



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:42 AM UTC

PDB ID : 7QBJ / pdb_00007qbj
Title : bacterial IMPDH chimera
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Deposited on : 2021-11-19
Resolution : 2.27 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

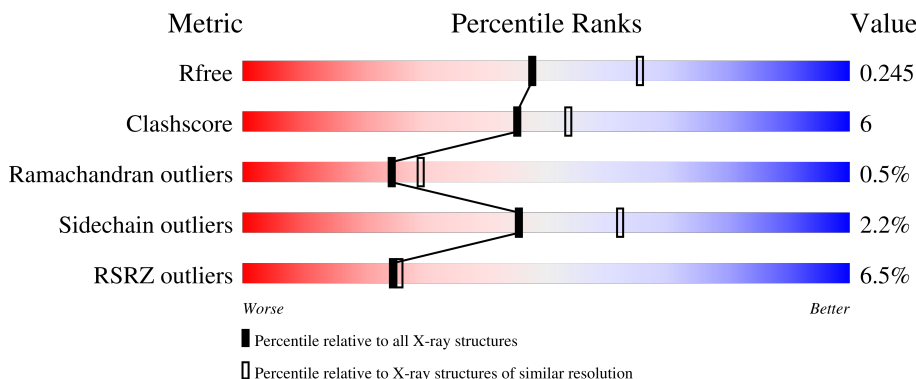
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	507	4% 75% 9% 16%
1	B	507	7% 75% 9% 15%
1	C	507	5% 55% 11% 33%
1	D	507	5% 73% 11% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12722 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	5	0
			3203	1995	579	611	18			
1	B	429	Total	C	N	O	S	2	0	0
			3199	1993	577	612	17			
1	C	341	Total	C	N	O	S	0	2	0
			2508	1556	460	478	14			
1	D	432	Total	C	N	O	S	0	1	0
			3222	2008	582	615	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0ADG7
A	-18	GLY	-	expression tag	UNP P0ADG7
A	-17	SER	-	expression tag	UNP P0ADG7
A	-16	SER	-	expression tag	UNP P0ADG7
A	-15	HIS	-	expression tag	UNP P0ADG7
A	-14	HIS	-	expression tag	UNP P0ADG7
A	-13	HIS	-	expression tag	UNP P0ADG7
A	-12	HIS	-	expression tag	UNP P0ADG7
A	-11	HIS	-	expression tag	UNP P0ADG7
A	-10	HIS	-	expression tag	UNP P0ADG7
A	-9	SER	-	expression tag	UNP P0ADG7
A	-8	SER	-	expression tag	UNP P0ADG7
A	-7	GLY	-	expression tag	UNP P0ADG7
A	-6	LEU	-	expression tag	UNP P0ADG7
A	-5	VAL	-	expression tag	UNP P0ADG7
A	-4	PRO	-	expression tag	UNP P0ADG7
A	-3	ARG	-	expression tag	UNP P0ADG7
A	-2	GLY	-	expression tag	UNP P0ADG7
A	-1	SER	-	expression tag	UNP P0ADG7
A	0	HIS	-	expression tag	UNP P0ADG7
B	-19	MET	-	initiating methionine	UNP P0ADG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0ADG7
B	-17	SER	-	expression tag	UNP P0ADG7
B	-16	SER	-	expression tag	UNP P0ADG7
B	-15	HIS	-	expression tag	UNP P0ADG7
B	-14	HIS	-	expression tag	UNP P0ADG7
B	-13	HIS	-	expression tag	UNP P0ADG7
B	-12	HIS	-	expression tag	UNP P0ADG7
B	-11	HIS	-	expression tag	UNP P0ADG7
B	-10	HIS	-	expression tag	UNP P0ADG7
B	-9	SER	-	expression tag	UNP P0ADG7
B	-8	SER	-	expression tag	UNP P0ADG7
B	-7	GLY	-	expression tag	UNP P0ADG7
B	-6	LEU	-	expression tag	UNP P0ADG7
B	-5	VAL	-	expression tag	UNP P0ADG7
B	-4	PRO	-	expression tag	UNP P0ADG7
B	-3	ARG	-	expression tag	UNP P0ADG7
B	-2	GLY	-	expression tag	UNP P0ADG7
B	-1	SER	-	expression tag	UNP P0ADG7
B	0	HIS	-	expression tag	UNP P0ADG7
C	-19	MET	-	initiating methionine	UNP P0ADG7
C	-18	GLY	-	expression tag	UNP P0ADG7
C	-17	SER	-	expression tag	UNP P0ADG7
C	-16	SER	-	expression tag	UNP P0ADG7
C	-15	HIS	-	expression tag	UNP P0ADG7
C	-14	HIS	-	expression tag	UNP P0ADG7
C	-13	HIS	-	expression tag	UNP P0ADG7
C	-12	HIS	-	expression tag	UNP P0ADG7
C	-11	HIS	-	expression tag	UNP P0ADG7
C	-10	HIS	-	expression tag	UNP P0ADG7
C	-9	SER	-	expression tag	UNP P0ADG7
C	-8	SER	-	expression tag	UNP P0ADG7
C	-7	GLY	-	expression tag	UNP P0ADG7
C	-6	LEU	-	expression tag	UNP P0ADG7
C	-5	VAL	-	expression tag	UNP P0ADG7
C	-4	PRO	-	expression tag	UNP P0ADG7
C	-3	ARG	-	expression tag	UNP P0ADG7
C	-2	GLY	-	expression tag	UNP P0ADG7
C	-1	SER	-	expression tag	UNP P0ADG7
C	0	HIS	-	expression tag	UNP P0ADG7
D	-19	MET	-	initiating methionine	UNP P0ADG7
D	-18	GLY	-	expression tag	UNP P0ADG7
D	-17	SER	-	expression tag	UNP P0ADG7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P0ADG7
D	-15	HIS	-	expression tag	UNP P0ADG7
D	-14	HIS	-	expression tag	UNP P0ADG7
D	-13	HIS	-	expression tag	UNP P0ADG7
D	-12	HIS	-	expression tag	UNP P0ADG7
D	-11	HIS	-	expression tag	UNP P0ADG7
D	-10	HIS	-	expression tag	UNP P0ADG7
D	-9	SER	-	expression tag	UNP P0ADG7
D	-8	SER	-	expression tag	UNP P0ADG7
D	-7	GLY	-	expression tag	UNP P0ADG7
D	-6	LEU	-	expression tag	UNP P0ADG7
D	-5	VAL	-	expression tag	UNP P0ADG7
D	-4	PRO	-	expression tag	UNP P0ADG7
D	-3	ARG	-	expression tag	UNP P0ADG7
D	-2	GLY	-	expression tag	UNP P0ADG7
D	-1	SER	-	expression tag	UNP P0ADG7
D	0	HIS	-	expression tag	UNP P0ADG7

