



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:09 PM UTC

PDB ID : 5OU5 / pdb_00005ou5
Title : Crystal structure of maize chloroplastic photosynthetic NADP(+)-dependent malic enzyme
Authors : Bovdilova, A.; Hoepfner, A.; Maurino, V.G.
Deposited on : 2017-08-23
Resolution : 2.20 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

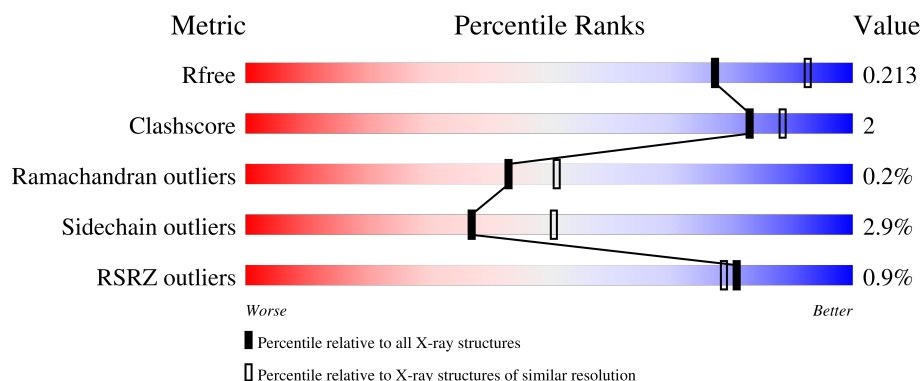
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	576	% 88% 7% . .
1	B	576	% 91% 6% . . .
1	C	576	% 90% 6% . .
1	D	576	% 87% 9% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18246 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 Malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	9	0
			4348	2795	729	806	18			
1	B	566	Total	C	N	O	S	0	11	0
			4424	2839	737	828	20			
1	C	557	Total	C	N	O	S	0	7	0
			4346	2791	719	817	19			
1	D	554	Total	C	N	O	S	0	13	0
			4382	2813	735	815	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	HIS	-	expression tag	UNP B4F8P6
B	61	HIS	-	expression tag	UNP B4F8P6
C	61	HIS	-	expression tag	UNP B4F8P6
D	61	HIS	-	expression tag	UNP B4F8P6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		
2	B	5	Total	Na	0	0
			5	5		
2	C	5	Total	Na	0	0
			5	5		
2	D	3	Total	Na	0	0
			3	3		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

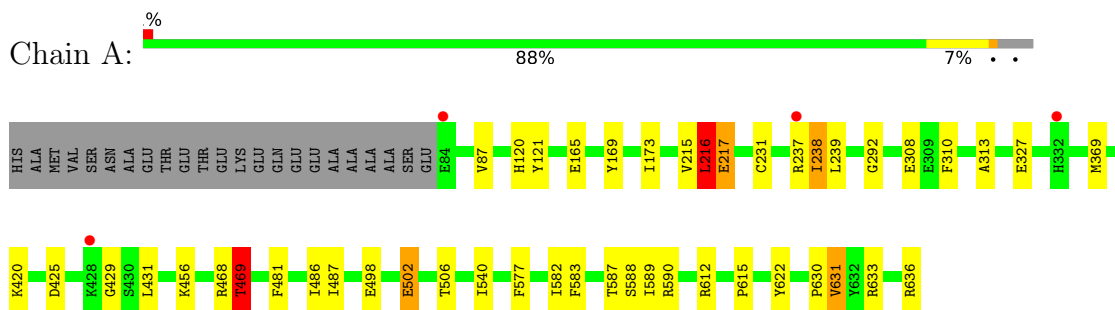
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0
4	B	144	Total O 144 144	0	0
4	C	164	Total O 164 164	0	0
4	D	217	Total O 217 217	0	0

