



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:10 pm BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

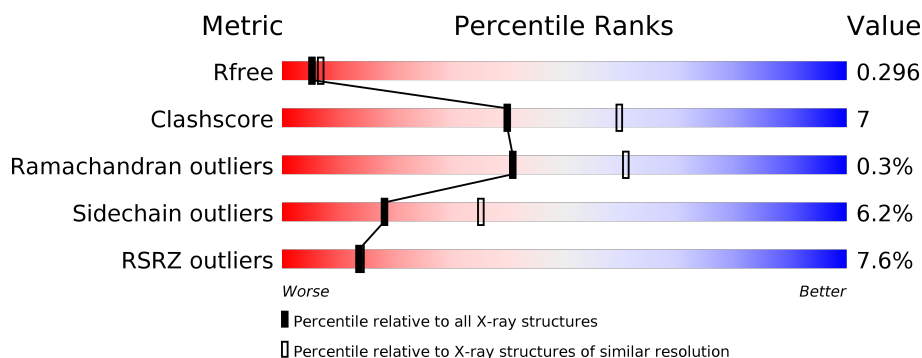
1 Overall quality at a glance

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}	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 on 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 $\leq 5\%$. 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>%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	B	575	<div> <div>16%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	C	575	<div> <div>5%</div> <div> <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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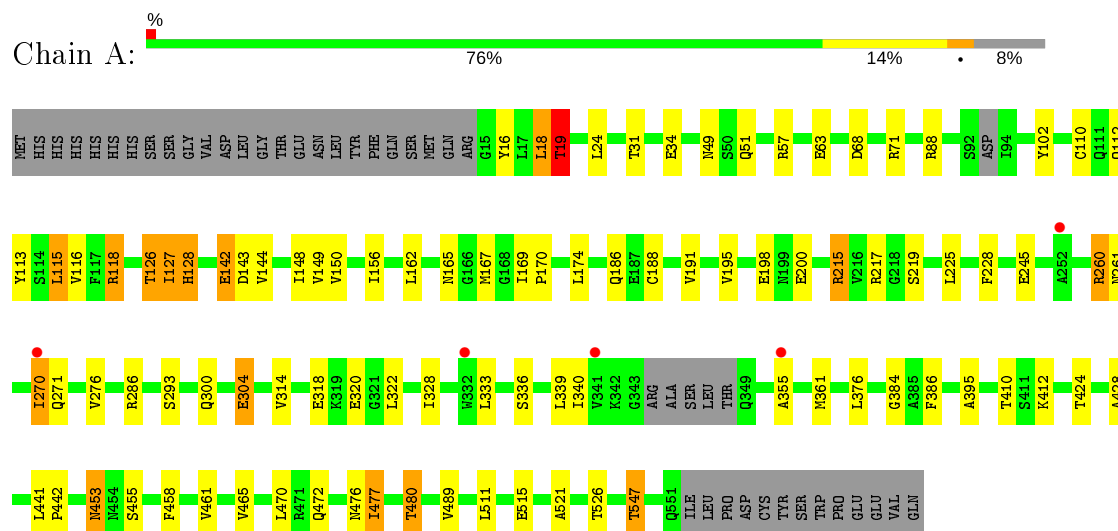
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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	PHE	-	CLONING ARTIFACT	UNP P48163
C	10	GLN	-	CLONING ARTIFACT	UNP P48163
C	11	SER	-	CLONING ARTIFACT	UNP P48163
C	12	MET	-	CLONING ARTIFACT	UNP P48163

