



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:42 am GMT

PDB ID : 2AW5  
Title : Crystal structure of a human malic enzyme  
Authors : Papagrigoriou, E.; Berridge, G.; Smee, C.; Bray, J.; Arrowsmith, C.; Edwards, A.; Weigelt, J.; Sundstrom, M.; Oppermann, U.; Gileadi, O.; von Delft, F.; Structural Genomics Consortium (SGC)  
Deposited on : 2005-08-31  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

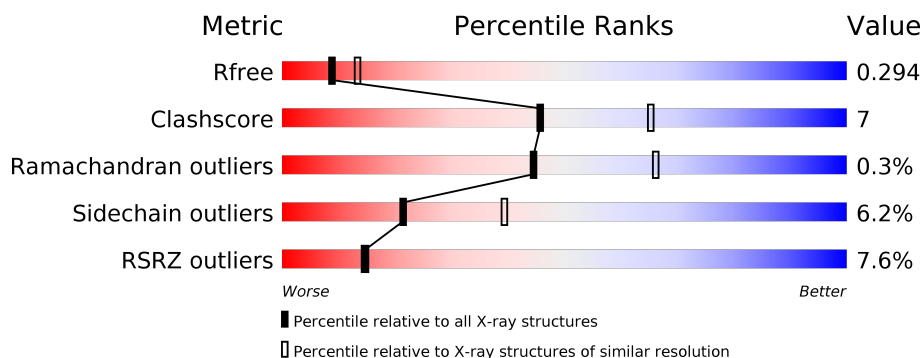
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>16%</div> <div> <div>76%</div> <div>14%</div> <div>8%</div> </div> </div>
1	B	575	<div> <div>16%</div> <div> <div>78%</div> <div>13%</div> <div>7%</div> </div> </div>
1	C	575	<div> <div>5%</div> <div> <div>74%</div> <div>17%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11920 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 NADP-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4004	2567	675	744	18			
1	B	536	Total	C	N	O	S	0	0	0
			3919	2500	670	730	19			
1	C	533	Total	C	N	O	S	0	0	0
			3997	2556	675	748	18			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	CLONING ARTIFACT	UNP P48163
A	-9	HIS	-	CLONING ARTIFACT	UNP P48163
A	-8	HIS	-	CLONING ARTIFACT	UNP P48163
A	-7	HIS	-	CLONING ARTIFACT	UNP P48163
A	-6	HIS	-	CLONING ARTIFACT	UNP P48163
A	-5	HIS	-	CLONING ARTIFACT	UNP P48163
A	-4	HIS	-	CLONING ARTIFACT	UNP P48163
A	-3	SER	-	CLONING ARTIFACT	UNP P48163
A	-2	SER	-	CLONING ARTIFACT	UNP P48163
A	-1	GLY	-	CLONING ARTIFACT	UNP P48163
A	0	VAL	-	CLONING ARTIFACT	UNP P48163
A	1	ASP	-	CLONING ARTIFACT	UNP P48163
A	2	LEU	-	CLONING ARTIFACT	UNP P48163
A	3	GLY	-	CLONING ARTIFACT	UNP P48163
A	4	THR	-	CLONING ARTIFACT	UNP P48163
A	5	GLU	-	CLONING ARTIFACT	UNP P48163
A	6	ASN	-	CLONING ARTIFACT	UNP P48163
A	7	LEU	-	CLONING ARTIFACT	UNP P48163
A	8	TYR	-	CLONING ARTIFACT	UNP P48163
A	9	PHE	-	CLONING ARTIFACT	UNP P48163
A	10	GLN	-	CLONING ARTIFACT	UNP P48163
A	11	SER	-	CLONING ARTIFACT	UNP P48163
A	12	MET	-	CLONING ARTIFACT	UNP P48163