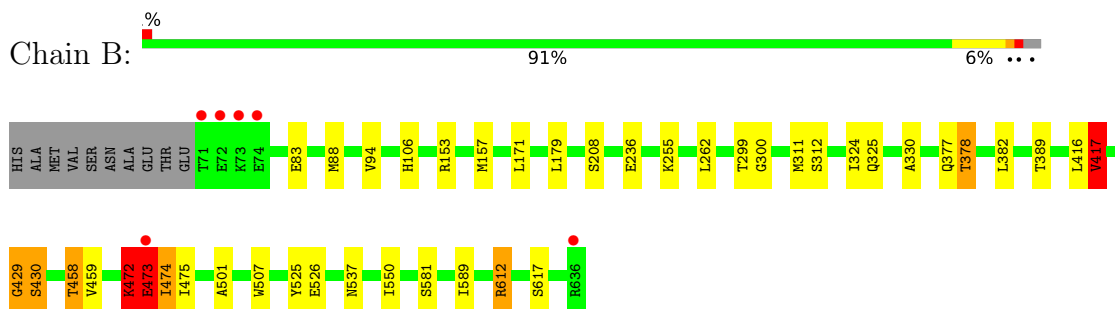
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

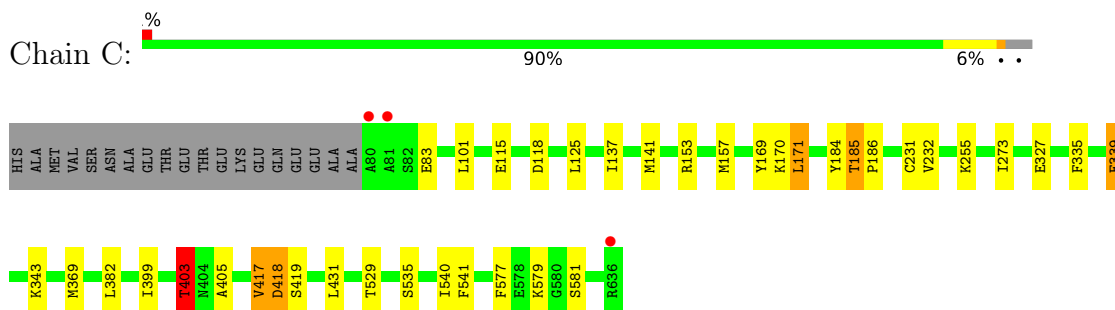
- Molecule 1: Malic enzyme



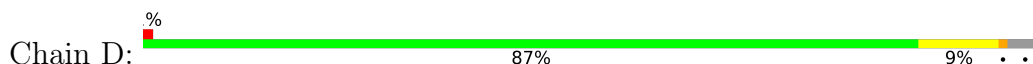
- Molecule 1: Malic enzyme

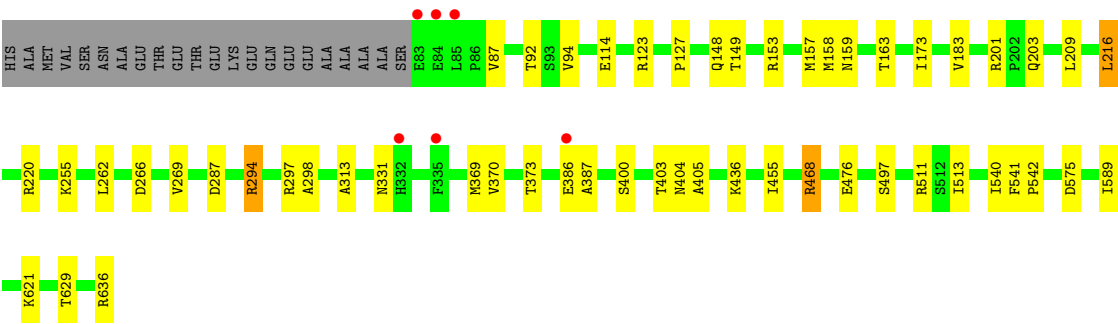


- Molecule 1: Malic enzyme



- Molecule 1: Malic enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.96Å 147.16Å 261.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.20 48.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.88-2.20) 99.7 (48.88-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.160 , 0.211 0.169 , 0.213	Depositor DCC
R_{free} test set	6725 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18246	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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](#)

