



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 3SR7 / pdb_00003sr7
Title : Crystal structure of S. mutans isopentenyl pyrophosphate isomerase
Authors : Liu, Y.H.; Fu, T.M.; Liu, X.; Su, X.D.
Deposited on : 2011-07-07
Resolution : 2.04 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

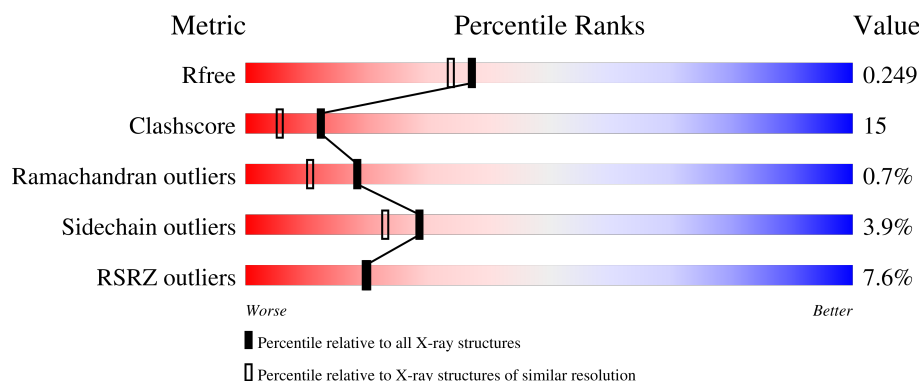
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

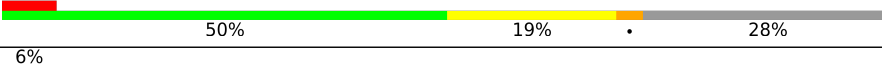
The reported resolution of this entry is 2.04 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	365	
1	B	365	
1	C	365	
1	D	365	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8467 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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2114	1358	357	389	10			
1	B	262	Total	C	N	O	S	0	0	0
			1991	1277	331	374	9			
1	C	272	Total	C	N	O	S	0	0	0
			2110	1352	366	383	9			
1	D	271	Total	C	N	O	S	0	0	0
			2094	1346	360	379	9			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP Q8DUI9
A	-32	GLY	-	expression tag	UNP Q8DUI9
A	-31	SER	-	expression tag	UNP Q8DUI9
A	-30	SER	-	expression tag	UNP Q8DUI9
A	-29	HIS	-	expression tag	UNP Q8DUI9
A	-28	HIS	-	expression tag	UNP Q8DUI9
A	-27	HIS	-	expression tag	UNP Q8DUI9
A	-26	HIS	-	expression tag	UNP Q8DUI9
A	-25	HIS	-	expression tag	UNP Q8DUI9
A	-24	HIS	-	expression tag	UNP Q8DUI9
A	-23	SER	-	expression tag	UNP Q8DUI9
A	-22	SER	-	expression tag	UNP Q8DUI9
A	-21	GLY	-	expression tag	UNP Q8DUI9
A	-20	LEU	-	expression tag	UNP Q8DUI9
A	-19	VAL	-	expression tag	UNP Q8DUI9
A	-18	PRO	-	expression tag	UNP Q8DUI9
A	-17	ARG	-	expression tag	UNP Q8DUI9
A	-16	GLY	-	expression tag	UNP Q8DUI9
A	-15	SER	-	expression tag	UNP Q8DUI9
A	-14	HIS	-	expression tag	UNP Q8DUI9
A	-13	MET	-	expression tag	UNP Q8DUI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP Q8DUI9
A	-11	SER	-	expression tag	UNP Q8DUI9
A	-10	MET	-	expression tag	UNP Q8DUI9
A	-9	THR	-	expression tag	UNP Q8DUI9
A	-8	GLY	-	expression tag	UNP Q8DUI9
A	-7	GLY	-	expression tag	UNP Q8DUI9
A	-6	GLN	-	expression tag	UNP Q8DUI9
A	-5	GLN	-	expression tag	UNP Q8DUI9
A	-4	MET	-	expression tag	UNP Q8DUI9
A	-3	GLY	-	expression tag	UNP Q8DUI9
A	-2	ARG	-	expression tag	UNP Q8DUI9
A	-1	GLY	-	expression tag	UNP Q8DUI9
A	0	SER	-	expression tag	UNP Q8DUI9
B	-33	MET	-	expression tag	UNP Q8DUI9
B	-32	GLY	-	expression tag	UNP Q8DUI9
B	-31	SER	-	expression tag	UNP Q8DUI9
B	-30	SER	-	expression tag	UNP Q8DUI9
B	-29	HIS	-	expression tag	UNP Q8DUI9
B	-28	HIS	-	expression tag	UNP Q8DUI9
B	-27	HIS	-	expression tag	UNP Q8DUI9
B	-26	HIS	-	expression tag	UNP Q8DUI9
B	-25	HIS	-	expression tag	UNP Q8DUI9
B	-24	HIS	-	expression tag	UNP Q8DUI9
B	-23	SER	-	expression tag	UNP Q8DUI9
B	-22	SER	-	expression tag	UNP Q8DUI9
B	-21	GLY	-	expression tag	UNP Q8DUI9
B	-20	LEU	-	expression tag	UNP Q8DUI9
B	-19	VAL	-	expression tag	UNP Q8DUI9
B	-18	PRO	-	expression tag	UNP Q8DUI9
B	-17	ARG	-	expression tag	UNP Q8DUI9
B	-16	GLY	-	expression tag	UNP Q8DUI9
B	-15	SER	-	expression tag	UNP Q8DUI9
B	-14	HIS	-	expression tag	UNP Q8DUI9
B	-13	MET	-	expression tag	UNP Q8DUI9
B	-12	ALA	-	expression tag	UNP Q8DUI9
B	-11	SER	-	expression tag	UNP Q8DUI9
B	-10	MET	-	expression tag	UNP Q8DUI9
B	-9	THR	-	expression tag	UNP Q8DUI9
B	-8	GLY	-	expression tag	UNP Q8DUI9
B	-7	GLY	-	expression tag	UNP Q8DUI9
B	-6	GLN	-	expression tag	UNP Q8DUI9
B	-5	GLN	-	expression tag	UNP Q8DUI9