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	CLONING ARTIFACT	UNP P48163
B	-9	HIS	-	CLONING ARTIFACT	UNP P48163
B	-8	HIS	-	CLONING ARTIFACT	UNP P48163
B	-7	HIS	-	CLONING ARTIFACT	UNP P48163
B	-6	HIS	-	CLONING ARTIFACT	UNP P48163
B	-5	HIS	-	CLONING ARTIFACT	UNP P48163
B	-4	HIS	-	CLONING ARTIFACT	UNP P48163
B	-3	SER	-	CLONING ARTIFACT	UNP P48163
B	-2	SER	-	CLONING ARTIFACT	UNP P48163
B	-1	GLY	-	CLONING ARTIFACT	UNP P48163
B	0	VAL	-	CLONING ARTIFACT	UNP P48163
B	1	ASP	-	CLONING ARTIFACT	UNP P48163
B	2	LEU	-	CLONING ARTIFACT	UNP P48163
B	3	GLY	-	CLONING ARTIFACT	UNP P48163
B	4	THR	-	CLONING ARTIFACT	UNP P48163
B	5	GLU	-	CLONING ARTIFACT	UNP P48163
B	6	ASN	-	CLONING ARTIFACT	UNP P48163
B	7	LEU	-	CLONING ARTIFACT	UNP P48163
B	8	TYR	-	CLONING ARTIFACT	UNP P48163
B	9	PHE	-	CLONING ARTIFACT	UNP P48163
B	10	GLN	-	CLONING ARTIFACT	UNP P48163
B	11	SER	-	CLONING ARTIFACT	UNP P48163
B	12	MET	-	CLONING ARTIFACT	UNP P48163
C	-10	MET	-	CLONING ARTIFACT	UNP P48163
C	-9	HIS	-	CLONING ARTIFACT	UNP P48163
C	-8	HIS	-	CLONING ARTIFACT	UNP P48163
C	-7	HIS	-	CLONING ARTIFACT	UNP P48163
C	-6	HIS	-	CLONING ARTIFACT	UNP P48163
C	-5	HIS	-	CLONING ARTIFACT	UNP P48163
C	-4	HIS	-	CLONING ARTIFACT	UNP P48163
C	-3	SER	-	CLONING ARTIFACT	UNP P48163
C	-2	SER	-	CLONING ARTIFACT	UNP P48163
C	-1	GLY	-	CLONING ARTIFACT	UNP P48163
C	0	VAL	-	CLONING ARTIFACT	UNP P48163
C	1	ASP	-	CLONING ARTIFACT	UNP P48163
C	2	LEU	-	CLONING ARTIFACT	UNP P48163
C	3	GLY	-	CLONING ARTIFACT	UNP P48163
C	4	THR	-	CLONING ARTIFACT	UNP P48163
C	5	GLU	-	CLONING ARTIFACT	UNP P48163
C	6	ASN	-	CLONING ARTIFACT	UNP P48163
C	7	LEU	-	CLONING ARTIFACT	UNP P48163
C	8	TYR	-	CLONING ARTIFACT	UNP P48163

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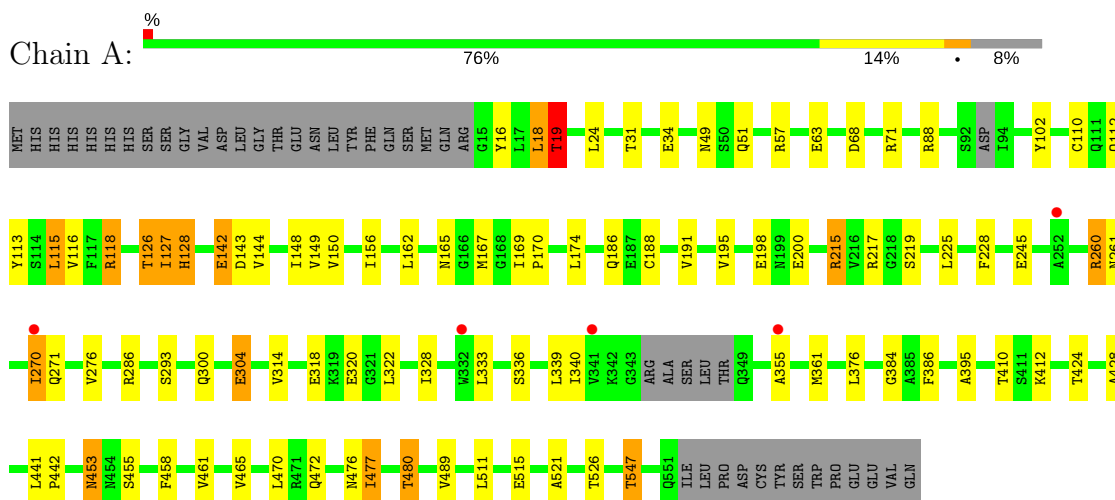
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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	PHE	-	CLONING ARTIFACT	UNP P48163
C	10	GLN	-	CLONING ARTIFACT	UNP P48163
C	11	SER	-	CLONING ARTIFACT	UNP P48163
C	12	MET	-	CLONING ARTIFACT	UNP P48163

