21	1:D:154:ARG:HH22	1.58	0.52
1:C:181:SER:H	1:C:184:ASN:ND2	2.08	0.52
1:A:56:ALA:HA	1:A:136:ILE:O	2.10	0.51
1:B:28:GLN:NE2	1:C:154:ARG:HH12	2.08	0.51
1:D:56:ALA:HA	1:D:136:ILE:O	2.11	0.50
1:A:77:GLN:HB2	1:A:380:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:O	1:A:206:ILE:HG22	2.11	0.50
1:B:35:HIS:HD2	1:B:64:LYS:HZ1	1.57	0.50
1:B:56:ALA:HA	1:B:136:ILE:O	2.11	0.50
1:C:181:SER:H	1:C:184:ASN:HD22	1.60	0.50
1:C:35:HIS:CD2	1:C:64:LYS:HZ1	2.29	0.49
1:A:181:SER:H	1:A:184:ASN:HD22	1.59	0.49
1:B:274:ASP:HB3	1:B:277:THR:CG2	2.43	0.49
1:B:52:ILE:HG21	1:B:134:VAL:HG13	1.95	0.48
1:B:180:PRO:HB2	1:C:420:ILE:HD13	1.95	0.48
1:C:203:ASN:O	1:C:206:ILE:HG22	2.12	0.48
1:B:154:ARG:HH12	1:C:28:GLN:NE2	2.11	0.48
1:B:274:ASP:CG	1:B:277:THR:HG22	2.34	0.48
1:D:35:HIS:CD2	1:D:64:LYS:HZ1	2.29	0.48
1:B:274:ASP:HB3	1:B:277:THR:HG23	1.97	0.47
1:A:5:LYS:HE3	1:A:76:ASP:HB2	1.97	0.47
1:C:138:HIS:HE1	1:C:365:HIS:O	1.97	0.47
1:A:25:THR:O	1:D:401:ARG:NH2	2.47	0.47
1:D:3:THR:HG21	1:D:6:PHE:CD1	2.46	0.47
1:B:246:ASP:OD1	1:B:248:THR:HG22	2.14	0.47
1:C:201:ARG:NH1	1:C:204:ARG:CD	2.75	0.47
1:D:330:ILE:O	1:D:334:ARG:HG3	2.15	0.47
1:A:138:HIS:HE1	1:A:365:HIS:O	1.98	0.46
1:A:330:ILE:O	1:A:334:ARG:HG3	2.16	0.46
1:A:66:LEU:HD21	1:A:218:MSE:HG2	1.98	0.46
1:A:165:LEU:HD12	1:A:328:LEU:HD21	1.98	0.46
1:C:330:ILE:O	1:C:334:ARG:HG3	2.16	0.45
1:A:50:ASP:OD1	1:A:50:ASP:N	2.42	0.45
1:A:77:GLN:HB2	1:A:380:ILE:HD11	1.98	0.45
1:A:185:TYR:CE1	1:D:420:ILE:HG13	2.52	0.45
1:C:409:VAL:HB	1:C:413:TRP:CD1	2.52	0.45
1:C:50:ASP:OD1	1:C:50:ASP:N	2.41	0.45
1:B:54:PHE:CD1	1:B:134:VAL:HG22	2.52	0.44
1:D:54:PHE:CD1	1:D:134:VAL:HG22	2.52	0.44
1:B:203:ASN:O	1:B:206:ILE:HG22	2.17	0.44
1:A:409:VAL:HB	1:A:413:TRP:CD1	2.52	0.44
1:B:330:ILE:O	1:B:334:ARG:HG3	2.17	0.44
1:C:48:PRO:HG2	1:C:82:HIS:CG	2.52	0.44
1:A:173:LEU:HA	1:A:184:ASN:HD21	1.83	0.43
1:C:173:LEU:HA	1:C:184:ASN:HD21	1.83	0.43
1:D:274:ASP:OD1	1:D:276:LYS:HG2	2.18	0.43
1:C:79:SER:OG	1:C:384:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:O	1:B:380:ILE:HG12	2.19	0.42
1:B:409:VAL:HB	1:B:413:TRP:CD1	2.55	0.42
1:D:409:VAL:HB	1:D:413:TRP:CD1	2.55	0.42
1:B:50:ASP:OD1	1:B:50:ASP:N	2.42	0.42
1:C:66:LEU:HD21	1:C:218:MSE:HG2	2.02	0.42
1:B:339:ILE:HD12	2:B:610:HOH:O	2.14	0.41
1:B:28:GLN:HE21	1:C:154:ARG:HH22	1.68	0.41
1:B:48:PRO:HG2	1:B:82:HIS:CG	2.55	0.41
1:A:48:PRO:HG2	1:A:82:HIS:CG	2.54	0.41
1:D:376:ALA:O	1:D:380:ILE:HG12	2.20	0.41
2:B:625:HOH:O	1:C:152:HIS:HD2	2.02	0.41
1:C:27:ASN:ND2	1:C:29:GLU:H	2.19	0.41
1:C:38:GLN:HE22	1:C:128:GLN:NE2	2.18	0.41
1:A:152:HIS:HD2	2:D:619:HOH:O	2.02	0.41
1:B:35:HIS:CD2	1:B:64:LYS:HZ1	2.39	0.41
1:A:28:GLN:NE2	1:D:154:ARG:HH22	2.17	0.41
1:C:165:LEU:HD12	1:C:328:LEU:HD21	2.03	0.41
1:D:48:PRO:HG2	1:D:82:HIS:CG	2.56	0.41
1:A:5:LYS:HB2	1:A:75:LEU:HD23	2.03	0.40
1:B:152:HIS:HD2	2:C:602:HOH:O	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:D:79:SER:OG[1_455]	2.11	0.09