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

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	1.24	8/4472 (0.2%)	1.13	12/6063 (0.2%)
1	B	1.19	7/4554 (0.2%)	1.09	7/6183 (0.1%)
1	C	1.18	6/4463 (0.1%)	1.12	8/6060 (0.1%)
1	D	1.21	6/4518 (0.1%)	1.07	7/6125 (0.1%)
All	All	1.21	27/18007 (0.1%)	1.10	34/24431 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185[A]	THR	CA-C	8.67	1.63	1.52
1	C	185[B]	THR	CA-C	8.67	1.63	1.52
1	A	217[A]	GLU	CA-C	7.95	1.64	1.52
1	A	217[B]	GLU	CA-C	7.95	1.64	1.52
1	A	292	GLY	N-CA	7.11	1.50	1.44
1	A	631	VAL	CA-CB	6.15	1.61	1.54
1	B	94	VAL	C-O	-5.96	1.17	1.24
1	A	238	ILE	C-O	-5.94	1.17	1.24
1	B	106	HIS	C-O	-5.82	1.16	1.23
1	B	458	THR	CA-C	5.79	1.60	1.52
1	C	101	LEU	C-O	-5.72	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	436	LYS	C-O	-5.51	1.19	1.24
1	A	308	GLU	CA-C	5.45	1.59	1.52
1	A	615	PRO	C-O	-5.39	1.20	1.25
1	C	541	PHE	C-O	-5.37	1.19	1.24
1	B	255	LYS	CA-C	-5.36	1.46	1.52
1	B	312	SER	CA-C	5.35	1.59	1.52
1	D	153	ARG	C-O	-5.33	1.17	1.24
1	C	125	LEU	C-O	-5.26	1.17	1.24
1	D	127	PRO	C-O	-5.22	1.18	1.24
1	D	476	GLU	C-O	-5.20	1.18	1.24
1	D	149	THR	C-O	-5.20	1.17	1.24
1	C	118	ASP	C-O	-5.18	1.18	1.24
1	B	325	GLN	N-CA	-5.14	1.39	1.46
1	B	501	ALA	C-O	5.04	1.29	1.24
1	D	173	ILE	C-O	-5.03	1.18	1.24
1	A	622	TYR	N-CA	-5.03	1.40	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	CA-C-N	9.27	133.63	120.28
1	A	216	LEU	C-N-CA	9.27	133.63	120.28
1	D	511	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	C	184	TYR	CA-C-N	7.84	140.94	121.80
1	C	184	TYR	C-N-CA	7.84	140.94	121.80
1	D	511	ARG	NE-CZ-NH2	7.59	126.03	119.20
1	D	387	ALA	N-CA-C	7.04	119.03	111.36
1	B	472	LYS	CA-C-N	6.70	133.76	121.70
1	B	472	LYS	C-N-CA	6.70	133.76	121.70
1	A	217[A]	GLU	CA-C-O	6.57	127.52	120.10
1	A	217[B]	GLU	CA-C-O	6.57	127.52	120.10
1	B	378	THR	CB-CA-C	6.50	121.61	109.71
1	A	469	THR	N-CA-CB	-6.42	101.10	110.53
1	B	474	ILE	N-CA-C	-6.23	104.21	111.00
1	A	583	PHE	CA-C-N	-6.15	114.05	120.38
1	A	583	PHE	C-N-CA	-6.15	114.05	120.38
1	C	418	ASP	CB-CA-C	-6.11	99.80	111.48
1	C	540	ILE	N-CA-C	6.05	116.77	111.56
1	D	297	ARG	CG-CD-NE	-6.01	98.77	112.00
1	A	631	VAL	N-CA-CB	5.93	119.38	110.13
1	B	473	GLU	N-CA-C	-5.92	94.43	111.00
1	D	405	ALA	CA-C-N	-5.75	113.86	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	ALA	C-N-CA	-5.75	113.86	119.78
1	A	469	THR	CB-CA-C	5.69	119.65	109.29
1	C	335	PHE	N-CA-C	5.51	117.37	111.36
1	C	403	THR	N-CA-CB	-5.44	103.36	110.59
1	C	403	THR	CB-CA-C	5.36	117.72	109.03
1	A	540	ILE	N-CA-C	5.27	116.09	111.56
1	B	472	LYS	N-CA-C	5.22	121.93	110.80
1	A	589	ILE	N-CA-C	5.22	115.94	110.62
1	D	540	ILE	N-CA-C	5.13	115.98	111.56
1	B	417	VAL	CB-CA-C	5.12	118.59	110.81
1	A	469	THR	N-CA-C	-5.09	107.24	113.50
1	C	184	TYR	N-CA-C	-5.09	99.96	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217[A]	GLU	Mainchain
1	B	429	GLY	Peptide
1	C	185[B]	THR	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4348	0	4391	24	0
1	B	4424	0	4437	22	0
1	C	4346	0	4363	17	0
1	D	4382	0	4425	25	0
2	A	3	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0
3	A	1	0	0	0	0
4	A	204	0	0	3	0
4	B	144	0	0	0	0
4	C	164	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	217	0	0	2	0
All	All	18246	0	17616	85	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 2.

