



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:06 AM UTC

PDB ID : 6FDG / pdb_00006fdg
Title : Novel crystal structure of DHNA-CoA Thioesterase from *Staphylococcus aureus*
Authors : Murad, A.M.; Betzel, C.; Wrenger, C.
Deposited on : 2017-12-22
Resolution : 1.30 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

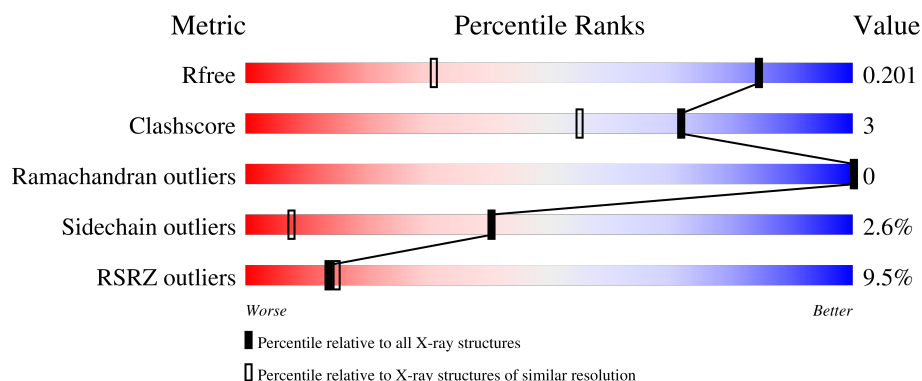
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	155	6% 72% 25% ..
1	B	155	15% 72% 23% ..
1	C	155	5% 79% 18% ..
1	D	155	12% 61% 30% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5483 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 4-hydroxybenzoyl-CoA thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	4	0
			1309	847	207	250	5			
1	B	149	Total	C	N	O	S	0	3	0
			1258	817	199	235	7			
1	C	155	Total	C	N	O	S	0	7	0
			1336	861	210	259	6			
1	D	149	Total	C	N	O	S	0	3	0
			1266	821	203	235	7			

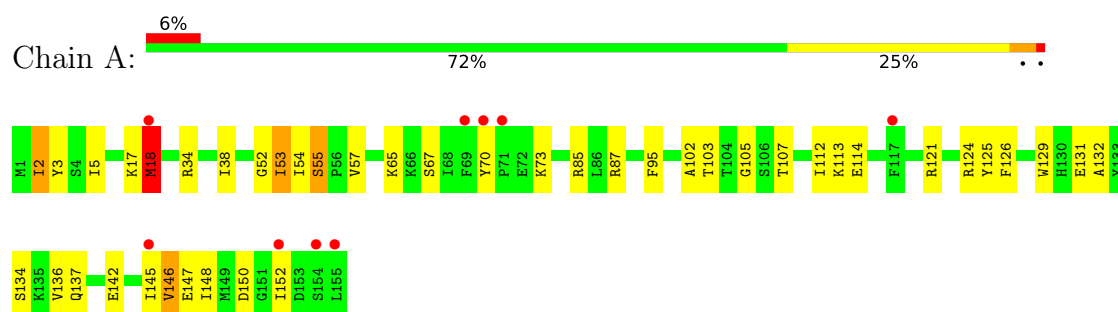
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	71	Total	O	0	0
			71	71		
2	C	85	Total	O	0	0
			85	85		
2	D	76	Total	O	0	0
			76	76		

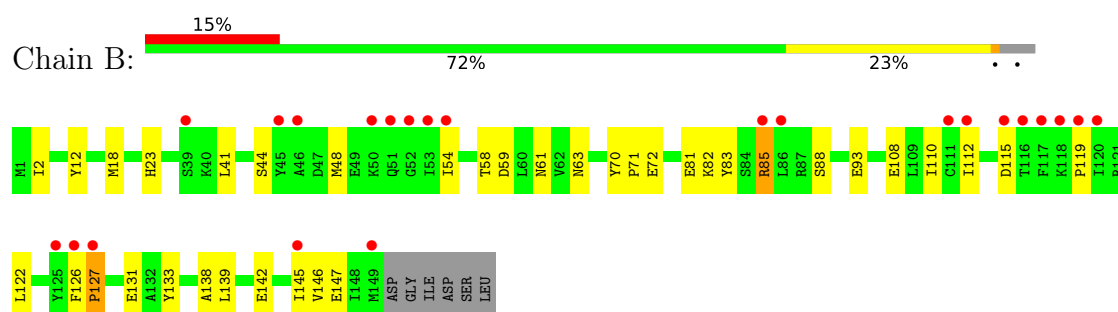
3 Residue-property plots [i](#)

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.