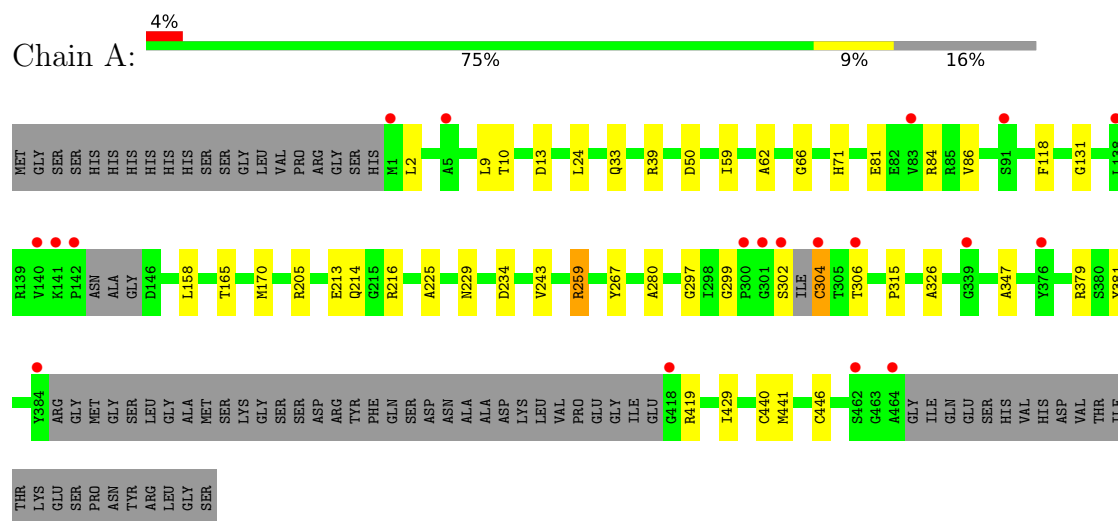
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	162	Total O 162 162	0	0
2	B	156	Total O 156 156	0	0
2	C	137	Total O 137 137	0	0
2	D	135	Total O 135 135	0	0

