



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:46 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

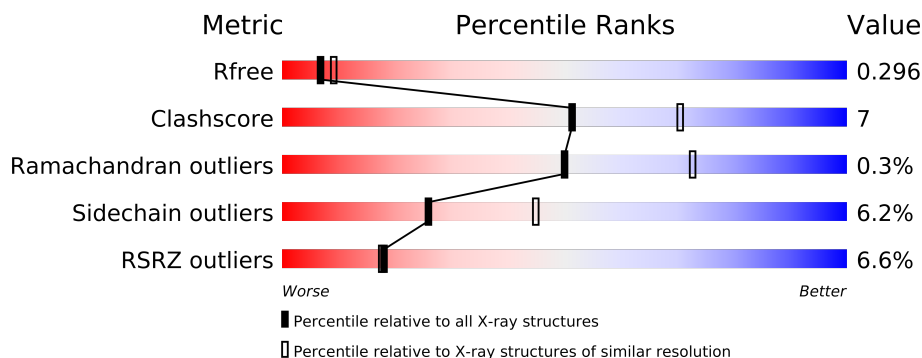
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	575	
1	B	575	
1	C	575	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11920 atoms, of which 0 are hydrogen and 0 are deuterium.

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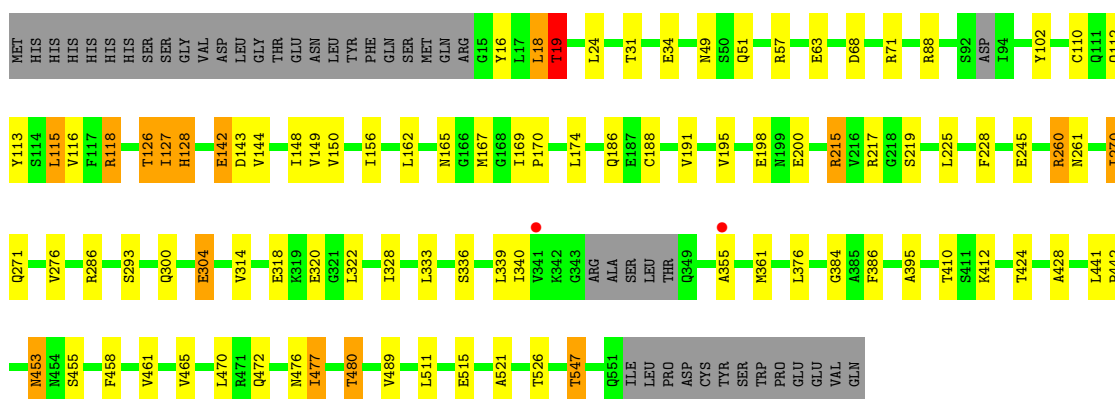
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	PHE	-	CLONING ARTIFACT	UNP P48163
C	10	GLN	-	CLONING ARTIFACT	UNP P48163
C	11	SER	-	CLONING ARTIFACT	UNP P48163
C	12	MET	-	CLONING ARTIFACT	UNP P48163

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 errors 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.