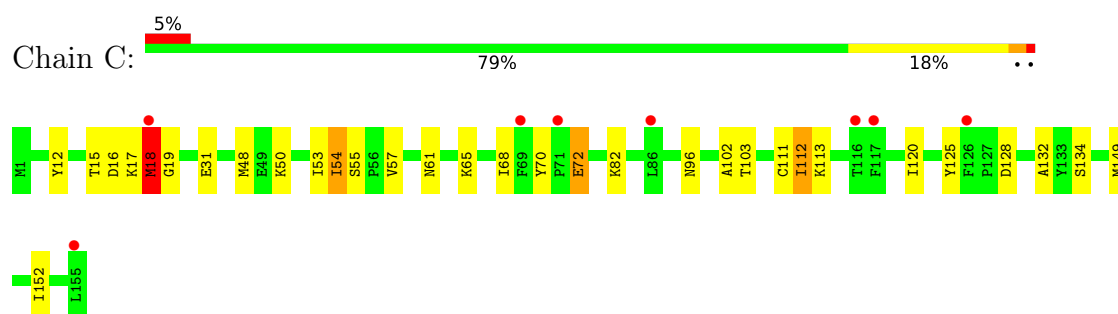
- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase



- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase

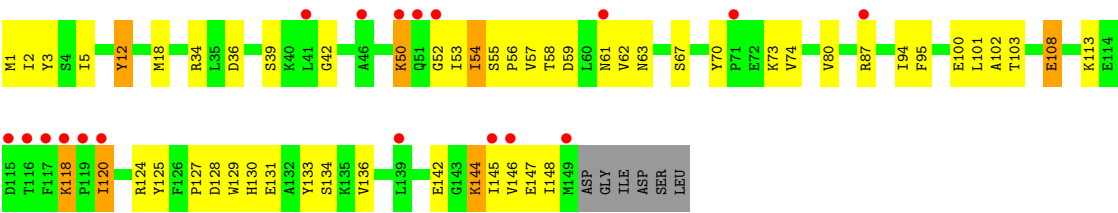


- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase



- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.61Å 90.78Å 75.38Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	75.33 – 1.30 75.33 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.33-1.30) 97.9 (75.33-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.198 0.185 , 0.201	Depositor DCC
R_{free} test set	8701 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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	1.97	34/1342 (2.5%)	1.60	15/1812 (0.8%)
1	B	1.91	25/1291 (1.9%)	1.55	9/1741 (0.5%)
1	C	1.83	23/1369 (1.7%)	1.49	11/1847 (0.6%)
1	D	2.08	40/1296 (3.1%)	1.67	12/1747 (0.7%)
All	All	1.95	122/5298 (2.3%)	1.58	47/7147 (0.7%)