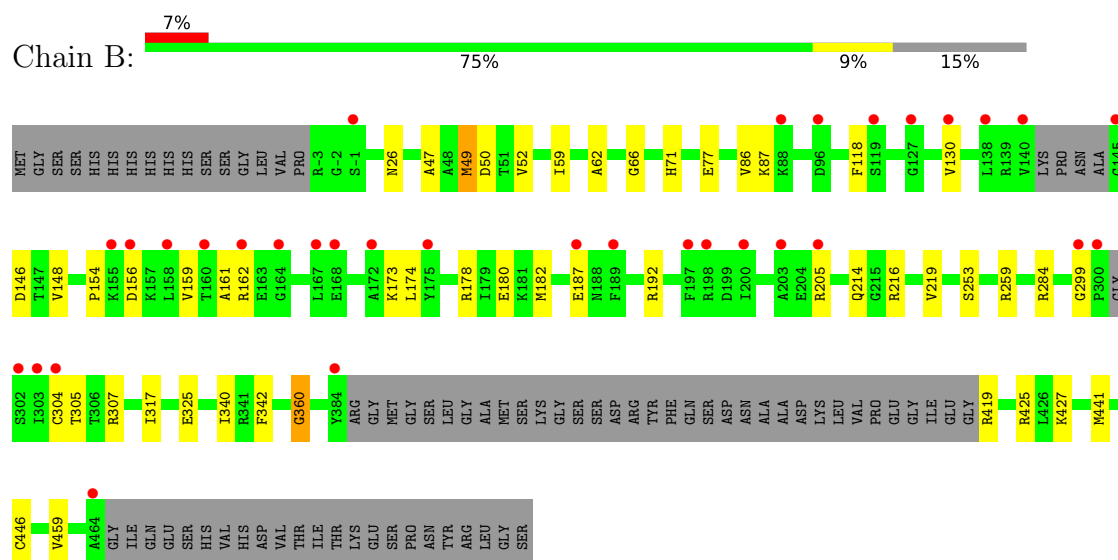
3 Residue-property plots

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

- Molecule 1: Inosine-5'-monophosphate dehydrogenase

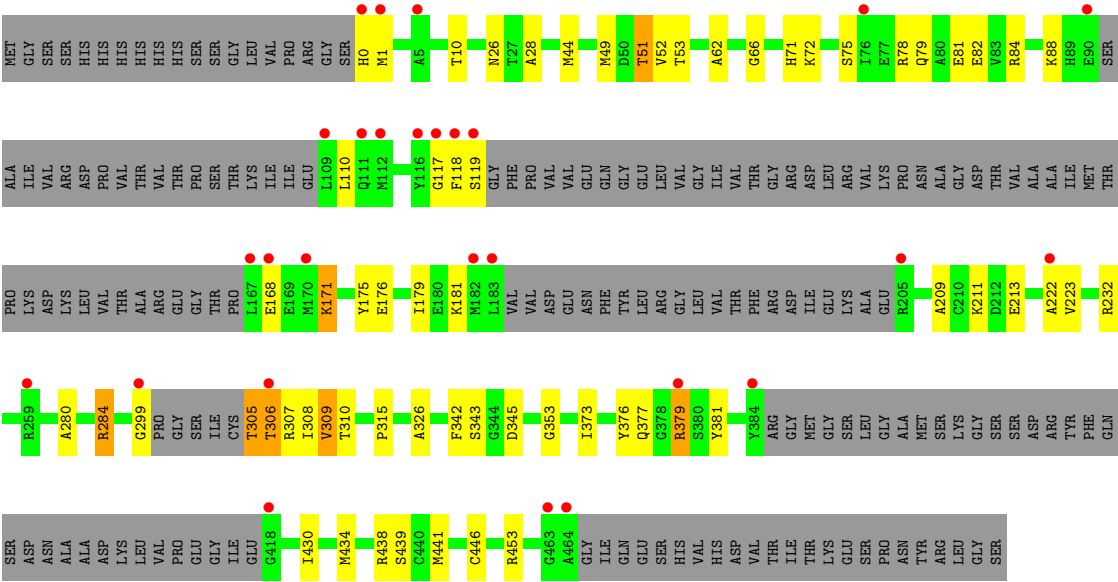


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

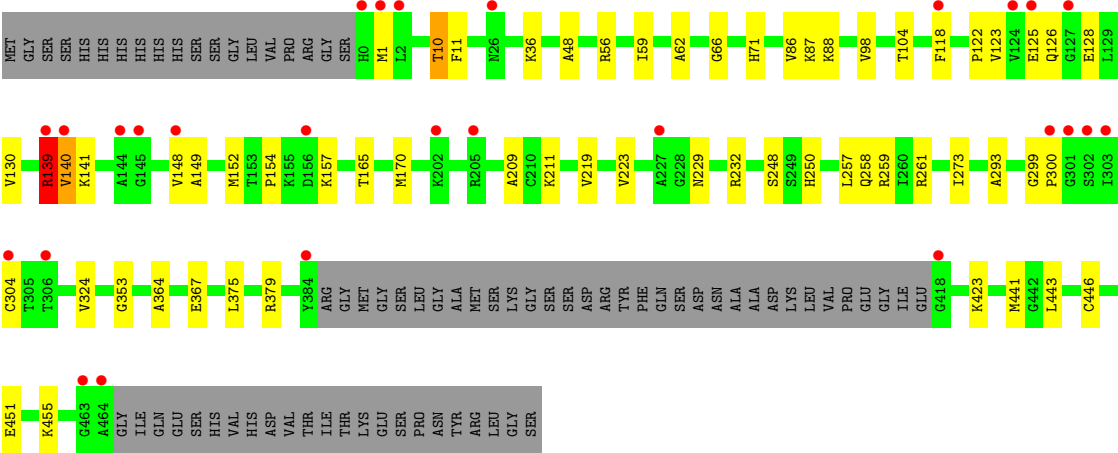


- Molecule 1: Inosine-5'-monophosphate dehydrogenase





● Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	145.04Å 145.04Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.27 48.32 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.32-2.27) 100.0 (48.32-2.27)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.193 , 0.226 (Not available) , 0.245	Depositor DCC
R_{free} test set	5858 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12722	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

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	0.41	0/3257	0.59	0/4390
1	B	0.42	1/3232 (0.0%)	0.58	0/4357
1	C	0.40	0/2535	0.61	0/3408
1	D	0.42	0/3262	0.63	2/4401 (0.0%)
All	All	0.41	1/12286 (0.0%)	0.60	2/16556 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	MET	SD-CE	-5.09	1.66	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	CA-C-N	6.17	133.08	121.97
1	D	139	ARG	C-N-CA	6.17	133.08	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	379	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	139	ARG	Sidechain

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	3203	0	3299	28	0
1	B	3199	0	3297	39	0
1	C	2508	0	2558	50	1
1	D	3222	0	3324	41	0
2	A	162	0	0	1	0
2	B	156	0	0	2	1
2	C	137	0	0	2	0
2	D	135	0	0	4	0
All	All	12722	0	12478	146	2