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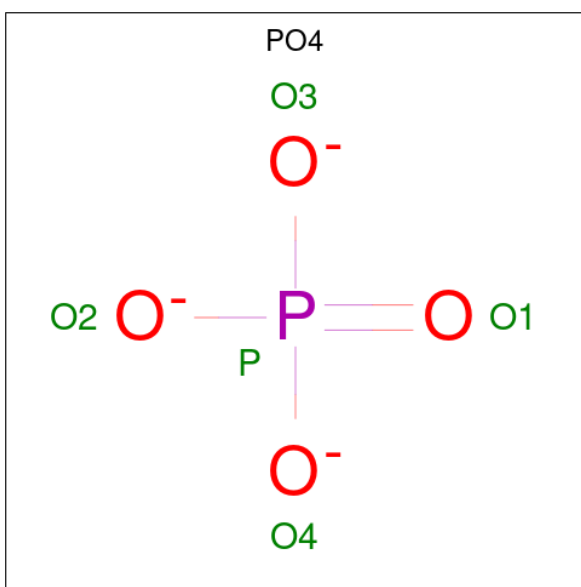
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP Q8DUI9
B	-3	GLY	-	expression tag	UNP Q8DUI9
B	-2	ARG	-	expression tag	UNP Q8DUI9
B	-1	GLY	-	expression tag	UNP Q8DUI9
B	0	SER	-	expression tag	UNP Q8DUI9
C	-33	MET	-	expression tag	UNP Q8DUI9
C	-32	GLY	-	expression tag	UNP Q8DUI9
C	-31	SER	-	expression tag	UNP Q8DUI9
C	-30	SER	-	expression tag	UNP Q8DUI9
C	-29	HIS	-	expression tag	UNP Q8DUI9
C	-28	HIS	-	expression tag	UNP Q8DUI9
C	-27	HIS	-	expression tag	UNP Q8DUI9
C	-26	HIS	-	expression tag	UNP Q8DUI9
C	-25	HIS	-	expression tag	UNP Q8DUI9
C	-24	HIS	-	expression tag	UNP Q8DUI9
C	-23	SER	-	expression tag	UNP Q8DUI9
C	-22	SER	-	expression tag	UNP Q8DUI9
C	-21	GLY	-	expression tag	UNP Q8DUI9
C	-20	LEU	-	expression tag	UNP Q8DUI9
C	-19	VAL	-	expression tag	UNP Q8DUI9
C	-18	PRO	-	expression tag	UNP Q8DUI9
C	-17	ARG	-	expression tag	UNP Q8DUI9
C	-16	GLY	-	expression tag	UNP Q8DUI9
C	-15	SER	-	expression tag	UNP Q8DUI9
C	-14	HIS	-	expression tag	UNP Q8DUI9
C	-13	MET	-	expression tag	UNP Q8DUI9
C	-12	ALA	-	expression tag	UNP Q8DUI9
C	-11	SER	-	expression tag	UNP Q8DUI9
C	-10	MET	-	expression tag	UNP Q8DUI9
C	-9	THR	-	expression tag	UNP Q8DUI9
C	-8	GLY	-	expression tag	UNP Q8DUI9
C	-7	GLY	-	expression tag	UNP Q8DUI9
C	-6	GLN	-	expression tag	UNP Q8DUI9
C	-5	GLN	-	expression tag	UNP Q8DUI9
C	-4	MET	-	expression tag	UNP Q8DUI9
C	-3	GLY	-	expression tag	UNP Q8DUI9
C	-2	ARG	-	expression tag	UNP Q8DUI9
C	-1	GLY	-	expression tag	UNP Q8DUI9
C	0	SER	-	expression tag	UNP Q8DUI9
D	-33	MET	-	expression tag	UNP Q8DUI9
D	-32	GLY	-	expression tag	UNP Q8DUI9
D	-31	SER	-	expression tag	UNP Q8DUI9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	expression tag	UNP Q8DUI9
D	-29	HIS	-	expression tag	UNP Q8DUI9
D	-28	HIS	-	expression tag	UNP Q8DUI9
D	-27	HIS	-	expression tag	UNP Q8DUI9
D	-26	HIS	-	expression tag	UNP Q8DUI9
D	-25	HIS	-	expression tag	UNP Q8DUI9
D	-24	HIS	-	expression tag	UNP Q8DUI9
D	-23	SER	-	expression tag	UNP Q8DUI9
D	-22	SER	-	expression tag	UNP Q8DUI9
D	-21	GLY	-	expression tag	UNP Q8DUI9
D	-20	LEU	-	expression tag	UNP Q8DUI9
D	-19	VAL	-	expression tag	UNP Q8DUI9
D	-18	PRO	-	expression tag	UNP Q8DUI9
D	-17	ARG	-	expression tag	UNP Q8DUI9
D	-16	GLY	-	expression tag	UNP Q8DUI9
D	-15	SER	-	expression tag	UNP Q8DUI9
D	-14	HIS	-	expression tag	UNP Q8DUI9
D	-13	MET	-	expression tag	UNP Q8DUI9
D	-12	ALA	-	expression tag	UNP Q8DUI9
D	-11	SER	-	expression tag	UNP Q8DUI9
D	-10	MET	-	expression tag	UNP Q8DUI9
D	-9	THR	-	expression tag	UNP Q8DUI9
D	-8	GLY	-	expression tag	UNP Q8DUI9
D	-7	GLY	-	expression tag	UNP Q8DUI9
D	-6	GLN	-	expression tag	UNP Q8DUI9
D	-5	GLN	-	expression tag	UNP Q8DUI9
D	-4	MET	-	expression tag	UNP Q8DUI9
D	-3	GLY	-	expression tag	UNP Q8DUI9
D	-2	ARG	-	expression tag	UNP Q8DUI9
D	-1	GLY	-	expression tag	UNP Q8DUI9
D	0	SER	-	expression tag	UNP Q8DUI9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		