All (85) 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:D:287:ASP:O	1:D:294:ARG:NH2	1.67	1.25
1:D:468[A]:ARG:HH11	1:D:468[A]:ARG:HG2	1.05	1.19
1:A:468[B]:ARG:HG3	1:A:468[B]:ARG:HH11	1.19	0.99
1:D:220[A]:ARG:NH1	4:D:801:HOH:O	2.01	0.94
1:D:468[A]:ARG:HH11	1:D:468[A]:ARG:CG	1.82	0.92
1:A:468[B]:ARG:HG3	1:A:468[B]:ARG:NH1	1.80	0.88
1:D:468[A]:ARG:HG2	1:D:468[A]:ARG:NH1	1.88	0.82
1:D:370:VAL:HG11	1:D:513:ILE:HD11	1.63	0.81
1:A:468[B]:ARG:HH11	1:A:468[B]:ARG:CG	1.94	0.80
1:D:159:ASN:O	1:D:163[B]:THR:HG22	1.83	0.78
1:B:472:LYS:CA	1:B:473:GLU:HB2	2.14	0.77
1:A:633[B]:ARG:NE	1:A:633[B]:ARG:HA	2.01	0.76
1:B:458:THR:HG23	1:B:459:VAL:HG23	1.67	0.74
1:B:377:GLN:OE1	1:B:458:THR:HG21	1.91	0.71
1:B:472:LYS:HB3	1:B:473:GLU:HB2	1.74	0.68
1:A:633[B]:ARG:NE	1:A:633[B]:ARG:CA	2.59	0.65
1:B:472:LYS:CB	1:B:473:GLU:HB2	2.27	0.65
1:B:157[B]:MET:HE1	1:B:179:LEU:HD13	1.79	0.65
1:D:403:THR:O	1:D:404:ASN:HB2	1.97	0.62
1:A:369:MET:HE2	1:A:577:PHE:CD1	2.35	0.62
1:A:633[B]:ARG:NH1	1:C:83:GLU:O	2.27	0.61
1:C:399:ILE:O	1:C:403:THR:HB	2.01	0.60
1:B:262:LEU:HD22	1:B:589:ILE:HG21	1.84	0.59
1:B:472:LYS:HA	1:B:507:TRP:CE3	2.37	0.59
1:A:369:MET:HE3	1:A:582:ILE:HG22	1.82	0.59
1:D:468[A]:ARG:CG	1:D:468[A]:ARG:NH1	2.51	0.57
1:C:339:GLU:O	1:C:343:LYS:HE2	2.04	0.57
1:B:472:LYS:N	1:B:473:GLU:HB2	2.19	0.56
1:B:475:ILE:HD13	1:B:507:TRP:HE3	1.71	0.56
1:A:633[B]:ARG:NE	4:A:804:HOH:O	2.41	0.54
1:D:114:GLU:OE1	1:D:123:ARG:NH2	2.44	0.51
1:C:231[A]:CYS:SG	1:C:327:GLU:HG3	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:O	1:B:157[B]:MET:HG3	2.11	0.51
1:C:403:THR:HG22	1:C:405:ALA:H	1.76	0.51
1:D:216:LEU:HD13	1:D:313:ALA:HB1	1.92	0.51
1:A:216:LEU:HD13	1:A:313:ALA:HB1	1.92	0.51
1:C:153:ARG:O	1:C:157[B]:MET:HE2	2.11	0.51
1:D:331:ASN:HB3	1:D:386:GLU:OE2	2.10	0.50
1:A:469:THR:HG22	1:A:498:GLU:HG3	1.93	0.49
1:A:633[B]:ARG:HA	1:A:633[B]:ARG:CZ	2.41	0.49
1:B:311:MET:HE1	1:B:324:ILE:HD13	1.93	0.49
1:A:502:GLU:O	1:A:506:THR:HG23	2.12	0.49
1:C:382:LEU:HD12	1:C:417:VAL:HG22	1.95	0.49
1:C:169:TYR:OH	4:C:801:HOH:O	2.20	0.48
1:D:157[B]:MET:HE2	1:D:183:VAL:CG1	2.43	0.48