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 6.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:HD3	1:B:182:MET:HE1	1.23	1.15
1:C:379:ARG:NH1	1:C:381:TYR:OH	1.96	0.98
1:B:178:ARG:HD3	1:C:118:PHE:HE1	1.25	0.98
1:B:162:ARG:HH22	1:B:187:GLU:HG3	1.48	0.78
1:C:0:HIS:CG	1:C:1:MET:H	2.01	0.78
1:A:213:GLU:H	1:A:213:GLU:CD	1.93	0.76
1:B:178:ARG:HD3	1:C:118:PHE:CE1	2.16	0.75
1:D:149:ALA:HA	1:D:152:MET:HE3	1.70	0.74
1:A:81[A]:GLU:OE1	1:A:84[A]:ARG:NH1	2.22	0.73
1:D:123:VAL:HG11	1:D:152:MET:HE1	1.73	0.69
1:C:81:GLU:OE1	1:C:84:ARG:NH1	2.24	0.69
1:B:173:LYS:CD	1:B:182:MET:HE1	2.14	0.68
1:C:110:LEU:O	1:C:110:LEU:HD23	1.94	0.68
1:C:376:TYR:CE1	1:C:377:GLN:HG3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASN:H	1:D:259:ARG:HH22	1.43	0.67
1:C:345:ASP:OD1	2:C:501:HOH:O	2.14	0.64
1:D:229:ASN:H	1:D:259:ARG:NH2	1.95	0.64
1:D:229:ASN:ND2	2:D:502:HOH:O	2.30	0.64
1:A:304[A]:CYS:SG	1:A:306:THR:HG22	2.38	0.64
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.33	0.62
1:A:205:ARG:NH2	2:A:503:HOH:O	2.29	0.62
1:B:118:PHE:HE1	1:C:175:TYR:HA	1.66	0.60
1:C:84:ARG:O	1:C:88:LYS:HG3	2.02	0.59
1:B:178:ARG:HA	1:C:118:PHE:CE1	2.37	0.59
1:B:304:CYS:HB2	1:B:307:ARG:HD3	1.84	0.58
1:C:44:MET:SD	1:C:434:MET:HE3	2.43	0.58
1:A:441:MET:HB3	1:A:446:CYS:O	2.03	0.57
1:C:305:THR:O	1:C:309:VAL:HG13	2.05	0.57
1:A:379:ARG:HE	1:D:379:ARG:CZ	2.17	0.57
1:A:381:TYR:CG	1:A:419:ARG:HD3	2.40	0.57
1:B:425:ARG:HH12	1:B:427:LYS:HD2	1.70	0.57
1:B:49:MET:HE3	1:B:52:VAL:HG21	1.87	0.56
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.40	0.56
1:B:159:VAL:HG12	1:B:182:MET:HE3	1.87	0.56
1:B:180:GLU:OE1	1:C:119:SER:HB3	2.06	0.56
1:D:154:PRO:HD2	1:D:157:LYS:HE3	1.87	0.55
1:D:441:MET:HB3	1:D:446:CYS:O	2.06	0.55
1:C:78:ARG:O	1:C:82:GLU:HG2	2.06	0.55
1:B:49:MET:HE2	1:B:360:GLY:HA3	1.88	0.54
1:B:299:GLY:O	1:B:307:ARG:HD2	2.08	0.54
1:C:213:GLU:H	1:C:213:GLU:CD	2.15	0.54
1:D:229:ASN:N	1:D:259:ARG:HH22	2.06	0.54
1:C:0:HIS:CD2	1:C:1:MET:H	2.25	0.54
1:B:154:PRO:HG2	1:B:156:ASP:OD1	2.08	0.54
1:D:364:ALA:O	1:D:423:LYS:NZ	2.39	0.54
1:C:0:HIS:CG	1:C:1:MET:N	2.72	0.53
1:A:59:ILE:HG13	1:A:86:VAL:HG22	1.89	0.53
1:B:47:ALA:HB3	1:B:49:MET:HE2	1.90	0.53