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

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	TYR	CA-C	12.43	1.68	1.53
1	D	144	LYS	N-CA	-8.59	1.35	1.45
1	C	70	TYR	CA-C	8.40	1.62	1.53
1	C	18	MET	N-CA	8.32	1.57	1.46
1	A	146	VAL	C-O	8.14	1.32	1.24
1	C	55	SER	CA-C	7.89	1.61	1.52
1	D	80	VAL	CA-C	-7.75	1.45	1.53
1	D	142	GLU	N-CA	7.54	1.56	1.46
1	B	139	LEU	N-CA	-7.54	1.37	1.46
1	B	81	GLU	C-O	7.43	1.32	1.24
1	C	57	VAL	C-O	7.40	1.32	1.24
1	D	95	PHE	CA-C	-7.36	1.43	1.52
1	D	50	LYS	N-CA	7.18	1.55	1.46
1	D	12	TYR	CE1-CZ	-7.07	1.21	1.38
1	A	18	MET	CA-C	7.05	1.62	1.52
1	D	118	LYS	CA-C	7.00	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLU	N-CA	6.96	1.55	1.46
1	A	65	LYS	CA-C	-6.96	1.43	1.52
1	A	67	SER	C-O	6.93	1.32	1.23
1	B	72	GLU	CA-C	-6.92	1.43	1.52
1	D	130	HIS	N-CA	-6.78	1.38	1.46
1	C	149	MET	SD-CE	-6.77	1.62	1.79
1	C	16	ASP	CA-C	6.75	1.62	1.53
1	D	108	GLU	N-CA	6.75	1.54	1.46
1	D	3	TYR	CA-C	-6.74	1.44	1.52
1	D	67	SER	CA-C	-6.73	1.44	1.52
1	D	147	GLU	CA-C	-6.60	1.44	1.52
1	A	126	PHE	CA-CB	6.58	1.60	1.53
1	C	152	ILE	C-O	6.58	1.30	1.24
1	D	55	SER	CA-C	6.50	1.59	1.52
1	C	55	SER	C-N	-6.49	1.25	1.33
1	A	57	VAL	CA-C	-6.46	1.45	1.52
1	A	147	GLU	CA-C	-6.44	1.45	1.52
1	A	53	ILE	C-O	-6.43	1.17	1.24
1	D	70	TYR	CA-C	6.40	1.60	1.53
1	D	5	ILE	C-O	-6.39	1.17	1.24
1	D	67	SER	C-O	6.37	1.31	1.23
1	D	128	ASP	CA-C	6.31	1.60	1.52
1	B	108	GLU	N-CA	6.28	1.53	1.46
1	D	57	VAL	C-O	6.25	1.31	1.24
1	A	18	MET	N-CA	6.23	1.54	1.46
1	B	58	THR	C-N	6.23	1.41	1.33
1	A	148	ILE	CA-C	-6.18	1.45	1.52
1	D	42	GLY	C-O	6.16	1.32	1.23
1	B	82	LYS	CA-C	-6.16	1.45	1.52
1	D	102	ALA	CA-CB	-6.15	1.44	1.53
1	D	56	PRO	C-O	-6.10	1.17	1.23
1	B	44	SER	CA-C	-6.08	1.45	1.52
1	A	147	GLU	C-O	6.07	1.31	1.24
1	A	112	ILE	C-O	-6.05	1.17	1.23
1	C	149	MET	CA-C	-6.02	1.45	1.52
1	C	54	ILE	C-O	-6.00	1.16	1.23
1	A	57	VAL	N-CA	6.00	1.53	1.46
1	D	56	PRO	CA-CB	-5.98	1.46	1.53
1	D	36	ASP	C-O	5.93	1.31	1.24
1	B	147	GLU	CA-C	-5.93	1.45	1.52
1	D	136	VAL	CA-C	-5.93	1.45	1.52
1	A	136	VAL	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	ASN	CA-C	-5.90	1.45	1.52
1	B	83	TYR	C-N	-5.90	1.25	1.33
1	B	146	VAL	N-CA	-5.85	1.39	1.46
1	A	107	THR	C-O	5.82	1.30	1.23
1	C	82	LYS	CA-C	-5.80	1.45	1.52
1	A	87	ARG	CA-C	-5.78	1.45	1.52
1	D	62	VAL	CA-C	-5.78	1.45	1.52
1	A	134	SER	C-N	-5.74	1.26	1.33
1	A	52	GLY	C-O	-5.69	1.16	1.23
1	B	122	LEU	CA-C	5.68	1.60	1.52
1	D	146	VAL	N-CA	-5.62	1.39	1.46
1	D	12	TYR	CZ-OH	5.62	1.49	1.38
1	B	142	GLU	N-CA	5.61	1.53	1.46
1	B	145	ILE	CA-C	-5.59	1.45	1.52
1	D	2	ILE	N-CA	-5.58	1.39	1.46
1	C	112	ILE	C-O	-5.53	1.17	1.23
1	C	132	ALA	CA-C	5.52	1.59	1.52
1	B	48	MET	CA-C	5.51	1.60	1.52
1	D	39	SER	C-O	5.50	1.30	1.24
1	D	133	TYR	C-O	-5.49	1.17	1.24
1	B	23	HIS	ND1-CE1	5.48	1.38	1.32
1	C	125	TYR	N-CA	-5.47	1.38	1.46
1	B	133	TYR	C-O	-5.43	1.17	1.24
1	A	102	ALA	CA-CB	-5.42	1.45	1.53
1	A	95	PHE	CA-C	-5.40	1.46	1.52
1	D	125	TYR	N-CA	-5.40	1.39	1.46
1	A	105	GLY	C-O	5.39	1.30	1.23
1	B	85	ARG	N-CA	-5.39	1.39	1.46
1	D	100	GLU	CA-C	5.38	1.59	1.52
1	A	3	TYR	CA-C	-5.37	1.46	1.52
1	A	132	ALA	CA-CB	-5.36	1.45	1.53
1	C	50	LYS	N-CA	5.35	1.53	1.46
1	D	148	ILE	N-CA	-5.34	1.40	1.46
1	A	38	ILE	C-O	5.33	1.30	1.24
1	C	102	ALA	CA-CB	-5.31	1.45	1.53