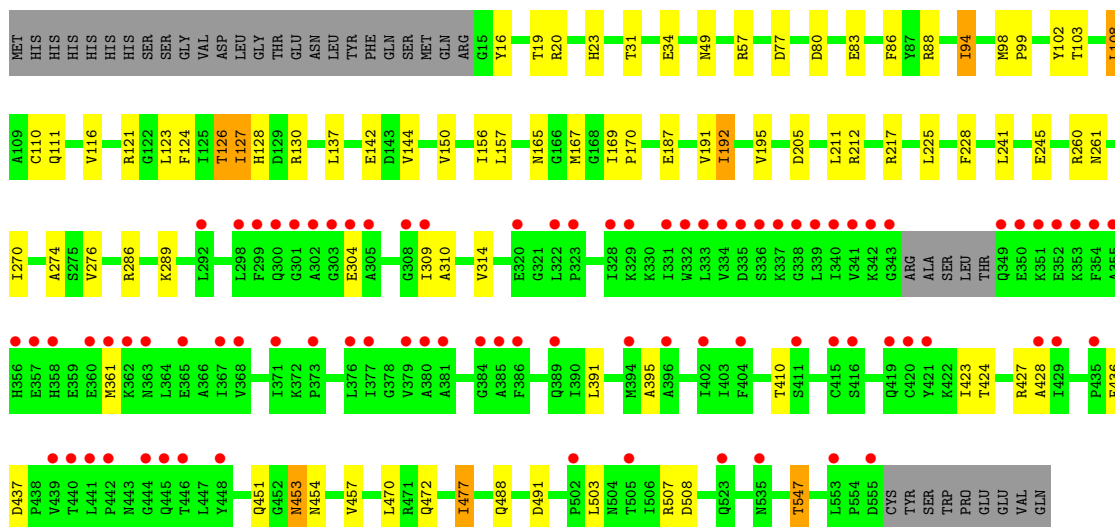
• Molecule 1: NADP-dependent malic enzyme

Chain A:



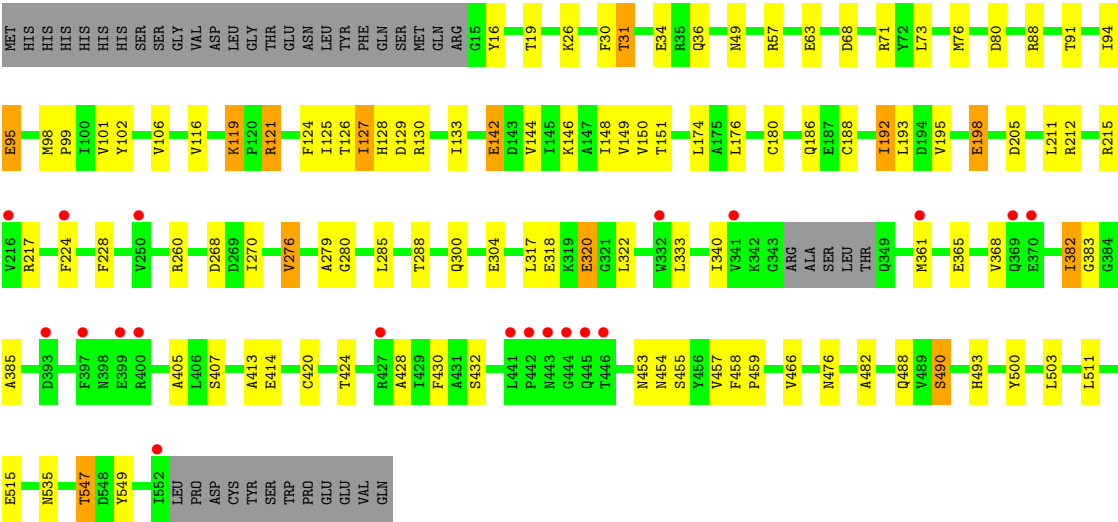
• Molecule 1: NADP-dependent malic enzyme

Chain B:



• Molecule 1: NADP-dependent malic enzyme

Chain C:



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	3517 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71047 reflections	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.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (169) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:C:124:PHE:CE2	1:C:192:ILE:HD11	2.41	0.56
1:A:286:ARG:NH2	1:A:489:VAL:O	2.36	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:ASN:HD22	1:A:455:SER:H	1.56	0.54
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:B:477:ILE:HD12	1:B:477:ILE:C	2.28	0.53
1:C:205:ASP:O	1:C:212:ARG:NH2	2.41	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: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:B:124:PHE:HA	1:B:192:ILE:HD12	1.90	0.52
1:A:142:GLU:HG2	1:A:186:GLN:O	2.08	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:C:68:ASP:HA	1:C:71:ARG:HD2	1.93	0.51
1:B:169:ILE:HB	1:B:170:PRO:HD3	1.92	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:C:150:VAL:CG1	1:C:151:THR:N	2.75	0.50
1:B:261:ASN:O	1:B:472:GLN:NE2	2.43	0.50
1:C:317:LEU:O	1:C:320:GLU:HG3	2.11	0.50
1:A:143:ASP:OD1	1:A:143:ASP:N	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:B:110:CYS:O	1:B:165:ASN:HB3	2.13	0.49
1:A:149:VAL:HG23	1:A:174:LEU:HD21	1.93	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: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
1:C:318:GLU:HA	1:C:322:LEU:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:126:THR:HG23	1:B:211:LEU:HD11	1.95	0.48
1:A:270:ILE:CG2	1:A:304:GLU:HB3	2.43	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:C:98:MET:O	1:C:102:TYR:HB3	2.13	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:126:THR:HB	1:C:129:ASP:OD2	2.13	0.48
1:C:80:ASP:OD1	1:C:119:LYS:HD2	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:B:23:HIS:HD1	1:B:83:GLU:CD	2.17	0.47
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: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:O	1:C:144:VAL:HG23	2.17	0.44
1:B:410:THR:HG23	1:B:436: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:A:376:LEU:HG	1:A:386:PHE:CZ	2.52	0.44
1:C:382:ILE:HG12	1:C:385:ALA:HB2	1.99	0.44
1:B:395:ALA:HB1	1:B:427:ARG:HH22	1.83	0.44
1:B:156:ILE:O	1:B:157:LEU:C	2.55	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
1:C:279:ALA:HB2	1:C:482:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:MET:O	1:B:170:PRO:HD2	2.19	0.43
1:A:441:LEU:HB3	1:A:442:PRO:HD2	2.01	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:B:424:THR:HG21	1:B:428:ALA:HB2	2.01	0.42
1:A:261:ASN:HA	1:A:472:GLN:HG2	2.01	0.42
1:A:384:GLY:HA3	1:B:289:LYS:HB3	2.02	0.42
1:B:477:ILE:HD12	1:B:477:ILE:O	2.20	0.42
1:C:127:ILE:HD11	1:C:211:LEU:HD13	2.01	0.42
1:C:142:GLU:OE2	1:C:186:GLN:NE2	2.53	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:118:ARG:CG	1:A:118:ARG:NH1	2.80	0.42
1:A:198:GLU:HG2	1:A:215:ARG:HG3	2.01	0.42
1:A:455:SER:HA	1:A:458:PHE:CE2	2.55	0.41
1:A:333:LEU:O	1:A:339:LEU:HD12	2.20	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:51:GLN:HE22	1:A:547:THR:HG23	1.84	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: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: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:B:241:LEU:C	1:B:241:LEU:HD23	2.42	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
1:B:144:VAL:O	1:B:144:VAL:HG23	2.22	0.40
1:A:31:THR:HG22	1:A:34:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:THR:CG2	1:A:34:GLU:H	2.34	0.40
1:B:94:ILE:HD13	1:B:98:MET:HB2	2.04	0.40
1:B:108:LEU:HA	1:B:111:GLN:HE21	1.86	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

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	525/575 (91%)	508 (97%)	14 (3%)	3 (1%)	33	55
1	B	532/575 (92%)	517 (97%)	14 (3%)	1 (0%)	56	79
1	C	529/575 (92%)	502 (95%)	27 (5%)	0	100	100
All	All	1586/1725 (92%)	1527 (96%)	55 (4%)	4 (0%)	50	73

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 ⓘ

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%)	26	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	372/492 (76%)	350 (94%)	22 (6%)	28	48
1	C	397/492 (81%)	372 (94%)	25 (6%)	25	44
All	All	1170/1476 (79%)	1098 (94%)	72 (6%)	26	45

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
1	B	130	ARG
1	B	142	GLU
1	B	192	ILE