1:B:77:GLU:H	1:B:77:GLU:CD	2.17	0.53
1:A:10:THR:HG22	1:A:13:ASP:OD2	2.09	0.53
1:C:284[A]:ARG:HG2	1:C:284[A]:ARG:HH11	1.73	0.53
1:C:441:MET:HB3	1:C:446:CYS:O	2.08	0.53
1:C:280:ALA:HB1	1:C:326:ALA:HB2	1.91	0.52
1:B:284:ARG:HD3	2:B:547:HOH:O	2.08	0.52
1:B:49:MET:CE	1:B:360:GLY:HA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ALA:HB3	1:C:211:LYS:HE2	1.92	0.52
1:C:284[A]:ARG:HH11	1:C:284[A]:ARG:CG	2.23	0.51
1:A:379:ARG:HH21	1:D:379:ARG:HD3	1.74	0.51
1:D:123:VAL:HG11	1:D:152:MET:CE	2.40	0.51
1:A:379:ARG:HE	1:D:379:ARG:HD3	1.76	0.51
1:A:62:ALA:HA	1:A:66:GLY:O	2.11	0.51
1:D:258:GLN:OE1	1:D:261:ARG:NH1	2.40	0.50
1:D:10:THR:HG23	2:D:501:HOH:O	2.10	0.50
1:C:379:ARG:NH1	1:C:381:TYR:HH	2.04	0.49
1:D:165:THR:HB	1:D:170:MET:HE3	1.94	0.49
1:D:273:ILE:HG12	1:D:293:ALA:HB3	1.95	0.49
1:B:325:GLU:OE2	1:D:141:LYS:NZ	2.41	0.48
1:C:353:GLY:O	1:C:453:ARG:HD2	2.11	0.48
1:D:257:LEU:O	1:D:261:ARG:HG3	2.12	0.48
1:A:229:ASN:HB3	1:A:259[B]:ARG:HH22	1.78	0.48
1:C:26:ASN:ND2	1:C:26:ASN:H	2.10	0.48
1:A:429:ILE:HG12	1:D:375:LEU:HD22	1.94	0.48
1:B:299:GLY:HA2	1:B:304:CYS:SG	2.54	0.48
1:C:175:TYR:HD2	1:C:176:GLU:HG2	1.78	0.48
1:A:33:GLN:OE1	1:A:39:ARG:HD2	2.13	0.48
1:D:299:GLY:N	1:D:300:PRO:HD3	2.28	0.48
1:C:28:ALA:O	1:C:438:ARG:NH1	2.47	0.47
1:D:56:ARG:NH2	1:D:367:GLU:HG3	2.29	0.47
1:D:62:ALA:HA	1:D:66:GLY:O	2.15	0.47
1:B:161:ALA:N	1:B:182:MET:HE2	2.29	0.47
1:C:179:ILE:HD12	1:C:181:LYS:O	2.15	0.47
1:C:51:THR:HG22	1:C:52:VAL:HG23	1.97	0.47
1:A:214:GLN:OE1	1:A:216:ARG:NH2	2.46	0.47
1:B:162:ARG:NH1	1:B:187:GLU:HA	2.29	0.46
1:A:234:ASP:OD1	1:A:267:TYR:OH	2.26	0.46
1:A:225:ALA:O	1:A:259[A]:ARG:NH1	2.48	0.46
1:D:104:THR:O	1:D:148:VAL:HG13	2.16	0.46
1:D:324:VAL:HG21	1:D:353:GLY:C	2.41	0.46
1:D:87:LYS:HD3	1:D:219:VAL:HG12	1.97	0.46
1:B:26:ASN:ND2	1:B:26:ASN:H	2.14	0.46
1:D:125:GLU:HG3	1:D:126:GLN:HG2	1.98	0.45
1:B:284:ARG:NH2	2:B:507:HOH:O	2.47	0.45
1:D:299:GLY:HA2	1:D:304:CYS:SG	2.56	0.45
1:C:62:ALA:HA	1:C:66:GLY:O	2.17	0.45
1:C:117:GLY:C	1:C:118:PHE:HD2	2.25	0.45
1:C:75:SER:OG	1:C:78:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ASN:H	1:B:26:ASN:HD22	1.65	0.45
1:C:168:GLU:HA	1:C:171:LYS:HB3	1.98	0.45