1	A	145	ILE	C-O	5.29	1.30	1.24
1	B	110	ILE	C-O	-5.29	1.17	1.24
1	A	124	ARG	CA-C	-5.28	1.45	1.52
1	C	12	TYR	CZ-OH	5.27	1.49	1.38
1	C	15	THR	C-O	5.26	1.30	1.23
1	D	133	TYR	C-N	5.23	1.41	1.33
1	D	73	LYS	CA-CB	5.22	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	MET	CG-SD	5.21	1.93	1.80
1	C	112	ILE	C-N	5.19	1.40	1.33
1	A	85	ARG	CD-NE	-5.17	1.39	1.46
1	A	5	ILE	CA-C	-5.16	1.45	1.52
1	C	134	SER	CB-OG	-5.12	1.31	1.42
1	B	71	PRO	N-CD	5.12	1.55	1.47
1	A	152	ILE	C-O	5.11	1.29	1.24
1	A	137	GLN	CA-C	5.10	1.59	1.52
1	B	88	SER	C-N	-5.10	1.26	1.33
1	C	149	MET	C-O	-5.09	1.17	1.23
1	C	65	LYS	C-O	5.09	1.30	1.24
1	C	48	MET	N-CA	-5.08	1.40	1.46
1	D	52	GLY	C-O	-5.08	1.17	1.24
1	B	108	GLU	CA-C	-5.07	1.46	1.52
1	B	85	ARG	CA-CB	5.06	1.62	1.53
1	D	63	ASN	CA-C	-5.06	1.46	1.52
1	D	124	ARG	CA-C	-5.05	1.45	1.52
1	A	55	SER	C-N	-5.04	1.27	1.33
1	D	101	LEU	CA-CB	-5.04	1.46	1.53
1	B	70	TYR	CA-C	5.03	1.58	1.53
1	D	148	ILE	C-O	5.03	1.30	1.24
1	B	93	GLU	CA-C	-5.01	1.46	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	SER	O-C-N	8.12	131.41	122.15
1	D	145	ILE	O-C-N	-7.81	115.45	123.03
1	A	145	ILE	O-C-N	-7.70	114.75	122.99
1	D	131	GLU	O-C-N	7.47	130.04	122.12
1	C	111	CYS	O-C-N	7.11	131.76	123.30
1	A	17	LYS	CA-C-O	-7.04	110.72	119.38
1	C	18	MET	O-C-N	-7.03	112.76	122.46
1	D	70	TYR	CA-C-O	-6.85	112.85	120.25
1	A	55	SER	O-C-N	6.52	127.25	121.32
1	C	17	LYS	CA-C-O	-6.47	113.64	120.63
1	B	126	PHE	O-C-N	-6.34	116.09	121.23
1	A	18	MET	CA-CB-CG	6.15	126.40	114.10
1	C	112	ILE	CA-C-O	6.08	127.66	121.63
1	B	110	ILE	CA-C-O	6.08	128.38	120.78
1	D	54	ILE	CA-C-O	6.06	128.03	121.67
1	A	125	TYR	CA-C-O	6.06	126.26	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	A	129	TRP	O-C-N	-5.88	116.01	122.07
1	B	72	GLU	N-CA-C	5.86	118.83	110.10
1	B	138	ALA	O-C-N	-5.73	115.62	122.15
1	A	147	GLU	CB-CG-CD	5.65	122.20	112.60
1	C	18	MET	CG-SD-CE	-5.64	88.48	100.90
1	A	73	LYS	O-C-N	-5.64	116.79	123.22
1	A	150	ASP	CA-C-O	-5.62	114.86	121.16
1	D	34	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	B	147	GLU	O-C-N	-5.51	116.79	123.13
1	C	70	TYR	CA-C-O	-5.50	114.31	120.25
1	D	120	ILE	CA-C-N	5.44	129.27	121.50
1	D	120	ILE	C-N-CA	5.44	129.27	121.50
1	D	127	PRO	O-C-N	5.42	129.21	122.22
1	A	146	VAL	CA-C-O	-5.35	114.60	120.43
1	B	127	PRO	CA-C-N	5.34	127.39	120.44
1	B	127	PRO	C-N-CA	5.34	127.39	120.44
1	A	95	PHE	CA-C-O	5.27	126.30	120.71
1	A	131	GLU	CA-C-O	-5.27	114.84	120.42
1	B	126	PHE	CA-C-O	5.26	127.07	121.28
1	D	74	VAL	O-C-N	5.26	128.23	122.76
1	C	19	GLY	CA-C-O	5.25	125.54	119.13
1	C	128	ASP	CB-CG-OD2	-5.25	106.33	118.40
1	B	70	TYR	CA-C-O	-5.19	114.64	120.25
1	C	112	ILE	O-C-N	-5.19	117.16	123.02
1	D	94	ILE	O-C-N	5.14	128.58	123.18
1	C	152	ILE	CA-C-O	-5.13	114.92	120.36
1	A	121	ARG	O-C-N	-5.10	117.41	123.22
1	D	129	TRP	O-C-N	-5.08	116.84	122.07
1	A	18	MET	O-C-N	-5.06	115.70	122.43
1	C	57	VAL	CA-C-O	-5.03	115.31	121.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	ILE	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	1309	0	1293	12	0
1	B	1258	0	1253	16	0
1	C	1336	0	1308	7	0
1	D	1266	0	1260	14	0
2	A	82	0	0	0	0
2	B	71	0	0	0	0
2	C	85	0	0	0	0
2	D	76	0	0	0	0
All	All	5483	0	5114	34	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 3.