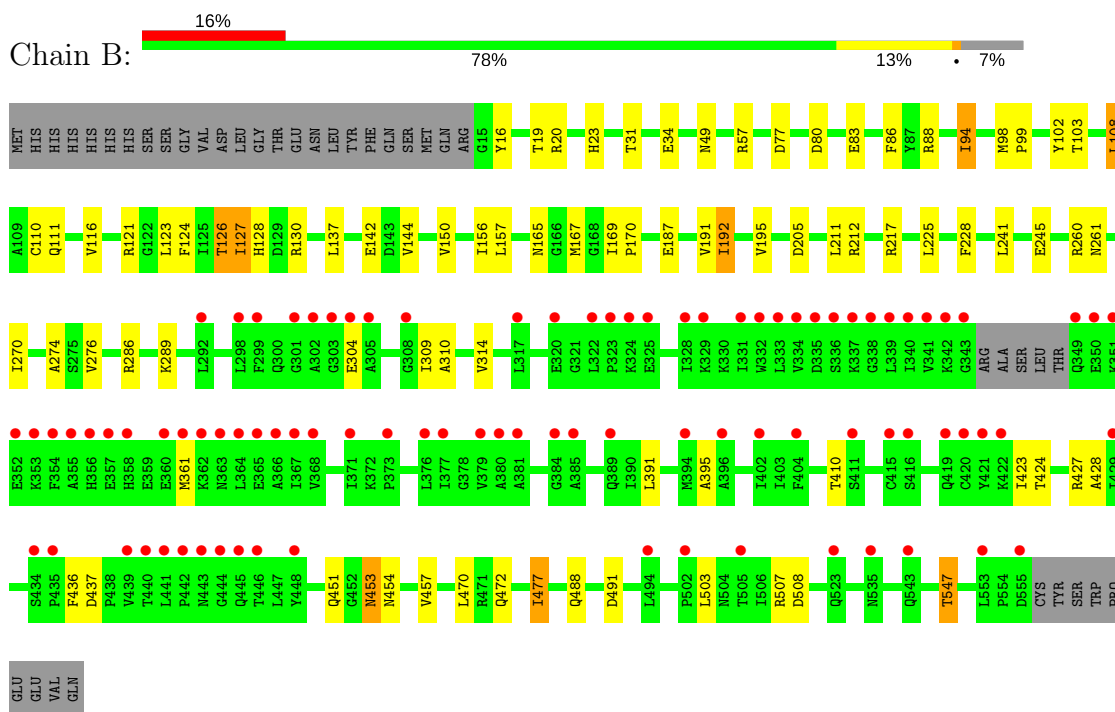
### 3 Residue-property plots

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

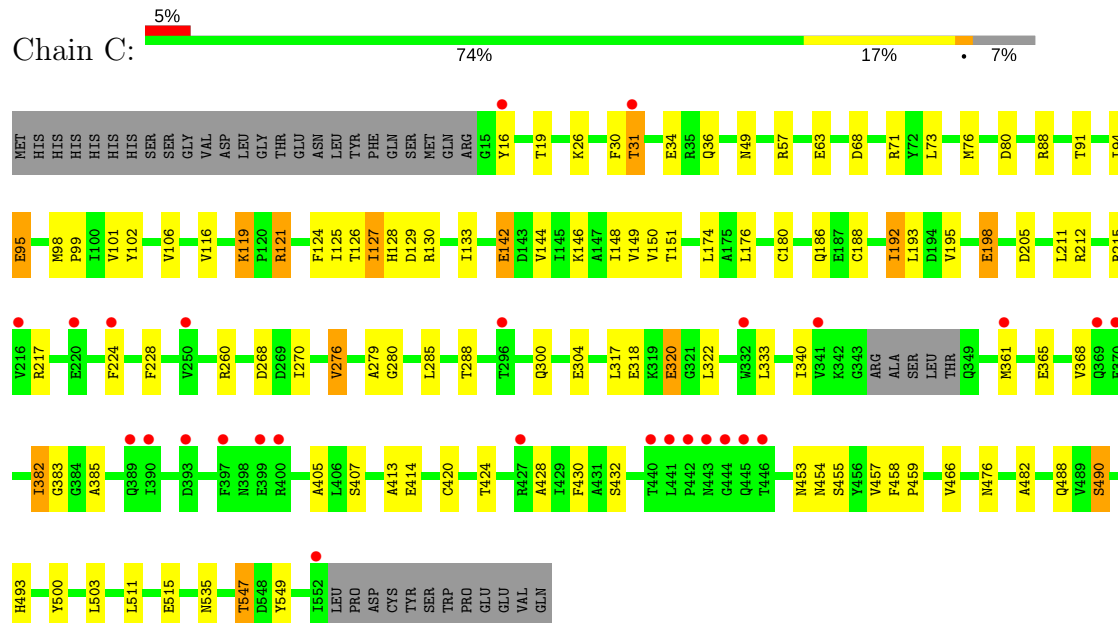
#### • Molecule 1: NADP-dependent malic enzyme