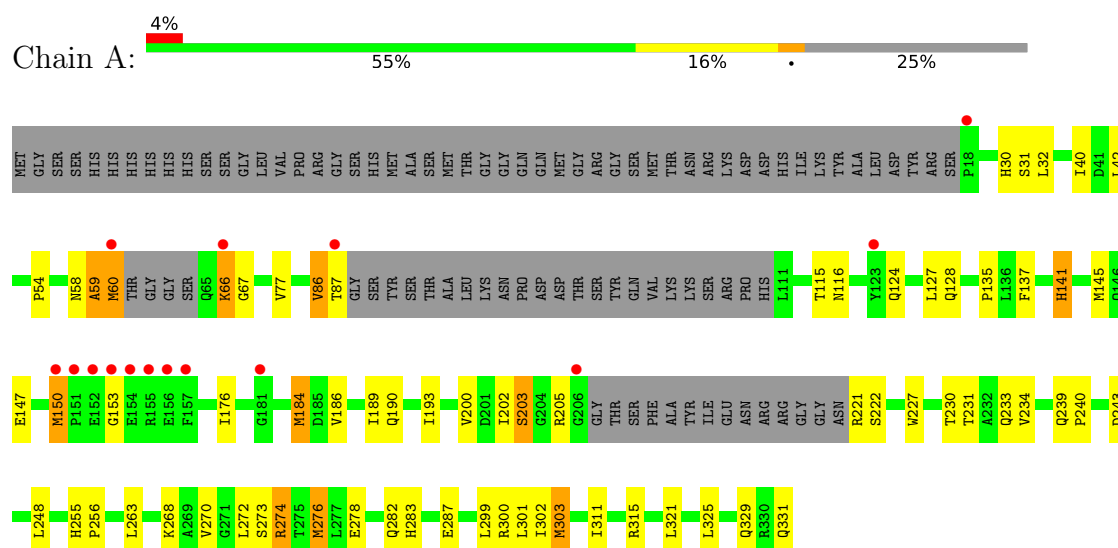
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	31	Total	O	0	0
			31	31		
3	C	42	Total	O	0	0
			42	42		
3	D	30	Total	O	0	0
			30	30		

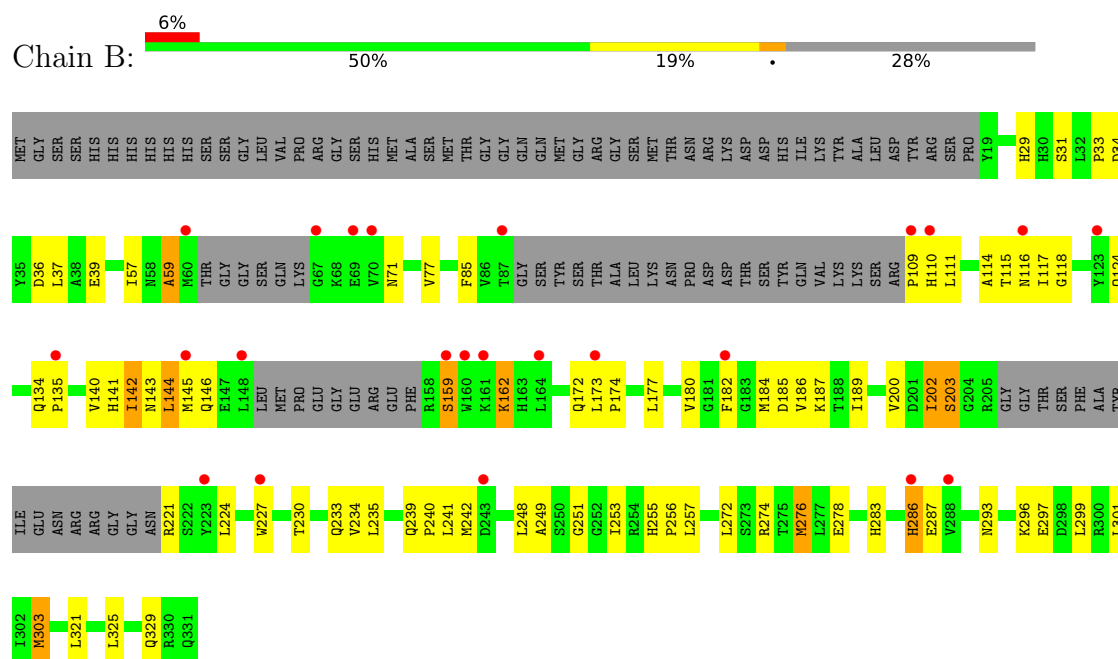
3 Residue-property plots [i](#)

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.

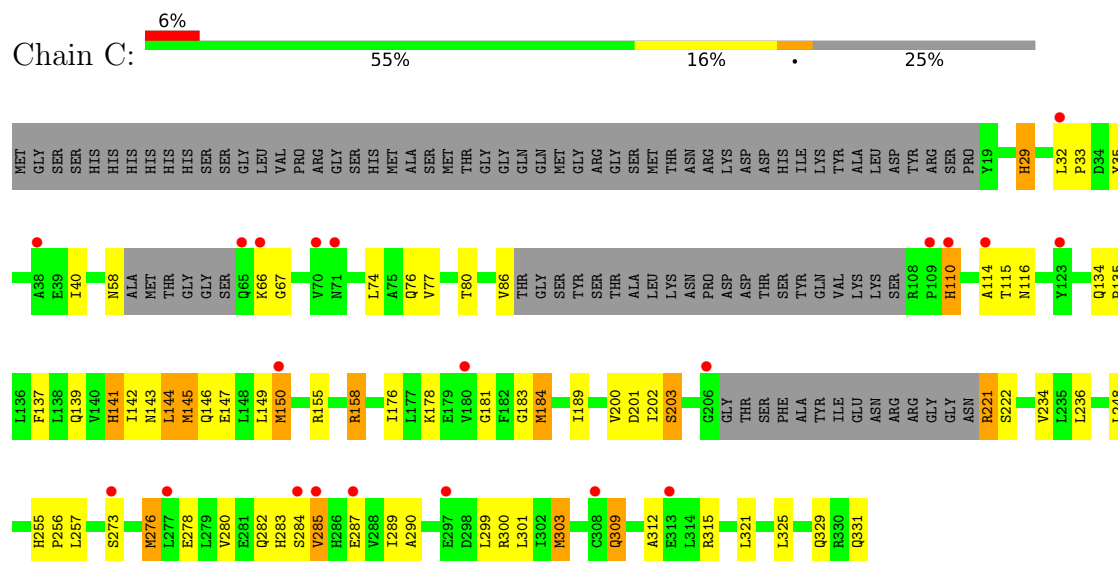
- Molecule 1: Isopentenyl-diphosphate delta-isomerase