1:D:203:GLN:NE2	4:D:808:HOH:O	2.46	0.48
1:B:550:ILE:O	1:B:612[A]:ARG:HG2	2.14	0.47
1:A:456:LYS:HE3	1:A:481:PHE:CD2	2.49	0.47
1:A:633[B]:ARG:CZ	4:A:804:HOH:O	2.63	0.46
1:C:369:MET:HE2	1:C:577:PHE:CD1	2.50	0.46
1:B:472:LYS:CA	1:B:473:GLU:CB	2.91	0.46
1:D:468[B]:ARG:NH1	1:D:497:SER:O	2.48	0.46
1:A:169:TYR:OH	4:A:801:HOH:O	2.20	0.46
1:B:525:TYR:CE1	1:B:526:GLU:HG3	2.51	0.46
1:C:157[B]:MET:HE2	1:C:157[B]:MET:HB2	1.52	0.45
1:D:370:VAL:CG1	1:D:513:ILE:HD11	2.40	0.45
1:A:231[A]:CYS:SG	1:A:327:GLU:HG3	2.56	0.45
1:B:472:LYS:O	1:B:475:ILE:HB	2.16	0.44
1:D:157[B]:MET:HE2	1:D:183:VAL:HG11	1.99	0.44
1:D:541:PHE:N	1:D:542:PRO:CD	2.81	0.44
1:B:299[B]:THR:HG22	1:B:300:GLY:H	1.83	0.44
1:C:141:MET:SD	1:C:171:LEU:HD11	2.58	0.43
1:A:469:THR:CG2	1:A:498:GLU:HG3	2.48	0.43
1:C:255:LYS:HE3	1:C:327:GLU:CD	2.44	0.43
1:D:262:LEU:HD22	1:D:589:ILE:HG21	2.01	0.42
1:C:137:ILE:HD11	1:C:170:LYS:HG2	2.00	0.42
1:A:173:ILE:HD12	1:A:630:PRO:HG3	2.01	0.42
1:C:137:ILE:HG23	1:C:171:LEU:HD12	2.01	0.42
1:D:266:ASP:O	1:D:269:VAL:HG22	2.20	0.42
1:B:382:LEU:HD12	1:B:417:VAL:HG22	2.02	0.42
1:A:120:HIS:NE2	1:A:636:ARG:O	2.53	0.42
1:A:238:ILE:O	1:A:239:LEU:C	2.60	0.41
1:A:486:ILE:C	1:A:487:ILE:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88[A]:MET:SD	1:D:636:ARG:NH1	2.93	0.41
1:B:236:GLU:HG2	1:B:330:ALA:HB2	2.03	0.41
1:C:232:VAL:HA	1:C:273:ILE:O	2.20	0.41
1:A:121:TYR:CE2	1:D:94:VAL:HG11	2.56	0.41
1:D:216:LEU:HD13	1:D:313:ALA:CB	2.50	0.41
1:B:429:GLY:O	1:B:430:SER:HB3	2.20	0.40
1:B:475:ILE:CD1	1:B:507:TRP:HE3	2.33	0.40
1:C:339:GLU:O	1:C:343:LYS:CE	2.68	0.40
1:A:215:VAL:HG11	1:A:310:PHE:HA	2.04	0.40
1:C:157[A]:MET:HE1	1:C:171:LEU:HD23	2.03	0.40
1:D:209:LEU:HD11	1:D:298:ALA:HB2	2.04	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	560/576 (97%)	550 (98%)	9 (2%)	1 (0%)	43	51
1	B	575/576 (100%)	563 (98%)	9 (2%)	3 (0%)	24	27
1	C	562/576 (98%)	553 (98%)	8 (1%)	1 (0%)	43	51
1	D	565/576 (98%)	552 (98%)	13 (2%)	0	100	100
All	All	2262/2304 (98%)	2218 (98%)	39 (2%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	SER
1	B	473	GLU
1	B	472	LYS
1	C	186	PRO