1:A:131:GLY:HA2	1:A:158:LEU:HD11	1.98	0.44
1:C:223:VAL:HG12	1:C:232:ARG:CD	2.47	0.44
1:A:280:ALA:HB1	1:A:326:ALA:HB2	1.99	0.44
1:B:180:GLU:HG3	1:C:118:PHE:H	1.81	0.44
1:C:175:TYR:CD2	1:C:176:GLU:HG2	2.52	0.44
1:B:59:ILE:HG13	1:B:86:VAL:HG22	2.00	0.44
1:B:441:MET:HB3	1:B:446:CYS:O	2.18	0.44
1:C:26:ASN:H	1:C:26:ASN:HD22	1.65	0.44
1:C:284[B]:ARG:NH1	2:C:508:HOH:O	2.48	0.44
1:C:373:ILE:HA	1:C:381:TYR:O	2.18	0.44
1:B:317:ILE:HD13	1:B:317:ILE:HA	1.85	0.43
1:D:59:ILE:HG13	1:D:86:VAL:HG22	1.99	0.43
1:D:10:THR:HG22	1:D:11:PHE:H	1.83	0.43
1:A:165:THR:HB	1:A:170:MET:HE3	2.01	0.43
1:A:299:GLY:HA2	1:A:304[A]:CYS:SG	2.59	0.43
1:A:379:ARG:HE	1:D:379:ARG:CD	2.31	0.43
1:B:214:GLN:HB2	1:B:216:ARG:HH21	1.83	0.43
1:D:250:HIS:HD2	2:D:580:HOH:O	2.02	0.43
1:C:79:GLN:OE1	1:C:232:ARG:NH1	2.38	0.42
1:D:88:LYS:HA	1:D:88:LYS:HD3	1.72	0.42
1:D:451:GLU:O	1:D:455:LYS:HB3	2.19	0.42
1:C:49:MET:C	1:C:51:THR:H	2.28	0.42
1:C:223:VAL:HG12	1:C:232:ARG:HD2	2.01	0.42
1:C:10:THR:HB	1:C:315:PRO:HB3	2.02	0.42
1:D:128:GLU:O	1:D:130:VAL:HG13	2.19	0.42
1:C:299:GLY:C	1:C:307:ARG:HE	2.27	0.42
1:C:376:TYR:CZ	1:C:377:GLN:HG3	2.53	0.42
1:D:48:ALA:HB1	1:D:71:HIS:HA	2.00	0.42
1:B:162:ARG:NH2	1:B:187:GLU:HG3	2.27	0.42
1:B:192:ARG:HD3	1:B:192:ARG:HA	1.73	0.42
1:C:306:THR:O	1:C:310:THR:OG1	2.30	0.42
1:C:53:THR:O	1:C:71:HIS:HD2	2.03	0.41
1:D:223:VAL:HG12	1:D:232:ARG:CD	2.49	0.41
1:B:259:ARG:HA	1:B:259:ARG:HD2	1.84	0.41
1:D:98:VAL:O	1:D:122:PRO:HD2	2.19	0.41
1:A:9:LEU:O	1:A:315:PRO:HB2	2.20	0.41
1:D:209:ALA:HB3	1:D:211:LYS:HE3	2.01	0.41
1:C:72:LYS:HB3	1:C:222:ALA:O	2.19	0.41
1:A:347:ALA:HB1	1:A:440:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD13	1:A:24:LEU:HA	1.90	0.41
1:A:304[A]:CYS:HG	1:A:306:THR:HG22	1.85	0.41
1:B:162:ARG:HH12	1:B:187:GLU:HA	1.84	0.41
1:B:174:LEU:HD11	1:B:182:MET:HB2	2.03	0.41
1:B:62:ALA:HA	1:B:66:GLY:O	2.21	0.40
1:D:209:ALA:CB	1:D:211:LYS:HE3	2.50	0.40
1:B:87:LYS:HD3	1:B:219:VAL:HG12	2.01	0.40
1:D:248:SER:HB2	2:D:618:HOH:O	2.21	0.40
1:C:309:VAL:HG22	1:C:310:THR:HG23	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:VAL:O	1:C:343:SER:OG[3_655]	2.09	0.11
2:B:549:HOH:O	2:B:553:HOH:O[3_655]	2.17	0.03