#### • Molecule 1: NADP-dependent malic enzyme



● Molecule 1: NADP-dependent malic enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.50Å 136.96Å 117.84Å 90.00° 121.75° 90.00°	Depositor
Resolution (Å)	37.30 – 2.50 47.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.30-2.50) 97.7 (47.40-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.256 0.245 , 0.294	Depositor DCC
$R_{free}$ test set	3517 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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](#)

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	0.60	0/4080	0.74	2/5546 (0.0%)
1	B	0.56	0/3993	0.70	0/5440
1	C	0.57	0/4074	0.71	1/5541 (0.0%)
All	All	0.58	0/12147	0.72	3/16527 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	215	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	276	VAL	CB-CA-C	-5.11	101.70	111.40

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	4004	0	3879	57	0
1	B	3919	0	3687	53	0
1	C	3997	0	3832	62	0
All	All	11920	0	11398	169	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 7.

All (169) 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:C:124:PHE:CD2	1:C:192:ILE:HD11	1.90	1.06
1:B:150:VAL:HG21	1:B:228:PHE:CZ	2.13	0.83
1:B:124:PHE:CD2	1:B:192:ILE:HD11	2.20	0.77
1:B:16:TYR:O	1:B:19:THR:HB	1.87	0.74
1:A:150:VAL:HG22	1:A:191:VAL:HB	1.69	0.73
1:B:150:VAL:HG22	1:B:191:VAL:HB	1.73	0.70
1:B:31:THR:HG23	1:B:34:GLU:H	1.59	0.67
1:B:286:ARG:O	1:B:289:LYS:NZ	2.28	0.66
1:B:274:ALA:HA	1:B:309:ILE:HG22	1.76	0.66
1:A:150:VAL:HG21	1:A:228:PHE:CZ	2.33	0.64
1:C:124:PHE:CD2	1:C:192:ILE:CD1	2.74	0.63
1:C:126:THR:HG22	1:C:128:HIS:N	2.14	0.63
1:A:88:ARG:HD3	1:A:547:THR:HG21	1.80	0.62
1:C:126:THR:HG22	1:C:128:HIS:H	1.64	0.62
1:B:453:ASN:HD22	1:B:454:ASN:N	1.98	0.62
1:C:285:LEU:HA	1:C:288:THR:HG22	1.81	0.61
1:A:340:ILE:HD12	1:A:355:ALA:HA	1.84	0.59
1:A:156:ILE:HD12	1:A:169:ILE:HG13	1.85	0.59
1:B:150:VAL:HG21	1:B:228:PHE:HZ	1.64	0.58
1:B:205:ASP:O	1:B:212:ARG:NH2	2.36	0.58
1:A:102:TYR:OH	1:A:245:GLU:OE1	2.22	0.58
1:C:333:LEU:HB2	1:C:340:ILE:HG12	1.84	0.58
1:B:124:PHE:CD2	1:B:192:ILE:CD1	2.87	0.57
1:C:49:ASN:ND2	1:C:57:ARG:HH12	2.03	0.57
1:C:285:LEU:HA	1:C:288:THR:CG2	2.35	0.57
1:C:150:VAL:HG21	1:C:228:PHE:CZ	2.40	0.56
1:B:102:TYR:CD2	1:B:103:THR:HG22	2.40	0.56
1:A:118:ARG:HH11	1:A:118:ARG:CG	2.18	0.56
1:A:286:ARG:NH2	1:A:489:VAL:O	2.36	0.56
1:C:124:PHE:CE2	1:C:192:ILE:HD11	2.41	0.56
1:C:150:VAL:HG12	1:C:151:THR:N	2.21	0.55
1:B:144:VAL:HG23	1:B:187:GLU:HG2	1.88	0.55
1:C:26:LYS:HE2	1:C:549:TYR:HB3	1.89	0.55
1:C:276:VAL:HG13	1:C:457:VAL:HG23	1.89	0.55
1:A:148:ILE:HG22	1:A:150:VAL:HG23	1.89	0.55
1:C:16:TYR:O	1:C:19:THR:HB	2.06	0.55
1:A:88:ARG:HD3	1:A:547:THR:CG2	2.37	0.54
1:A:476:ASN:O	1:A:480:THR:HG23	2.07	0.54
1:C:126:THR:HG23	1:C:211:LEU:HD11	1.90	0.54
1:A:453:ASN:HD22	1:A:455:SER:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ILE:HG22	1:C:304:GLU:C	2.27	0.54