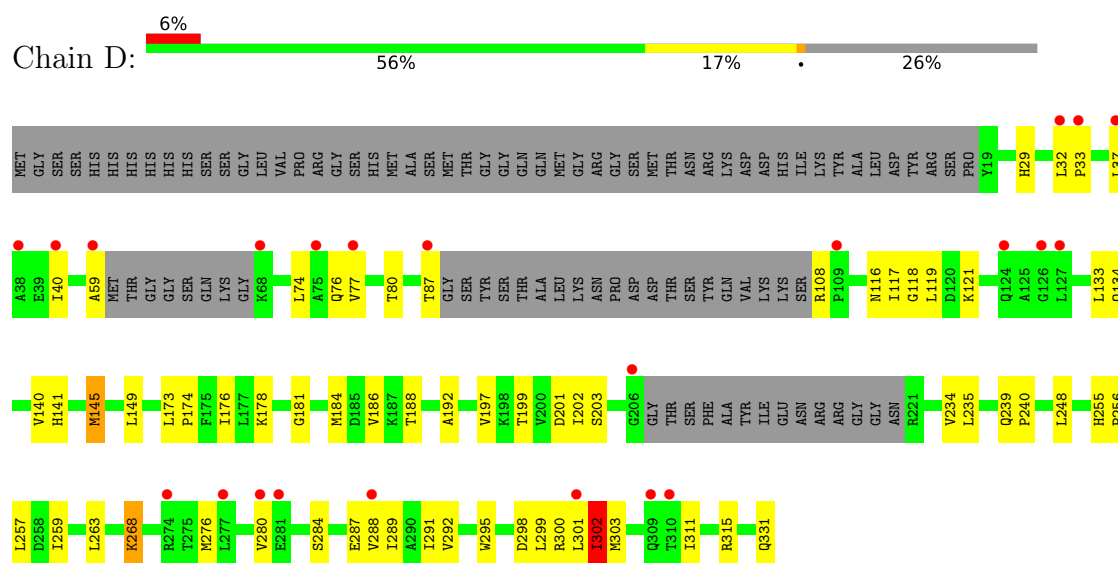
- Molecule 1: Isopentenyl-diphosphate delta-isomerase



• Molecule 1: Isopentenyl-diphosphate delta-isomerase



• Molecule 1: Isopentenyl-diphosphate delta-isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 76.42Å 92.53Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	41.92 – 2.04 41.92 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.92-2.04) 98.0 (41.92-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.285 0.245 , 0.249	Depositor DCC
R_{free} test set	3727 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	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	0.94	EDS
Total number of atoms	8467	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4893e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4

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	0.84	5/2151 (0.2%)	0.82	1/2916 (0.0%)
1	B	0.73	3/2024 (0.1%)	0.87	5/2749 (0.2%)
1	C	0.71	5/2147 (0.2%)	0.83	3/2909 (0.1%)
1	D	0.67	3/2132 (0.1%)	0.85	3/2891 (0.1%)
All	All	0.74	16/8454 (0.2%)	0.84	12/11465 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	MET	SD-CE	-10.85	1.52	1.79
1	C	184	MET	SD-CE	-8.87	1.57	1.79
1	D	184	MET	SD-CE	-7.95	1.59	1.79
1	A	303	MET	SD-CE	-7.73	1.60	1.79
1	A	276	MET	SD-CE	-6.96	1.62	1.79
1	D	145	MET	SD-CE	-6.76	1.62	1.79
1	B	303	MET	SD-CE	-6.71	1.62	1.79
1	C	145	MET	SD-CE	-6.64	1.62	1.79
1	A	302	ILE	C-O	-6.12	1.17	1.24
1	C	303	MET	SD-CE	-6.11	1.64	1.79
1	B	276	MET	SD-CE	-5.45	1.66	1.79
1	A	145	MET	SD-CE	-5.42	1.66	1.79
1	B	242	MET	SD-CE	-5.31	1.66	1.79
1	C	144	LEU	C-O	-5.30	1.17	1.24
1	C	276	MET	SD-CE	-5.12	1.66	1.79
1	D	302	ILE	C-O	-5.04	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	CA-C-N	-6.99	108.33	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	C-N-CA	-6.99	108.33	122.31
1	B	221	ARG	O-C-N	5.94	132.51	123.00
1	B	146	GLN	N-CA-C	-5.73	105.04	111.28
1	C	181	GLY	N-CA-C	5.58	121.33	114.69
1	D	181	GLY	N-CA-C	5.56	121.70	115.08
1	A	59	ALA	N-CA-C	5.43	117.54	110.43
1	C	32	LEU	CA-C-N	5.37	125.27	119.85
1	C	32	LEU	C-N-CA	5.37	125.27	119.85
1	D	32	LEU	CA-C-N	5.26	126.42	119.84
1	D	32	LEU	C-N-CA	5.26	126.42	119.84
1	B	59	ALA	N-CA-C	5.12	117.14	110.43

There are no chirality outliers.

There are no planarity outliers.

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	2114	0	2100	73	0
1	B	1991	0	1937	64	0
1	C	2110	0	2096	72	0
1	D	2094	0	2073	63	0
2	C	5	0	0	0	0
3	A	50	0	0	2	0
3	B	31	0	0	0	0
3	C	42	0	0	1	0
3	D	30	0	0	1	0
All	All	8467	0	8206	254	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 15.