All (34) 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:A:54[A]:ILE:HG21	1:B:18[A]:MET:SD	1.96	1.05
1:B:18[A]:MET:HG3	1:D:12:TYR:OH	1.68	0.93
1:A:54[A]:ILE:CG2	1:B:18[A]:MET:SD	2.59	0.89
1:D:59:ASP:OD2	1:D:61:ASN:ND2	2.15	0.79
1:B:12:TYR:OH	1:D:18[A]:MET:HG3	1.83	0.79
1:D:87[B]:ARG:HD2	1:D:108:GLU:HG3	1.73	0.70
1:A:54[A]:ILE:HG21	1:B:18[A]:MET:CG	2.29	0.62
1:B:18[A]:MET:HG3	1:D:12:TYR:HH	1.65	0.61
1:D:53:ILE:CD1	1:D:113:LYS:HD3	2.31	0.60
1:C:18:MET:HE3	1:D:54:ILE:HD12	1.86	0.57
1:A:54[B]:ILE:HD12	1:B:18[B]:MET:SD	2.46	0.54
1:A:54[A]:ILE:HG22	1:A:55:SER:N	2.22	0.54
1:A:54[A]:ILE:HG21	1:B:18[A]:MET:HG2	1.90	0.52
1:D:53:ILE:HD11	1:D:113:LYS:HD3	1.94	0.49
1:A:2:ILE:HD12	1:A:146:VAL:HB	1.95	0.48
1:B:12:TYR:HB3	1:C:31[A]:GLU:CD	2.38	0.47
1:D:58:THR:OG1	1:D:108:GLU:OE2	2.30	0.47
1:A:53:ILE:CD1	1:A:113:LYS:HD2	2.45	0.47
1:B:85:ARG:HE	1:B:85:ARG:HB3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:OD2	1:B:61:ASN:ND2	2.39	0.45
1:A:18:MET:HE3	1:B:54:ILE:HD12	1.98	0.45
1:C:54:ILE:HD12	1:D:18[B]:MET:SD	2.57	0.45
1:C:61[B]:ASN:OD1	1:D:61:ASN:OD1	2.36	0.44
1:B:127:PRO:O	1:B:131:GLU:HG3	2.18	0.44
1:C:54:ILE:HG13	1:C:112:ILE:CG1	2.48	0.43
1:D:87[A]:ARG:HH11	1:D:108:GLU:CD	2.26	0.43
1:D:1[B]:MET:N	1:D:144:LYS:O	2.32	0.42
1:B:112:ILE:HG22	1:B:119:PRO:HA	2.02	0.42
1:A:54[A]:ILE:HG22	1:B:18[A]:MET:SD	2.55	0.41
1:C:72[A]:GLU:OE1	1:C:96:ASN:HB2	2.20	0.41
1:D:87[B]:ARG:HE	1:D:87[B]:ARG:C	2.27	0.41
1:C:53:ILE:CD1	1:C:113:LYS:HD2	2.50	0.41
1:A:54[A]:ILE:HD13	1:B:18[A]:MET:HG2	2.02	0.41
1:A:54[A]:ILE:HD11	1:A:114:GLU:HG3	2.04	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	157/155 (101%)	157 (100%)	0	0	100	100
1	B	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
1	C	159/155 (103%)	158 (99%)	1 (1%)	0	100	100
1	D	149/155 (96%)	146 (98%)	3 (2%)	0	100	100
All	All	614/620 (99%)	608 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	143/139 (103%)	140 (98%)	3 (2%)	47	11
1	B	137/139 (99%)	134 (98%)	3 (2%)	45	10
1	C	146/139 (105%)	141 (97%)	5 (3%)	32	4
1	D	137/139 (99%)	133 (97%)	4 (3%)	37	5
All	All	563/556 (101%)	548 (97%)	15 (3%)	40	7