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	423/507 (83%)	411 (97%)	10 (2%)	2 (0%)	24	29
1	B	421/507 (83%)	405 (96%)	13 (3%)	3 (1%)	18	21
1	C	331/507 (65%)	323 (98%)	8 (2%)	0	100	100
1	D	429/507 (85%)	412 (96%)	14 (3%)	3 (1%)	18	21
All	All	1604/2028 (79%)	1551 (97%)	45 (3%)	8 (0%)	24	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	D	1	MET
1	D	139	ARG
1	A	2	LEU
1	B	146	ASP
1	B	205	ARG
1	A	297	GLY
1	B	360	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	336/397 (85%)	329 (98%)	7 (2%)	47	63
1	B	334/397 (84%)	326 (98%)	8 (2%)	43	59
1	C	252/397 (64%)	241 (96%)	11 (4%)	25	35
1	D	336/397 (85%)	331 (98%)	5 (2%)	57	72
All	All	1258/1588 (79%)	1227 (98%)	31 (2%)	45	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	PHE
1	A	243	VAL
1	A	259[A]	ARG
1	A	259[B]	ARG
1	A	302	SER
1	A	304[A]	CYS
1	A	304[B]	CYS
1	B	130	VAL
1	B	148	VAL
1	B	253	SER
1	B	305	THR
1	B	340	ILE
1	B	342	PHE
1	B	419	ARG