All (254) 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:145:MET:CE	1:C:149:LEU:HG	1.71	1.19
1:D:145:MET:HE3	1:D:149:LEU:HG	1.23	1.16
1:A:184:MET:HE2	1:A:189:ILE:HG12	1.13	1.12
1:D:299:LEU:O	1:D:303:MET:HG3	1.51	1.10
1:D:145:MET:CE	1:D:149:LEU:HG	1.82	1.08
1:C:184:MET:HE2	1:C:189:ILE:HG12	1.27	1.08
1:B:116:ASN:HD21	1:B:141:HIS:CD2	1.71	1.07
1:B:184:MET:HE2	1:B:189:ILE:HG12	1.35	1.07
1:C:145:MET:HE3	1:C:149:LEU:HG	1.34	1.05
1:A:221:ARG:HG2	1:A:222:SER:H	1.23	1.02
1:A:184:MET:HE2	1:A:189:ILE:CG1	1.89	1.02
1:C:145:MET:CE	1:C:149:LEU:CG	2.45	0.95
1:D:145:MET:CE	1:D:149:LEU:CG	2.47	0.93
1:D:116:ASN:HD21	1:D:141:HIS:HD2	1.16	0.92
1:B:116:ASN:HD21	1:B:141:HIS:HD2	1.05	0.90
1:A:60:MET:HA	1:A:60:MET:CE	2.02	0.89
1:A:116:ASN:HD21	1:A:141:HIS:HD2	1.15	0.89
1:A:184:MET:CE	1:A:189:ILE:HG12	2.03	0.88
1:D:116:ASN:HD21	1:D:141:HIS:CD2	1.92	0.85
1:D:145:MET:HE3	1:D:149:LEU:CG	2.03	0.85
1:A:116:ASN:HD21	1:A:141:HIS:CD2	1.93	0.85
1:B:272:LEU:HD12	1:B:276:MET:HE2	1.57	0.85
1:C:145:MET:HE2	1:C:149:LEU:HD11	1.59	0.84
1:D:145:MET:HE2	1:D:149:LEU:HD11	1.60	0.82
1:A:321:LEU:H	1:D:331:GLN:HE22	1.29	0.80
1:B:299:LEU:O	1:B:303:MET:HG3	1.82	0.80
1:A:60:MET:CA	1:A:60:MET:HE3	2.12	0.80
1:C:145:MET:HE2	1:C:149:LEU:CD1	2.13	0.78
1:B:321:LEU:H	1:C:331:GLN:HE22	1.31	0.78
1:C:66:LYS:N	1:C:67:GLY:HA3	1.99	0.78
1:C:116:ASN:HD21	1:C:141:HIS:CD2	2.02	0.78
1:C:147:GLU:HA	1:C:150:MET:HE2	1.66	0.77
1:B:116:ASN:ND2	1:B:141:HIS:HD2	1.81	0.77
1:A:60:MET:HE3	1:A:60:MET:N	2.02	0.75
1:A:60:MET:CE	1:A:60:MET:CA	2.66	0.73
1:A:329:GLN:HB3	3:A:376:HOH:O	1.89	0.73
1:A:272:LEU:CD1	1:A:276:MET:CE	2.66	0.73
1:A:60:MET:HA	1:A:60:MET:HE2	1.70	0.72
1:A:272:LEU:HD12	1:A:276:MET:CE	2.18	0.72
1:B:272:LEU:CD1	1:B:276:MET:HE2	2.20	0.72
1:B:31:SER:HB3	1:C:142:ILE:HD12	1.71	0.72
1:C:116:ASN:HD21	1:C:141:HIS:HD2	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD22	1:D:33:PRO:HD3	1.73	0.70
1:D:288:VAL:HA	1:D:291:ILE:HD12	1.72	0.70
1:A:331:GLN:HE22	1:C:321:LEU:H	1.40	0.70
1:D:145:MET:CE	1:D:149:LEU:CD1	2.69	0.70
1:C:184:MET:CE	1:C:189:ILE:HG12	2.16	0.69
1:D:202:ILE:HD13	1:D:234:VAL:CG2	2.22	0.69
1:B:145:MET:HE3	1:B:145:MET:O	1.94	0.68
1:A:60:MET:HA	1:A:60:MET:HE3	1.74	0.68
1:A:221:ARG:HG2	1:A:222:SER:N	2.01	0.68
1:C:76:GLN:HG2	1:C:285:VAL:HG11	1.76	0.67
1:A:116:ASN:ND2	1:A:141:HIS:HD2	1.91	0.67
1:D:202:ILE:HD13	1:D:234:VAL:HG23	1.77	0.66
1:C:86:VAL:HG22	1:C:114:ALA:HB3	1.78	0.65
1:B:180:VAL:HG12	1:B:180:VAL:O	1.96	0.65
1:A:137:PHE:CE1	1:A:176:ILE:HD12	2.33	0.64
1:D:255:HIS:HB2	1:D:256:PRO:HD2	1.80	0.64
1:D:145:MET:CE	1:D:149:LEU:HD11	2.28	0.63
1:C:178:LYS:HG3	1:C:201:ASP:HB3	1.80	0.63
1:C:137:PHE:CE1	1:C:176:ILE:HD12	2.34	0.63
1:A:40:ILE:O	1:A:300:ARG:NH1	2.32	0.63
1:C:145:MET:HE2	1:C:149:LEU:CG	2.23	0.62
1:D:119:LEU:HD13	1:D:140:VAL:HG21	1.81	0.62
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.65	0.62
1:D:59:ALA:HB3	1:D:87:THR:C	2.25	0.62
1:A:221:ARG:CG	1:A:222:SER:H	2.05	0.62
1:D:255:HIS:HB2	1:D:256:PRO:CD	2.31	0.61
1:A:87:THR:OG1	1:A:115:THR:HA	2.01	0.60
1:B:34:ASP:O	1:C:158:ARG:HD3	2.01	0.60
1:B:325:LEU:O	1:B:329:GLN:HG2	2.02	0.60
1:A:255:HIS:HB2	1:A:256:PRO:CD	2.31	0.59
1:D:145:MET:HE2	1:D:149:LEU:CD1	2.29	0.59
1:C:221:ARG:CZ	1:C:221:ARG:HA	2.33	0.58
1:A:272:LEU:HD13	1:A:276:MET:HE2	1.85	0.58
1:B:272:LEU:HD12	1:B:276:MET:CE	2.29	0.58
1:C:145:MET:CE	1:C:149:LEU:CD1	2.79	0.58
1:C:184:MET:HE1	1:C:200:VAL:HG11	1.85	0.58
1:D:76:GLN:CD	1:D:108:ARG:HH12	2.11	0.58
1:A:30:HIS:CE1	1:A:32:LEU:O	2.57	0.58
1:A:58:ASN:HA	1:A:86:VAL:O	2.04	0.57
1:A:184:MET:CE	1:A:189:ILE:CG1	2.73	0.57
1:C:80:THR:HG21	1:C:289:ILE:HD13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:CD1	1:A:276:MET:HE2	2.34	0.57
1:C:35:TYR:CD1	1:C:309:GLN:HG3	2.40	0.57
1:B:109:PRO:O	1:B:110:HIS:HB2	2.05	0.57
1:C:184:MET:HE2	1:C:189:ILE:CG1	2.18	0.57