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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%)	0.08	2 (0%) 90 92	25, 60, 79, 87	0
1	B	536/575 (93%)	0.73	84 (15%) 3 2	25, 63, 84, 95	0
1	C	533/575 (92%)	0.43	20 (3%) 38 40	25, 63, 79, 93	0
All	All	1600/1725 (92%)	0.42	106 (6%) 18 17	25, 62, 81, 95	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	9.0
1	B	358	HIS	7.7
1	C	552	ILE	6.8
1	B	380	ALA	6.5
1	C	442	PRO	6.5
1	B	355	ALA	6.3
1	B	298	LEU	5.9
1	B	367	ILE	5.4
1	B	341	VAL	5.4
1	B	305	ALA	5.4
1	B	441	LEU	5.3
1	B	360	GLU	5.0
1	B	333	LEU	4.9
1	C	441	LEU	4.9
1	B	332	TRP	4.8
1	B	299	PHE	4.8
1	B	337	LYS	4.7
1	C	443	ASN	4.6
1	B	343	GLY	4.6
1	B	350	GLU	4.5
1	B	357	GLU	4.5
1	B	420	CYS	4.5
1	B	396	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	442	PRO	4.5
1	B	446	THR	4.2
1	B	377	ILE	4.2
1	C	332	TRP	4.1
1	B	371	ILE	4.1
1	C	445	GLN	4.1
1	B	445	GLN	4.0
1	C	397	PHE	4.0
1	C	444	GLY	4.0
1	B	339	LEU	3.9
1	B	349	GLN	3.9
1	B	444	GLY	3.9
1	B	335	ASP	3.9
1	B	553	LEU	3.8
1	B	328	ILE	3.8
1	B	440	THR	3.7
1	B	331	ILE	3.7
1	B	338	GLY	3.6
1	B	381	ALA	3.6
1	B	368	VAL	3.5
1	B	394	MET	3.5
1	B	308	GLY	3.5
1	B	302	ALA	3.5
1	B	535	ASN	3.5
1	B	416	SER	3.4
1	B	411	SER	3.4
1	B	351	LYS	3.3
1	B	303	GLY	3.3
1	B	336	SER	3.3
1	B	384	GLY	3.2
1	C	361	MET	3.2
1	B	292	LEU	3.2
1	B	340	ILE	3.2
1	B	555	ASP	3.2
1	B	342	LYS	3.2
1	B	353	LYS	3.2
1	B	376	LEU	3.2
1	B	356	HIS	3.1
1	C	399	GLU	3.1
1	B	352	GLU	3.1
1	B	334	VAL	3.0
1	B	365	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	370	GLU	2.9
1	C	216	VAL	2.9
1	B	404	PHE	2.8
1	B	363	ASN	2.8
1	A	341	VAL	2.8
1	C	369	GLN	2.8
1	B	379	VAL	2.7
1	B	304	GLU	2.7
1	B	435	PRO	2.7
1	B	361	MET	2.7
1	B	448	TYR	2.7
1	B	421	TYR	2.7
1	C	400	ARG	2.7
1	B	402	ILE	2.7
1	B	386	PHE	2.7
1	C	393	ASP	2.6
1	B	373	PRO	2.5
1	B	415	CYS	2.5
1	B	301	GLY	2.5
1	B	428	ALA	2.4
1	B	309	ILE	2.4
1	B	502	PRO	2.4
1	C	250	VAL	2.4
1	C	341	VAL	2.4
1	A	355	ALA	2.4
1	B	439	VAL	2.3
1	B	362	LYS	2.3
1	B	385	ALA	2.3
1	B	505	THR	2.3
1	B	419	GLN	2.2
1	C	446	THR	2.2
1	B	329	LYS	2.2
1	B	429	ILE	2.1
1	B	389	GLN	2.1
1	B	523	GLN	2.1
1	B	320	GLU	2.1
1	C	427	ARG	2.1
1	C	224	PHE	2.0
1	B	300	GLN	2.0
1	B	323	PRO	2.0
1	B	322	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.