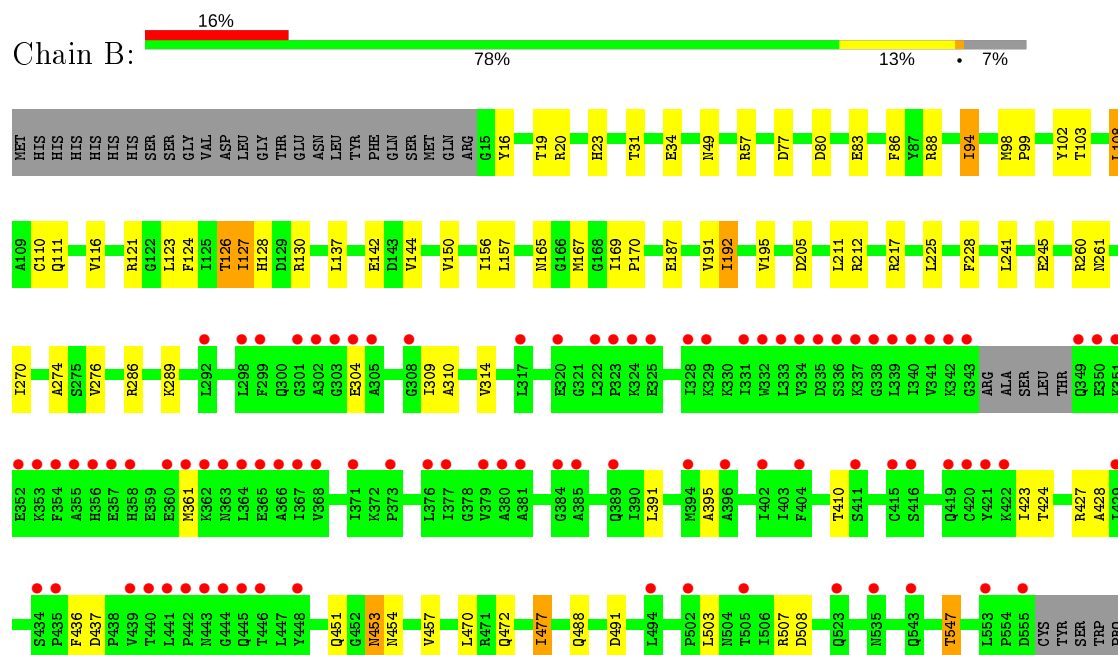
3 Residue-property plots

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

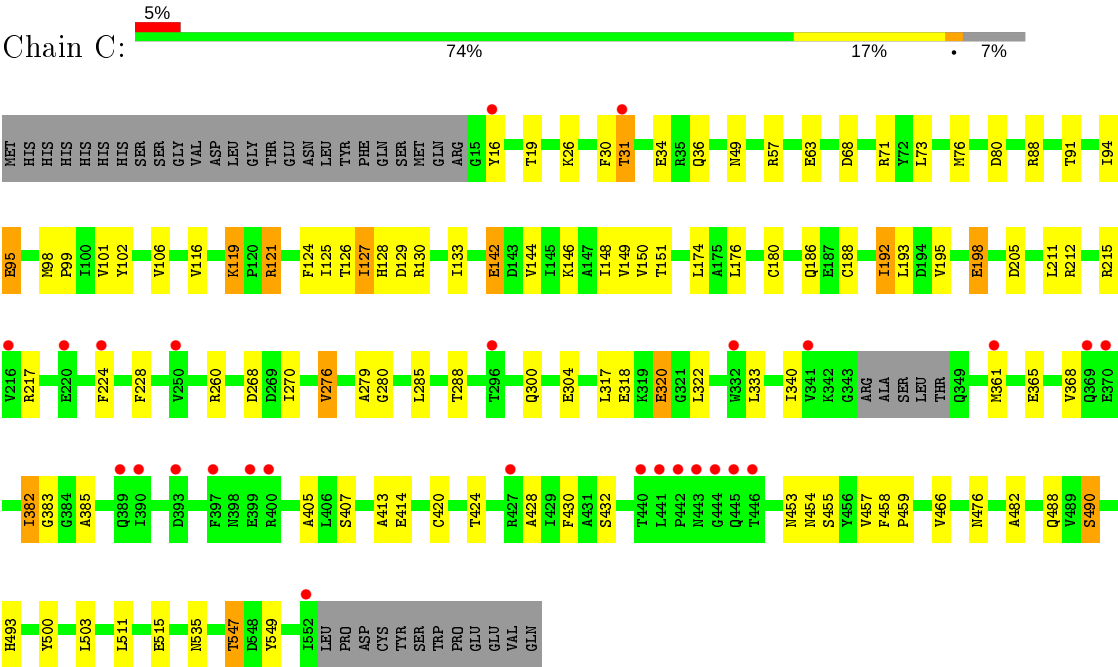


• Molecule 1: NADP-dependent malic enzyme



GLU
GLU
VAL
GLN

● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.256 0.250 , 0.296	Depositor DCC
R_{free} test set	3520 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	25	43
1	B	532/575 (92%)	517 (97%)	14 (3%)	1 (0%)	47	68
1	C	529/575 (92%)	502 (95%)	27 (5%)	0	100	100
All	All	1586/1725 (92%)	1527 (96%)	55 (4%)	4 (0%)	41	61