1:A:233:GLN:HE22	1:A:329:GLN:HE22	1.53	0.56
1:A:255:HIS:HB2	1:A:256:PRO:HD2	1.88	0.56
1:C:147:GLU:HA	1:C:150:MET:CE	2.34	0.56
1:C:221:ARG:HD3	1:C:222:SER:H	1.71	0.56
1:C:312:ALA:O	1:C:315:ARG:HG3	2.06	0.56
1:A:272:LEU:HD13	1:A:276:MET:CE	2.34	0.55
1:A:283:HIS:HB3	1:A:287:GLU:HB2	1.87	0.55
1:B:321:LEU:H	1:C:331:GLN:NE2	2.01	0.55
1:A:299:LEU:O	1:A:303:MET:HG3	2.06	0.55
1:D:76:GLN:NE2	1:D:108:ARG:HH12	2.05	0.55
1:C:145:MET:HE1	1:C:149:LEU:HG	1.79	0.54
1:C:299:LEU:O	1:C:303:MET:HG3	2.07	0.54
1:B:184:MET:HE1	1:B:200:VAL:HG11	1.89	0.54
1:B:57:ILE:HG13	1:B:276:MET:HE3	1.88	0.53
1:A:66:LYS:N	1:A:67:GLY:HA3	2.23	0.53
1:C:74:LEU:O	1:C:77:VAL:HG22	2.06	0.53
1:D:145:MET:HE1	1:D:149:LEU:CD2	2.38	0.53
1:A:202:ILE:HD13	1:A:234:VAL:HG23	1.90	0.53
1:B:255:HIS:HB2	1:B:256:PRO:CD	2.38	0.53
1:B:301:LEU:C	1:B:301:LEU:HD23	2.33	0.53
1:B:173:LEU:HD12	1:B:174:PRO:HD2	1.90	0.53
1:C:284:SER:O	1:C:285:VAL:C	2.51	0.53
1:D:118:GLY:HA2	1:D:141:HIS:CE1	2.45	0.52
1:A:321:LEU:H	1:D:331:GLN:NE2	2.02	0.52
1:B:255:HIS:HB2	1:B:256:PRO:HD2	1.91	0.52
1:A:243:ASP:OD1	1:A:243:ASP:N	2.30	0.52
1:D:284:SER:OG	1:D:287:GLU:HG3	2.08	0.52
1:A:202:ILE:HD13	1:A:234:VAL:CG2	2.39	0.52
1:B:115:THR:HG22	1:B:135:PRO:HG3	1.90	0.52
1:C:74:LEU:HD21	1:C:276:MET:HB3	1.91	0.52
1:C:115:THR:HG22	1:C:135:PRO:HG3	1.92	0.51
1:A:331:GLN:NE2	1:C:321:LEU:H	2.08	0.51
1:D:145:MET:HE1	1:D:149:LEU:HD21	1.93	0.51
1:B:230:THR:H	1:B:233:GLN:HE21	1.57	0.51
1:B:142:ILE:HD13	1:B:177:LEU:HD11	1.92	0.51
1:D:145:MET:HE1	1:D:149:LEU:HG	1.83	0.51
1:B:286:HIS:C	1:B:286:HIS:CD2	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ASN:ND2	1:D:141:HIS:HD2	1.97	0.51
1:C:255:HIS:HB2	1:C:256:PRO:HD2	1.93	0.51
1:D:145:MET:HE1	1:D:149:LEU:CG	2.38	0.50
1:B:182:PHE:CD1	1:B:227:TRP:HD1	2.29	0.50
1:D:80:THR:HG21	1:D:289:ILE:HD13	1.94	0.50
1:D:268:LYS:HE3	3:D:353:HOH:O	2.10	0.50
1:B:186:VAL:HG13	1:B:241:LEU:HD11	1.93	0.50
1:D:284:SER:HG	1:D:287:GLU:HG3	1.76	0.50
1:A:42:LEU:O	1:A:54:PRO:HD3	2.11	0.50
1:A:30:HIS:HE1	1:A:32:LEU:O	1.94	0.50
1:B:184:MET:CE	1:B:189:ILE:HG12	2.24	0.49
1:B:274:ARG:O	1:B:278:GLU:HG3	2.12	0.49
1:A:147:GLU:HA	1:A:150:MET:HE2	1.94	0.49
1:A:301:LEU:C	1:A:301:LEU:HD23	2.37	0.49
1:A:272:LEU:HD12	1:A:276:MET:HE3	1.94	0.49
1:A:278:GLU:O	1:A:282:GLN:HG2	2.13	0.49
1:D:263:LEU:HD13	1:D:311:ILE:HD12	1.95	0.49
1:C:255:HIS:HB2	1:C:256:PRO:CD	2.43	0.48
1:D:276:MET:O	1:D:280:VAL:HG22	2.12	0.48
1:B:59:ALA:HB2	1:B:85:PHE:CZ	2.48	0.48
1:C:325:LEU:O	1:C:329:GLN:HG2	2.13	0.48
1:B:185:ASP:OD2	1:B:187:LYS:HB2	2.12	0.48
1:D:121:LYS:HD2	1:D:121:LYS:N	2.27	0.48
1:D:145:MET:HE3	1:D:149:LEU:CD1	2.40	0.48
1:B:255:HIS:CE1	1:B:257:LEU:HB3	2.49	0.48
1:C:139:GLN:NE2	1:C:178:LYS:HD2	2.28	0.48
1:A:124:GLN:O	1:A:128:GLN:HG3	2.14	0.48
1:A:274:ARG:NH1	1:A:274:ARG:HG2	2.28	0.48
1:D:133:LEU:O	1:D:134:GLN:C	2.56	0.48
1:A:184:MET:HE1	1:A:200:VAL:HG11	1.96	0.48
1:D:255:HIS:CE1	1:D:257:LEU:HB3	2.48	0.48
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.78	0.47
1:B:118:GLY:HA2	1:B:141:HIS:CE1	2.49	0.47
1:D:284:SER:O	1:D:288:VAL:HG23	2.14	0.47
1:D:176:ILE:HG12	1:D:199:THR:HB	1.95	0.47
1:C:202:ILE:C	1:C:202:ILE:HD12	2.39	0.47
1:C:29:HIS:C	1:C:29:HIS:CD2	2.90	0.47
1:C:145:MET:HE3	1:C:149:LEU:CG	2.22	0.47
1:C:276:MET:O	1:C:280:VAL:HG22	2.15	0.47
1:D:287:GLU:O	1:D:291:ILE:HG13	2.15	0.47
1:C:202:ILE:O	1:C:203:SER:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:N	1:A:240:PRO:CD	2.78	0.47
1:B:235:LEU:HD21	1:B:249:ALA:HB2	1.96	0.46
1:C:110:HIS:ND1	1:C:110:HIS:N	2.62	0.46
1:A:205:ARG:O	1:A:230:THR:HA	2.16	0.46
1:B:143:ASN:O	1:B:144:LEU:C	2.56	0.46
1:C:301:LEU:C	1:C:301:LEU:HD23	2.40	0.46
1:D:173:LEU:HD12	1:D:174:PRO:HD2	1.98	0.46
1:A:263:LEU:HD13	1:A:311:ILE:HD12	1.98	0.46
1:B:202:ILE:HD12	1:B:202:ILE:HA	1.78	0.46
1:B:37:LEU:HD23	1:C:155:ARG:HD2	1.96	0.46