## 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	418/433 (96%)	406 (97%)	11 (3%)	1 (0%)	47    44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	415/433 (96%)	406 (98%)	8 (2%)	1 (0%)	47 44
1	C	418/433 (96%)	410 (98%)	7 (2%)	1 (0%)	47 44
1	D	416/433 (96%)	405 (97%)	10 (2%)	1 (0%)	47 44
All	All	1667/1732 (96%)	1627 (98%)	36 (2%)	4 (0%)	47 44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	18	ILE
1	A	18	ILE
1	B	18	ILE
1	D	18	ILE

### 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	368/366 (100%)	361 (98%)	7 (2%)	57 61
1	B	364/366 (100%)	358 (98%)	6 (2%)	62 67
1	C	368/366 (100%)	360 (98%)	8 (2%)	52 55
1	D	366/366 (100%)	357 (98%)	9 (2%)	47 49
All	All	1466/1464 (100%)	1436 (98%)	30 (2%)	55 58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	140	PHE
1	A	163	ASP
1	A	204	ARG
1	A	384	GLN
1	A	401	ARG
1	A	420	ILE

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Mol	Chain	Res	Type
1	B	140	PHE
1	B	163	ASP
1	B	208	GLN
1	B	276	LYS
1	B	401	ARG
1	B	420	ILE
1	C	14	PRO
1	C	140	PHE
1	C	163	ASP
1	C	201	ARG
1	C	238	LYS
1	C	276	LYS
1	C	417	LEU
1	C	422	SER
1	D	4	GLU
1	D	20	GLU
1	D	140	PHE
1	D	163	ASP
1	D	215	LEU
1	D	276	LYS
1	D	401	ARG
1	D	418	LYS
1	D	420	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	35	HIS
1	A	77	GLN
1	A	95	ASN
1	A	128	GLN
1	A	138	HIS
1	A	152	HIS
1	A	184	ASN
1	B	28	GLN
1	B	35	HIS
1	B	77	GLN
1	B	128	GLN
1	B	152	HIS
1	B	184	ASN
1	B	384	GLN

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Mol	Chain	Res	Type
1	C	27	ASN
1	C	28	GLN
1	C	35	HIS
1	C	77	GLN
1	C	95	ASN
1	C	128	GLN
1	C	138	HIS
1	C	152	HIS
1	C	184	ASN
1	C	384	GLN
1	D	35	HIS
1	D	77	GLN
1	D	95	ASN
1	D	128	GLN
1	D	152	HIS
1	D	184	ASN

### 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 [\(i\)](#)

There are no ligands in this entry.

### 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 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	408/433 (94%)	0.05	13 (3%) 47 46	19, 26, 47, 82	0
1	B	405/433 (93%)	0.16	11 (2%) 54 53	18, 27, 49, 88	0
1	C	408/433 (94%)	0.04	15 (3%) 41 41	19, 26, 48, 76	0
1	D	406/433 (93%)	0.14	12 (2%) 50 49	19, 26, 49, 77	0
All	All	1627/1732 (93%)	0.10	51 (3%) 49 48	18, 26, 49, 88	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	GLY	6.0
1	B	276	LYS	5.2
1	A	276	LYS	4.7
1	C	275	PRO	4.6
1	B	44	GLU	4.4
1	A	275	PRO	3.9
1	C	44	GLU	3.8
1	A	248	THR	3.7
1	A	44	GLU	3.6
1	C	3	THR	3.6
1	C	4	GLU	3.5
1	C	277	THR	3.4
1	B	402	ASP	3.4
1	B	403	GLY	3.4
1	D	4	GLU	3.3
1	D	45	GLY	3.2
1	D	206	ILE	3.2
1	D	44	GLU	3.1
1	C	276	LYS	3.0
1	D	208	GLN	2.9
1	B	275	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	211	ASP	2.8
1	B	208	GLN	2.7
1	A	4	GLU	2.7
1	B	49	ASP	2.7
1	C	185	TYR	2.7
1	A	185	TYR	2.6
1	A	3	THR	2.6
1	A	403	GLY	2.6
1	C	402	ASP	2.6
1	C	399	GLU	2.6
1	C	45	GLY	2.5
1	A	277	THR	2.5
1	D	3	THR	2.5
1	A	402	ASP	2.5
1	A	236	ALA	2.5
1	D	212	PRO	2.4
1	A	46	PRO	2.4
1	B	212	PRO	2.4
1	D	215	LEU	2.3
1	B	215	LEU	2.3
1	D	403	GLY	2.3
1	B	401	ARG	2.3
1	C	46	PRO	2.2
1	D	209	GLY	2.2
1	C	396	GLN	2.2
1	D	276	LYS	2.2
1	C	395	ARG	2.1
1	C	392	GLN	2.1
1	B	277	THR	2.0
1	C	240	LEU	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 [\(i\)](#)

There are no ligands in this entry.

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

There are no such residues in this entry.