1:C:174:LEU:HD22	1:C:188:CYS:HB3	1.89	0.53
1:C:31:THR:HG22	1:C:34:GLU:H	1.73	0.53
1:A:461:VAL:HG13	1:A:477:ILE:HD11	1.89	0.53
1:B:391:LEU:HB2	1:B:423:ILE:HG21	1.90	0.53
1:B:477:ILE:C	1:B:477:ILE:HD12	2.28	0.53
1:C:205:ASP:O	1:C:212:ARG:NH2	2.41	0.53
1:C:511:LEU:O	1:C:515:GLU:HG3	2.08	0.53
1:A:126:THR:HG22	1:A:128:HIS:N	2.24	0.53
1:A:148:ILE:CG2	1:A:150:VAL:HG23	2.40	0.52
1:B:127:ILE:HG13	1:B:195:VAL:HA	1.90	0.52
1:C:133:ILE:HD11	1:C:224:PHE:CE1	2.44	0.52
1:A:142:GLU:HG2	1:A:186:GLN:O	2.08	0.52
1:B:124:PHE:HA	1:B:192:ILE:HD12	1.90	0.52
1:A:465:VAL:HG13	1:A:470:LEU:HB2	1.91	0.52
1:A:167:MET:O	1:A:170:PRO:HD2	2.09	0.52
1:A:49:ASN:ND2	1:A:57:ARG:HH12	2.08	0.52
1:B:169:ILE:HB	1:B:170:PRO:HD3	1.92	0.51
1:C:68:ASP:HA	1:C:71:ARG:HD2	1.93	0.51
1:C:198:GLU:OE1	1:C:215:ARG:HG3	2.11	0.51
1:B:276:VAL:HG13	1:B:457:VAL:HG23	1.91	0.51
1:A:31:THR:HG22	1:A:34:GLU:CG	2.40	0.51
1:A:461:VAL:O	1:A:465:VAL:HG23	2.11	0.51
1:B:80:ASP:HB2	1:B:121:ARG:HH21	1.77	0.50
1:B:126:THR:HG22	1:B:128:HIS:N	2.26	0.50
1:B:261:ASN:O	1:B:472:GLN:NE2	2.43	0.50
1:C:150:VAL:CG1	1:C:151:THR:N	2.75	0.50
1:C:317:LEU:O	1:C:320:GLU:HG3	2.11	0.50
1:A:143:ASP:N	1:A:143:ASP:OD1	2.40	0.49
1:B:102:TYR:OH	1:B:245:GLU:OE1	2.30	0.49
1:B:98:MET:CE	1:B:503:LEU:HD21	2.42	0.49
1:C:127:ILE:HG13	1:C:195:VAL:HA	1.94	0.49
1:A:149:VAL:HG23	1:A:174:LEU:HD21	1.93	0.49
1:B:110:CYS:O	1:B:165:ASN:HB3	2.13	0.49
1:A:127:ILE:HG13	1:A:195:VAL:HA	1.95	0.49
1:A:395:ALA:HB2	1:A:424:THR:HG22	1.95	0.49
1:B:83:GLU:O	1:B:86:PHE:HB3	2.13	0.49
1:B:451:GLN:NE2	1:B:453:ASN:OD1	2.46	0.48
1:C:318:GLU:HA	1:C:322:LEU:O	2.14	0.48
1:C:49:ASN:HD22	1:C:57:ARG:HH12	1.61	0.48
1:C:73:LEU:HD21	1:C:116:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:CG2	1:A:304:GLU:HB3	2.43	0.48
1:B:126:THR:HG23	1:B:211:LEU:HD11	1.95	0.48
1:C:407:SER:OG	1:C:414:GLU:OE2	2.31	0.48
1:B:98:MET:HE3	1:B:503:LEU:HD21	1.96	0.48
1:C:176:LEU:O	1:C:180:CYS:HB2	2.14	0.48
1:A:112:GLN:HE21	1:A:115:LEU:HD12	1.78	0.48
1:C:146:LYS:HD3	1:C:466:VAL:CG1	2.43	0.48
1:C:98:MET:O	1:C:102:TYR:HB3	2.13	0.48
1:C:80:ASP:OD1	1:C:119:LYS:HD2	2.13	0.48
1:C:126:THR:HB	1:C:129:ASP:OD2	2.13	0.48
1:B:309:ILE:HG13	1:B:310:ALA:N	2.29	0.48
1:C:280:GLY:HA3	1:C:500:TYR:OH	2.13	0.48
1:A:270:ILE:HG22	1:A:304:GLU:C	2.35	0.48
1:A:18:LEU:HD21	1:A:24:LEU:HB3	1.96	0.47
1:B:49:ASN:ND2	1:B:57:ARG:HH12	2.12	0.47
1:B:23:HIS:HD1	1:B:83:GLU:CD	2.17	0.47
1:C:125:ILE:O	1:C:193:LEU:HA	2.15	0.47
1:C:405:ALA:O	1:C:432:SER:HA	2.15	0.47
1:A:16:TYR:O	1:A:19:THR:HB	2.15	0.46
1:A:412:LYS:HE2	1:B:491:ASP:OD1	2.16	0.46
1:A:162:LEU:O	1:A:165:ASN:HB2	2.16	0.46
1:C:95:GLU:HG3	1:C:503:LEU:HB2	1.97	0.46
1:C:149:VAL:HG23	1:C:174:LEU:HD21	1.97	0.45
1:B:20:ARG:NH2	1:C:80:ASP:OD2	2.48	0.45
1:A:150:VAL:HG21	1:A:228:PHE:HZ	1.80	0.45
1:A:260:ARG:NH1	1:A:271:GLN:HE22	2.15	0.45
1:C:26:LYS:HD2	1:C:30:PHE:CD2	2.52	0.45
1:C:144:VAL:HG23	1:C:144:VAL:O	2.17	0.44