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%)	18	35
1	B	372/492 (76%)	350 (94%)	22 (6%)	19	37
1	C	397/492 (81%)	372 (94%)	25 (6%)	18	34
All	All	1170/1476 (79%)	1098 (94%)	72 (6%)	18	35

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	531/575 (92%)	0.15	5 (0%) 84 86	25, 60, 79, 87	0
1	B	536/575 (93%)	0.82	90 (16%) 1 1	25, 63, 84, 95	0
1	C	533/575 (92%)	0.48	27 (5%) 28 29	25, 63, 79, 93	0
All	All	1600/1725 (92%)	0.48	122 (7%) 13 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	7.8
1	B	355	ALA	7.4
1	B	380	ALA	7.3
1	B	298	LEU	6.9
1	C	442	PRO	6.7
1	B	341	VAL	6.4
1	C	552	ILE	6.4
1	B	360	GLU	6.4
1	B	420	CYS	5.8
1	B	333	LEU	5.4
1	B	367	ILE	5.3
1	B	396	ALA	5.3
1	C	441	LEU	5.3
1	B	343	GLY	5.1
1	B	299	PHE	5.0
1	B	357	GLU	4.9
1	B	332	TRP	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	337	LYS	4.5
1	C	332	TRP	4.4
1	B	335	ASP	4.4
1	B	442	PRO	4.4
1	B	336	SER	4.3
1	B	339	LEU	4.3
1	B	381	ALA	4.3
1	B	349	GLN	4.3
1	C	445	GLN	4.3
1	B	553	LEU	4.2
1	B	308	GLY	4.1
1	C	397	PHE	4.1
1	B	331	ILE	4.1
1	B	338	GLY	4.0
1	B	340	ILE	3.9
1	B	371	ILE	3.9
1	B	416	SER	3.9
1	B	440	THR	3.9
1	B	303	GLY	3.8
1	B	445	GLN	3.8
1	B	305	ALA	3.8
1	B	394	MET	3.7
1	B	328	ILE	3.7
1	B	411	SER	3.7
1	B	444	GLY	3.6
1	A	341	VAL	3.6
1	B	363	ASN	3.6
1	B	535	ASN	3.6
1	B	356	HIS	3.5
1	B	351	LYS	3.5
1	B	415	CYS	3.5
1	B	435	PRO	3.5
1	B	365	GLU	3.5
1	B	368	VAL	3.4
1	C	370	GLU	3.4
1	B	334	VAL	3.4
1	B	384	GLY	3.3
1	B	379	VAL	3.3
1	B	421	TYR	3.3
1	C	361	MET	3.2
1	B	302	ALA	3.2
1	B	342	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	369	GLN	3.1
1	C	393	ASP	3.0
1	C	399	GLU	3.0
1	B	377	ILE	3.0
1	B	292	LEU	3.0
1	B	352	GLU	3.0
1	B	402	ILE	2.9
1	B	361	MET	2.9
1	B	422	LYS	2.9
1	B	505	THR	2.9
1	B	362	LYS	2.8
1	B	448	TYR	2.8
1	B	555	ASP	2.8
1	B	376	LEU	2.8
1	B	325	GLU	2.8
1	A	355	ALA	2.8
1	B	322	LEU	2.8
1	B	353	LYS	2.7
1	B	419	GLN	2.7
1	B	373	PRO	2.7
1	B	502	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	2.5
1	C	31	THR	2.5
1	B	329	LYS	2.5
1	B	389	GLN	2.5
1	C	390	ILE	2.4
1	B	320	GLU	2.4
1	C	446	THR	2.4
1	B	317	LEU	2.4
1	B	324	LYS	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	2.2
1	B	429	ILE	2.2
1	B	364	LEU	2.2
1	C	224	PHE	2.2
1	C	296	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	434	SER	2.2
1	A	270	ILE	2.2
1	C	427	ARG	2.2
1	B	523	GLN	2.1
1	A	332	TRP	2.1
1	C	341	VAL	2.1
1	C	389	GLN	2.1
1	C	440	THR	2.1
1	B	443	ASN	2.1
1	B	301	GLY	2.1
1	B	366	ALA	2.1
1	B	304	GLU	2.1
1	A	252	ALA	2.1
1	C	220	GLU	2.0
1	C	16	TYR	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.