1:B:184:MET:CE	1:B:189:ILE:HA	2.46	0.45
1:C:282:GLN:O	1:C:283:HIS:CG	2.70	0.45
1:D:40:ILE:HG21	1:D:300:ARG:HA	1.98	0.45
1:D:192:ALA:HB1	1:D:197:VAL:HB	1.97	0.45
1:B:227:TRP:HZ2	1:D:29:HIS:HB2	1.80	0.45
1:B:57:ILE:HD12	1:B:57:ILE:N	2.32	0.45
1:D:40:ILE:O	1:D:300:ARG:NH1	2.49	0.45
1:D:117:ILE:O	1:D:140:VAL:HA	2.16	0.45
1:D:202:ILE:HD13	1:D:234:VAL:HG21	1.98	0.45
1:C:287:GLU:O	1:C:290:ALA:HB3	2.17	0.45
1:A:31:SER:HB2	1:D:188:THR:HG21	1.99	0.45
1:B:59:ALA:HB1	1:B:71:ASN:OD1	2.17	0.45
1:B:230:THR:H	1:B:233:GLN:NE2	2.14	0.45
1:A:87:THR:O	1:A:87:THR:HG23	2.16	0.45
1:C:202:ILE:HD13	1:C:234:VAL:CG2	2.46	0.45
1:B:114:ALA:HA	1:B:135:PRO:HB2	1.98	0.45
1:B:251:GLY:O	1:B:253:ILE:HD12	2.17	0.45
1:A:141:HIS:ND1	1:A:141:HIS:C	2.75	0.44
1:C:33:PRO:HA	3:C:374:HOH:O	2.17	0.44
1:A:190:GLN:NE2	1:A:193:ILE:HB	2.33	0.44
1:B:31:SER:HB3	1:C:142:ILE:CD1	2.46	0.44
1:B:184:MET:HE3	1:B:189:ILE:HA	1.99	0.44
1:A:59:ALA:N	1:A:86:VAL:O	2.40	0.44
1:B:36:ASP:O	1:B:39:GLU:HG2	2.18	0.44
1:C:284:SER:O	1:C:287:GLU:N	2.50	0.44
1:C:278:GLU:O	1:C:282:GLN:HG2	2.18	0.44
1:B:29:HIS:HD2	1:C:183:GLY:O	2.01	0.44
1:B:184:MET:HB3	1:B:202:ILE:CD1	2.47	0.44
1:C:221:ARG:HA	1:C:221:ARG:NE	2.32	0.44
1:D:298:ASP:O	1:D:302:ILE:HG12	2.18	0.44
1:D:239:GLN:N	1:D:240:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:LEU:HD23	1:D:301:LEU:C	2.43	0.43
1:A:227:TRP:NE1	1:C:29:HIS:HB2	2.32	0.43
1:C:202:ILE:HD12	1:C:203:SER:N	2.33	0.43
1:A:221:ARG:HH11	1:A:221:ARG:CG	2.31	0.43
1:B:202:ILE:HG23	1:B:234:VAL:CG2	2.49	0.43
1:D:74:LEU:HA	1:D:77:VAL:HG22	1.99	0.43
1:B:145:MET:HE3	1:B:145:MET:C	2.44	0.43
1:D:315:ARG:CZ	1:D:315:ARG:CB	2.97	0.43
1:A:184:MET:CE	1:A:189:ILE:HA	2.49	0.42
1:C:116:ASN:ND2	1:C:141:HIS:HD2	2.11	0.42
1:A:227:TRP:CE2	1:C:29:HIS:HB2	2.54	0.42
1:A:325:LEU:HD12	1:A:325:LEU:HA	1.84	0.42
1:C:143:ASN:HB2	1:C:146:GLN:HB3	2.00	0.42
1:A:268:LYS:HE2	3:A:378:HOH:O	2.20	0.42
1:B:33:PRO:HB3	1:C:144:LEU:HD22	2.01	0.42
1:C:236:LEU:HD13	1:C:329:GLN:HG3	2.01	0.42
1:D:202:ILE:HD12	1:D:202:ILE:C	2.45	0.42
1:A:87:THR:O	1:A:87:THR:CG2	2.68	0.42
1:C:178:LYS:HG3	1:C:201:ASP:CB	2.47	0.42
1:D:292:VAL:O	1:D:295:TRP:HB2	2.20	0.42
1:A:315:ARG:HE	1:A:315:ARG:HB2	1.46	0.42
1:A:202:ILE:O	1:A:203:SER:C	2.63	0.41
1:B:202:ILE:O	1:B:203:SER:C	2.62	0.41
1:A:273:SER:OG	1:A:274:ARG:N	2.53	0.41
1:B:184:MET:HE2	1:B:189:ILE:CG1	2.26	0.41
1:C:58:ASN:HB2	1:C:273:SER:OG	2.20	0.41
1:A:231:THR:O	1:A:234:VAL:HG22	2.20	0.41
1:B:159:SER:O	1:B:162:LYS:HB3	2.20	0.41
1:B:239:GLN:N	1:B:240:PRO:CD	2.83	0.41
1:C:134:GLN:N	1:C:135:PRO:CD	2.84	0.41
1:C:221:ARG:HH21	1:C:222:SER:N	2.19	0.41
1:A:147:GLU:OE1	1:A:153:GLY:HA2	2.20	0.41
1:B:224:LEU:O	1:B:227:TRP:HB2	2.21	0.41
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.90	0.41
1:B:117:ILE:HG22	1:B:140:VAL:HG12	2.02	0.41
1:B:143:ASN:OD1	1:B:143:ASN:N	2.53	0.41
1:C:255:HIS:CE1	1:C:257:LEU:HB3	2.56	0.41
1:D:118:GLY:CA	1:D:141:HIS:CE1	3.03	0.41
1:D:140:VAL:O	1:D:140:VAL:HG13	2.21	0.41
1:B:124:GLN:H	1:B:124:GLN:CD	2.27	0.41
1:B:293:ASN:O	1:B:296:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:O	1:C:300:ARG:NH1	2.54	0.41
1:D:256:PRO:HA	1:D:259:ILE:HD12	2.01	0.41
1:A:227:TRP:CZ2	1:C:29:HIS:HB2	2.56	0.40
1:D:141:HIS:HA	1:D:178:LYS:O	2.21	0.40
1:B:283:HIS:HB3	1:B:287:GLU:HB2	2.03	0.40
1:A:115:THR:HG22	1:A:135:PRO:HG3	2.03	0.40
1:D:178:LYS:HG3	1:D:201:ASP:HB3	2.02	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	265/365 (73%)	252 (95%)	11 (4%)	2 (1%)	16	9
1	B	252/365 (69%)	242 (96%)	8 (3%)	2 (1%)	16	9
1	C	264/365 (72%)	251 (95%)	11 (4%)	2 (1%)	16	9
1	D	263/365 (72%)	252 (96%)	10 (4%)	1 (0%)	30	22
All	All	1044/1460 (72%)	997 (96%)	40 (4%)	7 (1%)	18	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	SER
1	C	203	SER
1	D	203	SER
1	A	66	LYS
1	A	203	SER
1	B	144	LEU
1	C	285	VAL