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Mol	Chain	Res	Type
1	B	459	VAL
1	C	51	THR
1	C	171	LYS
1	C	284[A]	ARG
1	C	284[B]	ARG
1	C	305	THR
1	C	306	THR
1	C	308	ILE
1	C	309	VAL
1	C	342	PHE
1	C	430	ILE
1	C	439	SER
1	D	10	THR
1	D	36	LYS
1	D	118	PHE
1	D	140	VAL
1	D	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	188	ASN
1	A	250	HIS
1	A	432	GLN
1	A	433	GLN
1	B	26	ASN
1	B	89	HIS
1	B	208	ASN
1	B	229	ASN
1	B	258	GLN
1	B	433	GLN
1	C	0	HIS
1	C	26	ASN
1	C	63	GLN
1	C	177	ASN
1	C	214	GLN
1	D	188	ASN
1	D	229	ASN
1	D	250	HIS
1	D	433	GLN

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 oligosaccharides 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 [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	427/507 (84%)	0.28	19 (4%)	39	40	28, 44, 67, 101	9 (2%)
1	B	429/507 (84%)	0.57	33 (7%)	19	20	30, 45, 99, 126	2 (0%)
1	C	341/507 (67%)	0.56	27 (7%)	18	19	26, 47, 88, 107	3 (0%)
1	D	432/507 (85%)	0.52	27 (6%)	26	27	33, 48, 78, 115	3 (0%)
All	All	1629/2028 (80%)	0.48	106 (6%)	25	26	26, 46, 91, 126	17 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	7.2
1	D	303	ILE	6.1
1	B	140	VAL	6.0
1	D	144	ALA	5.6
1	C	0	HIS	4.7
1	C	464	ALA	4.6
1	C	183	LEU	4.3
1	A	464	ALA	4.2
1	D	140	VAL	4.1
1	B	127	GLY	4.1
1	D	384	TYR	4.0
1	B	464	ALA	4.0
1	A	142	PRO	3.9
1	D	418	GLY	3.9
1	C	109	LEU	3.8
1	D	1	MET	3.7
1	C	167	LEU	3.7
1	D	301	GLY	3.6
1	A	384	TYR	3.6
1	A	376	TYR	3.5
1	C	182	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	299	GLY	3.4
1	B	384	TYR	3.3
1	D	302	SER	3.3
1	C	418	GLY	3.3
1	D	300	PRO	3.3
1	D	127	GLY	3.2
1	D	148	VAL	3.2
1	D	125	GLU	3.1
1	D	464	ALA	3.1
1	D	304	CYS	3.1
1	B	145	GLY	3.0
1	A	306	THR	3.0
1	A	141	LYS	2.9
1	C	463	GLY	2.9
1	B	300	PRO	2.9
1	A	1	MET	2.9
1	D	26	ASN	2.9
1	B	304	CYS	2.8
1	A	300	PRO	2.8
1	C	170	MET	2.8
1	A	418	GLY	2.8
1	B	172	ALA	2.8
1	D	145	GLY	2.7
1	C	205	ARG	2.7
1	A	462	SER	2.7
1	B	302	SER	2.7
1	B	198	ARG	2.7
1	A	301	GLY	2.7
1	C	119	SER	2.6
1	A	138	LEU	2.6
1	D	463	GLY	2.6
1	C	76	ILE	2.6
1	D	227	ALA	2.6
1	C	5	ALA	2.5
1	B	175	TYR	2.5
1	B	96	ASP	2.5
1	B	187	GLU	2.5
1	C	118	PHE	2.5
1	C	168	GLU	2.5
1	C	1	MET	2.5
1	B	130	VAL	2.4
1	D	0	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	-1	SER	2.4
1	B	155	LYS	2.4
1	B	189	PHE	2.4
1	B	205	ARG	2.4
1	D	156	ASP	2.4
1	B	299	GLY	2.4
1	B	167	LEU	2.4
1	B	168	GLU	2.3
1	C	384	TYR	2.3
1	C	112	MET	2.3
1	D	306	THR	2.3
1	C	111	GLN	2.3
1	D	118	PHE	2.3
1	C	116	TYR	2.2
1	A	302	SER	2.2
1	B	200	ILE	2.2
1	C	259	ARG	2.2
1	C	379	ARG	2.2
1	D	139	ARG	2.2
1	C	117	GLY	2.2
1	A	91	SER	2.2
1	D	124	VAL	2.2
1	B	164	GLY	2.2
1	A	304[A]	CYS	2.2
1	D	205	ARG	2.1
1	A	5	ALA	2.1
1	B	88	LYS	2.1
1	D	202	LYS	2.1
1	A	140	VAL	2.1
1	A	339	GLY	2.1
1	B	119	SER	2.1
1	C	222	ALA	2.1
1	B	138	LEU	2.1
1	C	306	THR	2.1
1	B	203	ALA	2.1
1	D	2	LEU	2.1
1	B	156	ASP	2.1
1	A	83	VAL	2.1
1	B	158	LEU	2.0
1	B	197	PHE	2.0
1	B	160	THR	2.0
1	C	90	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	162	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.