1:B:410:THR:HG23	1:B:436:PHE:CZ	2.52	0.44
1:A:376:LEU:HG	1:A:386:PHE:CZ	2.52	0.44
1:B:123:LEU:HD11	1:B:137:LEU:HA	1.99	0.44
1:C:424:THR:HG21	1:C:428:ALA:HB2	2.00	0.44
1:C:382:ILE:HG12	1:C:385:ALA:HB2	1.99	0.44
1:B:156:ILE:O	1:B:157:LEU:C	2.55	0.44
1:B:395:ALA:HB1	1:B:427:ARG:HH22	1.83	0.44
1:C:490:SER:HB3	1:C:493:HIS:CE1	2.53	0.44
1:B:124:PHE:HA	1:B:192:ILE:CD1	2.48	0.44
1:C:276:VAL:HG11	1:C:453:ASN:O	2.18	0.43
1:A:314:VAL:HG21	1:A:328:ILE:HD13	2.00	0.43
1:C:458:PHE:N	1:C:459:PRO:CD	2.81	0.43
1:A:68:ASP:HA	1:A:71:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:HB2	1:C:482:ALA:HA	2.01	0.43
1:A:441:LEU:HB3	1:A:442:PRO:HD2	2.01	0.43
1:B:167:MET:O	1:B:170:PRO:HD2	2.19	0.43
1:A:521:ALA:HA	1:A:526:THR:OG1	2.19	0.43
1:A:110:CYS:O	1:A:165:ASN:HB3	2.18	0.43
1:C:383:GLY:HA2	1:C:413:ALA:O	2.19	0.43
1:A:424:THR:HG21	1:A:428:ALA:HB2	1.99	0.43
1:C:420:CYS:HG	1:C:430:PHE:HD1	1.57	0.43
1:A:49:ASN:HD22	1:A:57:ARG:HH12	1.66	0.43
1:A:293:SER:OG	1:A:320:GLU:OE1	2.31	0.42
1:B:98:MET:N	1:B:99:PRO:CD	2.82	0.42
1:C:268:ASP:CG	1:C:454:ASN:HD22	2.22	0.42
1:A:169:ILE:HB	1:A:170:PRO:HD3	2.01	0.42
1:A:511:LEU:O	1:A:515:GLU:HG3	2.19	0.42
1:A:261:ASN:HA	1:A:472:GLN:HG2	2.01	0.42
1:B:424:THR:HG21	1:B:428:ALA:HB2	2.01	0.42
1:A:384:GLY:HA3	1:B:289:LYS:HB3	2.02	0.42
1:B:477:ILE:O	1:B:477:ILE:HD12	2.20	0.42
1:C:142:GLU:OE2	1:C:186:GLN:NE2	2.53	0.42
1:C:127:ILE:HD11	1:C:211:LEU:HD13	2.01	0.42
1:A:118:ARG:CG	1:A:118:ARG:NH1	2.80	0.42
1:B:310:ALA:O	1:B:314:VAL:HG23	2.20	0.42
1:B:453:ASN:C	1:B:453:ASN:HD22	2.23	0.42
1:A:198:GLU:HG2	1:A:215:ARG:HG3	2.01	0.42
1:A:333:LEU:O	1:A:339:LEU:HD12	2.20	0.41
1:A:455:SER:HA	1:A:458:PHE:CE2	2.55	0.41
1:C:102:TYR:CG	1:C:176:LEU:HD11	2.56	0.41
1:C:365:GLU:O	1:C:368:VAL:HG22	2.21	0.41
1:B:127:ILE:CG1	1:B:195:VAL:HA	2.50	0.41
1:C:535:ASN:OD1	1:C:535:ASN:C	2.58	0.41
1:A:174:LEU:HD13	1:A:188:CYS:HB3	2.02	0.41
1:A:18:LEU:HD21	1:A:24:LEU:CB	2.51	0.41
1:A:51:GLN:HE22	1:A:547:THR:HG23	1.84	0.41
1:B:88:ARG:HD3	1:B:547:THR:HG23	2.03	0.41
1:C:476:ASN:N	1:C:476:ASN:HD22	2.19	0.41
1:B:241:LEU:C	1:B:241:LEU:HD23	2.42	0.41
1:C:148:ILE:HG22	1:C:150:VAL:HG23	2.02	0.41
1:C:98:MET:N	1:C:99:PRO:CD	2.84	0.41
1:A:318:GLU:HA	1:A:322:LEU:O	2.22	0.40
1:B:286:ARG:O	1:B:289:LYS:CE	2.69	0.40
1:C:88:ARG:HD3	1:C:547:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG22	1:A:34:GLU:HG3	2.02	0.40
1:A:31:THR:CG2	1:A:34:GLU:H	2.34	0.40
1:B:108:LEU:HA	1:B:111:GLN:HE21	1.86	0.40
1:B:144:VAL:O	1:B:144:VAL:HG23	2.22	0.40
1:B:94:ILE:HD13	1:B:98:MET:HB2	2.04	0.40
1:C:76:MET:O	1:C:121:ARG:NH2	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	525/575 (91%)	508 (97%)	14 (3%)	3 (1%)	28	48
1	B	532/575 (92%)	517 (97%)	14 (3%)	1 (0%)	51	73
1	C	529/575 (92%)	502 (95%)	27 (5%)	0	100	100
All	All	1586/1725 (92%)	1527 (96%)	55 (4%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLU
1	A	128	HIS
1	B	304	GLU
1	A	19	THR