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	223/310 (72%)	213 (96%)	10 (4%)	24	18
1	B	207/310 (67%)	196 (95%)	11 (5%)	20	13
1	C	221/310 (71%)	213 (96%)	8 (4%)	31	26
1	D	217/310 (70%)	212 (98%)	5 (2%)	44	42
All	All	868/1240 (70%)	834 (96%)	34 (4%)	28	23

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	MET
1	A	77	VAL
1	A	86	VAL
1	A	127	LEU
1	A	141	HIS
1	A	150	MET
1	A	186	VAL
1	A	248	LEU
1	A	270	VAL
1	A	274	ARG
1	B	77	VAL
1	B	111	LEU
1	B	134	GLN
1	B	142	ILE
1	B	159	SER
1	B	162	LYS
1	B	172	GLN
1	B	202	ILE
1	B	248	LEU
1	B	286	HIS
1	B	297	GLU
1	C	29	HIS
1	C	110	HIS
1	C	141	HIS

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Mol	Chain	Res	Type
1	C	150	MET
1	C	158	ARG
1	C	221	ARG
1	C	248	LEU
1	C	309	GLN
1	D	37	LEU
1	D	186	VAL
1	D	248	LEU
1	D	268	LYS
1	D	302	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	139	GLN
1	A	141	HIS
1	A	172	GLN
1	A	190	GLN
1	A	329	GLN
1	A	331	GLN
1	B	29	HIS
1	B	30	HIS
1	B	116	ASN
1	B	139	GLN
1	B	141	HIS
1	B	172	GLN
1	B	233	GLN
1	B	286	HIS
1	C	30	HIS
1	C	134	GLN
1	C	139	GLN
1	C	141	HIS
1	C	282	GLN
1	C	283	HIS
1	C	329	GLN
1	C	331	GLN
1	D	116	ASN
1	D	139	GLN
1	D	141	HIS
1	D	331	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	C	332	-	4,4,4	1.20	0	6,6,6	0.62	0

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 ⓘ

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	273/365 (74%)	0.56	15 (5%)	30 30	25, 38, 56, 75	0
1	B	262/365 (71%)	0.84	23 (8%)	15 16	27, 45, 63, 70	0
1	C	272/365 (74%)	0.75	21 (7%)	19 20	27, 43, 66, 77	0
1	D	271/365 (74%)	0.93	23 (8%)	16 17	27, 46, 66, 72	0
All	All	1078/1460 (73%)	0.77	82 (7%)	20 20	25, 43, 65, 77	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	PRO	4.3
1	C	38	ALA	3.9
1	B	160	TRP	3.9
1	A	155	ARG	3.9
1	D	206	GLY	3.9
1	D	38	ALA	3.8
1	A	154	GLU	3.7
1	B	67	GLY	3.6
1	B	87	THR	3.5
1	B	159	SER	3.5
1	D	87	THR	3.4
1	B	227	TRP	3.3
1	B	60	MET	3.3
1	A	151	PRO	3.3
1	C	206	GLY	3.3
1	C	66	LYS	3.3
1	C	285	VAL	3.2
1	B	286	HIS	3.1
1	C	110	HIS	3.1
1	D	301	LEU	3.1
1	C	277	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	126	GLY	3.0
1	A	87	THR	3.0
1	C	297	GLU	3.0
1	B	243	ASP	3.0
1	C	65	GLN	3.0
1	D	127	LEU	3.0
1	D	310	THR	3.0
1	B	173	LEU	2.9
1	D	33	PRO	2.9
1	A	206	GLY	2.9
1	D	288	VAL	2.8
1	B	145	MET	2.8
1	B	182	PHE	2.7
1	A	60	MET	2.7
1	D	277	LEU	2.6
1	C	109	PRO	2.6
1	C	313	GLU	2.6
1	D	281	GLU	2.6
1	A	150	MET	2.6
1	C	70	VAL	2.6
1	B	164	LEU	2.6
1	A	157	PHE	2.5
1	B	148	LEU	2.5
1	D	32	LEU	2.5
1	C	71	ASN	2.5
1	D	109	PRO	2.5
1	D	68	LYS	2.5
1	D	124	GLN	2.5
1	B	116	ASN	2.5
1	D	280	VAL	2.4
1	A	123	TYR	2.4
1	D	75	ALA	2.4
1	C	287	GLU	2.4
1	B	69	GLU	2.3
1	B	70	VAL	2.3
1	B	123	TYR	2.3
1	C	150	MET	2.3
1	A	153	GLY	2.3
1	A	181	GLY	2.3
1	C	114	ALA	2.2
1	B	135	PRO	2.2
1	C	308	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	110	HIS	2.2
1	B	161	LYS	2.2
1	B	223	TYR	2.2
1	C	123	TYR	2.2
1	A	18	PRO	2.1
1	C	180	VAL	2.1
1	D	77	VAL	2.1
1	C	284	SER	2.1
1	D	37	LEU	2.1
1	D	40	ILE	2.1
1	B	288	VAL	2.1
1	C	32	LEU	2.1
1	A	156	GLU	2.1
1	A	66	LYS	2.1
1	A	152	GLU	2.0
1	D	309	GLN	2.0
1	C	273	SER	2.0
1	D	59	ALA	2.0
1	D	274	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](#)

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
2	PO4	C	332	5/5	0.93	0.14	47,48,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.