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	18	MET
1	A	103	THR
1	B	2	ILE
1	B	41	LEU
1	B	115	ASP
1	C	18	MET
1	C	72[A]	GLU
1	C	72[B]	GLU
1	C	103	THR
1	C	120	ILE
1	D	50	LYS
1	D	103	THR
1	D	118	LYS
1	D	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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	155/155 (100%)	0.75	9 (5%) 29 33	10, 22, 36, 44	4 (2%)
1	B	149/155 (96%)	0.83	23 (15%) 5 5	10, 21, 50, 66	3 (2%)
1	C	155/155 (100%)	0.66	8 (5%) 33 37	8, 20, 34, 48	7 (4%)
1	D	149/155 (96%)	0.73	18 (12%) 8 9	10, 21, 39, 49	3 (2%)
All	All	608/620 (98%)	0.74	58 (9%) 14 15	8, 21, 39, 66	17 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PHE	5.9
1	D	119	PRO	3.8
1	B	46	ALA	3.8
1	B	120	ILE	3.7
1	A	69	PHE	3.6
1	C	18	MET	3.5
1	D	117	PHE	3.5
1	A	18	MET	3.4
1	D	149	MET	3.4
1	B	116	THR	3.4
1	C	69	PHE	3.3
1	B	53	ILE	3.3
1	B	145	ILE	3.2
1	D	120	ILE	3.2
1	B	118	LYS	3.2
1	D	116	THR	3.1
1	B	50	LYS	3.0
1	D	46	ALA	2.9
1	D	146	VAL	2.9
1	B	119	PRO	2.9
1	B	127	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	155	LEU	2.8
1	D	87[A]	ARG	2.7
1	A	155	LEU	2.7
1	D	139	LEU	2.7
1	D	41	LEU	2.7
1	B	149	MET	2.6
1	B	85	ARG	2.6
1	D	71	PRO	2.6
1	A	154	SER	2.5
1	C	71	PRO	2.5
1	D	50	LYS	2.5
1	A	152	ILE	2.5
1	B	54	ILE	2.5
1	B	112	ILE	2.4
1	B	86	LEU	2.4
1	B	51	GLN	2.4
1	D	118	LYS	2.4
1	B	126	PHE	2.4
1	B	52	GLY	2.4
1	D	52	GLY	2.4
1	B	125	TYR	2.4
1	D	145	ILE	2.3
1	C	86	LEU	2.3
1	B	115	ASP	2.3
1	A	71	PRO	2.2
1	A	117	PHE	2.2
1	C	117	PHE	2.2
1	B	45	TYR	2.2
1	D	51	GLN	2.2
1	B	39[A]	SER	2.2
1	C	126	PHE	2.1
1	D	61	ASN	2.1
1	C	116	THR	2.1
1	A	70	TYR	2.1
1	D	115	ASP	2.0
1	B	111	CYS	2.0
1	A	145	ILE	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 [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.