### 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	401/492 (82%)	376 (94%)	25 (6%)	21	39
1	B	372/492 (76%)	350 (94%)	22 (6%)	23	42
1	C	397/492 (81%)	372 (94%)	25 (6%)	21	38
All	All	1170/1476 (79%)	1098 (94%)	72 (6%)	21	39

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	THR
1	A	63	GLU
1	A	113	TYR
1	A	115	LEU
1	A	116	VAL
1	A	126	THR
1	A	127	ILE
1	A	142	GLU
1	A	144	VAL
1	A	200	GLU
1	A	217	ARG
1	A	219	SER
1	A	225	LEU
1	A	260	ARG
1	A	270	ILE
1	A	276	VAL
1	A	300	GLN
1	A	336	SER
1	A	361	MET
1	A	410	THR
1	A	453	ASN
1	A	477	ILE
1	A	480	THR
1	A	547	THR
1	B	77	ASP
1	B	94	ILE
1	B	108	LEU
1	B	116	VAL
1	B	126	THR
1	B	127	ILE

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Mol	Chain	Res	Type
1	B	130	ARG
1	B	142	GLU
1	B	192	ILE
1	B	217	ARG
1	B	225	LEU
1	B	260	ARG
1	B	270	ILE
1	B	361	MET
1	B	437	ASP
1	B	453	ASN
1	B	470	LEU
1	B	477	ILE
1	B	488	GLN
1	B	507	ARG
1	B	508	ASP
1	B	547	THR
1	C	31	THR
1	C	36	GLN
1	C	63	GLU
1	C	91	THR
1	C	94	ILE
1	C	95	GLU
1	C	101	VAL
1	C	106	VAL
1	C	119	LYS
1	C	121	ARG
1	C	127	ILE
1	C	130	ARG
1	C	142	GLU
1	C	192	ILE
1	C	198	GLU
1	C	217	ARG
1	C	260	ARG
1	C	300	GLN
1	C	320	GLU
1	C	361	MET
1	C	382	ILE
1	C	455	SER
1	C	488	GLN
1	C	490	SER
1	C	547	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	51	GLN
1	A	111	GLN
1	A	112	GLN
1	A	186	GLN
1	A	443	ASN
1	A	453	ASN
1	A	488	GLN
1	B	49	ASN
1	B	61	ASN
1	B	111	GLN
1	B	451	GLN
1	B	453	ASN
1	C	36	GLN
1	C	49	ASN
1	C	186	GLN
1	C	369	GLN
1	C	476	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 carbohydrates 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