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Mol	Chain	Res	Type
1	A	429	GLY

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	469/480 (98%)	455 (97%)	14 (3%)	36	49
1	B	474/480 (99%)	460 (97%)	14 (3%)	36	49
1	C	469/480 (98%)	456 (97%)	13 (3%)	38	52
1	D	475/480 (99%)	458 (96%)	17 (4%)	31	42
All	All	1887/1920 (98%)	1829 (97%)	58 (3%)	37	48

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	165	GLU
1	A	216	LEU
1	A	237	ARG
1	A	420	LYS
1	A	425	ASP
1	A	431	LEU
1	A	469	THR
1	A	502	GLU
1	A	587	THR
1	A	588	SER
1	A	590	ARG
1	A	612	ARG
1	A	631	VAL
1	B	83	GLU
1	B	171	LEU
1	B	208	SER
1	B	378	THR
1	B	389	THR
1	B	416	LEU

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Mol	Chain	Res	Type
1	B	417	VAL
1	B	473	GLU
1	B	474	ILE
1	B	537	ASN
1	B	581	SER
1	B	612[A]	ARG
1	B	612[B]	ARG
1	B	617	SER
1	C	115	GLU
1	C	171	LEU
1	C	339	GLU
1	C	403	THR
1	C	417	VAL
1	C	418	ASP
1	C	419	SER
1	C	431	LEU
1	C	529[A]	THR
1	C	529[B]	THR
1	C	535	SER
1	C	579	LYS
1	C	581	SER
1	D	87	VAL
1	D	92	THR
1	D	148	GLN
1	D	201	ARG
1	D	216	LEU
1	D	255	LYS
1	D	294	ARG
1	D	369	MET
1	D	373	THR
1	D	400[A]	SER
1	D	400[B]	SER
1	D	455	ILE
1	D	468[A]	ARG
1	D	468[B]	ARG
1	D	575	ASP
1	D	621	LYS
1	D	629	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	224	HIS
1	A	228	GLN
1	A	247	GLN
1	A	574	GLN
1	B	152	GLN
1	B	175	ASN
1	B	332	HIS
1	C	226	ASN
1	C	228	GLN
1	C	295	GLN
1	C	331	ASN
1	C	571	GLN
1	D	161	GLN
1	D	228	GLN
1	D	247	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	553/576 (96%)	-0.38	4 (0%) 84 82	17, 35, 64, 84	9 (1%)
1	B	566/576 (98%)	-0.24	6 (1%) 78 76	18, 40, 69, 124	11 (1%)
1	C	557/576 (96%)	-0.38	3 (0%) 87 85	16, 36, 62, 94	7 (1%)
1	D	554/576 (96%)	-0.43	6 (1%) 78 76	16, 35, 58, 90	13 (2%)
All	All	2230/2304 (96%)	-0.36	19 (0%) 81 79	16, 36, 63, 124	40 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	THR	4.6
1	C	80	ALA	4.2
1	D	85	LEU	3.3
1	A	84	GLU	3.2
1	B	72	GLU	3.0
1	D	84	GLU	2.9
1	B	73	LYS	2.8
1	D	83	GLU	2.8
1	A	428	LYS	2.6
1	C	81	ALA	2.5
1	B	636	ARG	2.4
1	B	473	GLU	2.4
1	D	386	GLU	2.3
1	B	74	GLU	2.2
1	C	636	ARG	2.2
1	D	335	PHE	2.2
1	A	237	ARG	2.1
1	A	332	HIS	2.1
1	D	332	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	A	704	1/1	0.88	0.14	66,66,66,66	0
2	NA	C	702	1/1	0.90	0.13	55,55,55,55	0
2	NA	B	705	1/1	0.96	0.05	46,46,46,46	0
2	NA	A	703	1/1	0.96	0.11	44,44,44,44	0
2	NA	C	704	1/1	0.96	0.10	44,44,44,44	0
2	NA	D	702	1/1	0.96	0.10	43,43,43,43	0
2	NA	B	704	1/1	0.96	0.18	45,45,45,45	0
2	NA	A	702	1/1	0.97	0.08	55,55,55,55	0
2	NA	D	703	1/1	0.97	0.13	50,50,50,50	0
2	NA	B	702	1/1	0.97	0.18	45,45,45,45	0
2	NA	B	701	1/1	0.98	0.07	37,37,37,37	0
2	NA	C	705	1/1	0.98	0.15	46,46,46,46	0
2	NA	D	701	1/1	0.98	0.12	36,36,36,36	0
2	NA	A	701	1/1	0.98	0.12	41,41,41,41	0
2	NA	C	701	1/1	0.98	0.12	37,37,37,37	0
2	NA	B	703	1/1	0.98	0.12	45,45,45,45	0
2	NA	C	703	1/1	0.99	0.14	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.