### 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	531/575 (92%)	0.15	5 (0%) 84 85	25, 60, 79, 87	0
1	B	536/575 (93%)	0.82	90 (16%) 2 1	25, 63, 84, 95	0
1	C	533/575 (92%)	0.48	27 (5%) 29 30	25, 63, 79, 93	0
All	All	1600/1725 (92%)	0.48	122 (7%) 15 14	25, 62, 81, 95	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	9.4
1	B	358	HIS	7.9
1	B	355	ALA	7.3
1	B	380	ALA	7.3
1	B	298	LEU	6.9
1	C	442	PRO	6.7
1	C	552	ILE	6.5
1	B	341	VAL	6.4
1	B	360	GLU	6.4
1	B	420	CYS	5.9
1	B	333	LEU	5.4
1	B	396	ALA	5.4
1	B	367	ILE	5.3
1	C	441	LEU	5.3
1	B	343	GLY	5.0
1	B	299	PHE	5.0
1	B	332	TRP	5.0
1	B	357	GLU	4.9
1	B	441	LEU	4.9
1	B	350	GLU	4.8
1	C	444	GLY	4.7
1	B	446	THR	4.7
1	C	443	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	335	ASP	4.5
1	C	332	TRP	4.4
1	B	337	LYS	4.4
1	B	339	LEU	4.4
1	B	442	PRO	4.4
1	B	381	ALA	4.3
1	B	336	SER	4.3
1	B	349	GLN	4.3
1	C	445	GLN	4.2
1	B	553	LEU	4.2
1	B	308	GLY	4.2
1	B	331	ILE	4.1
1	C	397	PHE	4.1
1	B	338	GLY	4.0
1	B	340	ILE	4.0
1	B	416	SER	3.9
1	B	371	ILE	3.9
1	B	440	THR	3.9
1	B	445	GLN	3.8
1	B	303	GLY	3.8
1	B	305	ALA	3.7
1	B	394	MET	3.7
1	A	341	VAL	3.7
1	B	328	ILE	3.6
1	B	444	GLY	3.6
1	B	411	SER	3.6
1	B	535	ASN	3.6
1	B	363	ASN	3.6
1	B	356	HIS	3.5
1	B	415	CYS	3.5
1	B	351	LYS	3.5
1	B	435	PRO	3.5
1	B	365	GLU	3.5
1	C	370	GLU	3.5
1	B	334	VAL	3.4
1	B	368	VAL	3.4
1	B	384	GLY	3.3
1	B	421	TYR	3.3
1	B	379	VAL	3.2
1	B	302	ALA	3.2
1	C	361	MET	3.2
1	C	369	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	342	LYS	3.1
1	B	292	LEU	3.1
1	C	399	GLU	3.0
1	C	393	ASP	3.0
1	B	352	GLU	3.0
1	B	377	ILE	3.0
1	B	402	ILE	2.9
1	B	422	LYS	2.9
1	B	505	THR	2.9
1	B	361	MET	2.9
1	B	448	TYR	2.8
1	B	362	LYS	2.8
1	B	555	ASP	2.8
1	A	355	ALA	2.8
1	B	322	LEU	2.8
1	B	419	GLN	2.8
1	B	376	LEU	2.8
1	B	353	LYS	2.7
1	B	325	GLU	2.7
1	B	502	PRO	2.7
1	B	373	PRO	2.7
1	C	400	ARG	2.7
1	B	404	PHE	2.6
1	B	494	LEU	2.6
1	B	385	ALA	2.6
1	B	329	LYS	2.5
1	B	389	GLN	2.5
1	C	31	THR	2.5
1	C	390	ILE	2.5
1	B	320	GLU	2.5
1	B	317	LEU	2.4
1	B	324	LYS	2.4
1	C	446	THR	2.4
1	C	250	VAL	2.4
1	B	439	VAL	2.3
1	C	216	VAL	2.3
1	B	543	GLN	2.3
1	B	323	PRO	2.3
1	B	364	LEU	2.3
1	B	429	ILE	2.2
1	C	296	THR	2.2
1	B	434	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	224	PHE	2.2
1	C	427	ARG	2.2
1	C	341	VAL	2.2
1	A	270	ILE	2.2
1	C	440	THR	2.2
1	C	389	GLN	2.1
1	A	332	TRP	2.1
1	B	523	GLN	2.1
1	A	252	ALA	2.1
1	B	304	GLU	2.1
1	B	443	ASN	2.1
1	B	301	GLY	2.1
1	B	366	ALA	2.0
1	C	16	TYR	2.0
1	C	220	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.