



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:20 PM UTC

PDB ID : 7YVY / pdb_00007yvy
Title : Crystal structure of thiolase PFC_04095 from Pyrococcus furiosus
Authors : Singh, R.; Das, A.K.
Deposited on : 2022-08-20
Resolution : 2.70 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

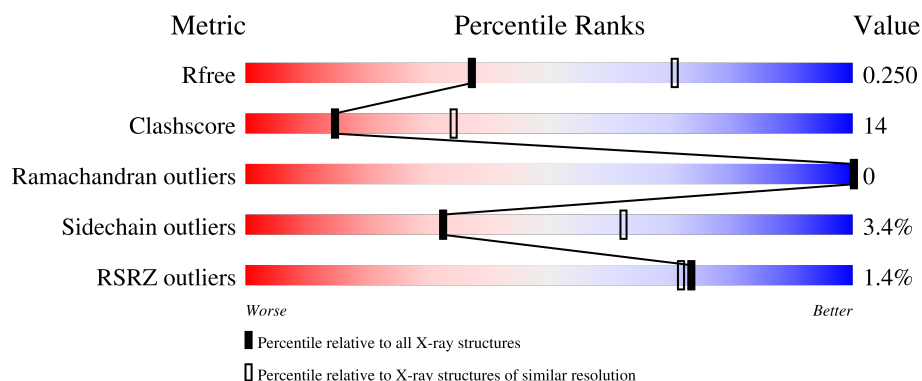
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	388	
1	B	388	
1	C	388	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7760 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.

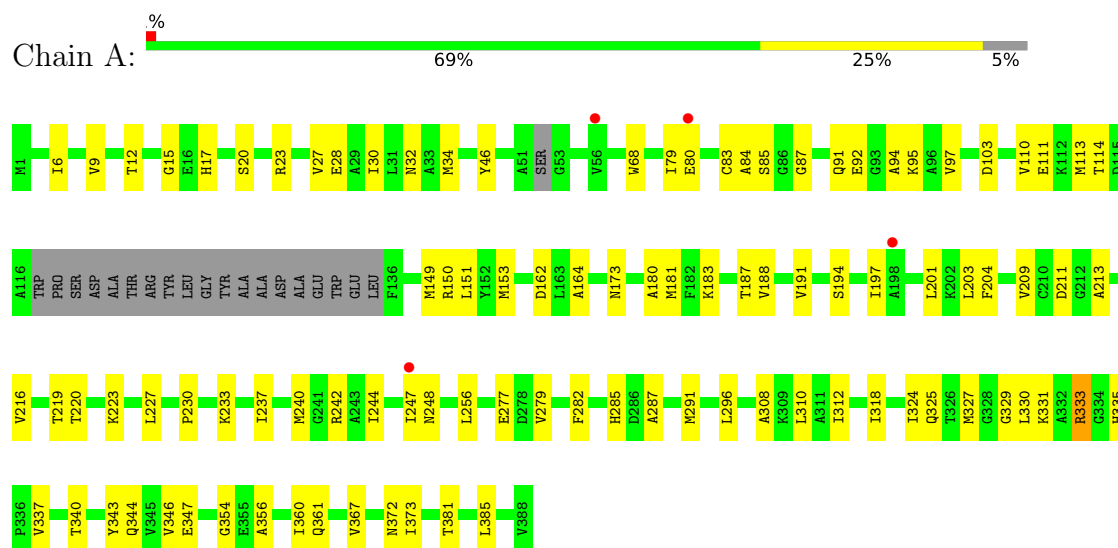
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2637	1674	440	509	14			
1	B	364	Total	C	N	O	S	0	0	0
			2592	1643	435	501	13			
1	C	359	Total	C	N	O	S	0	0	0
			2531	1606	427	484	14			

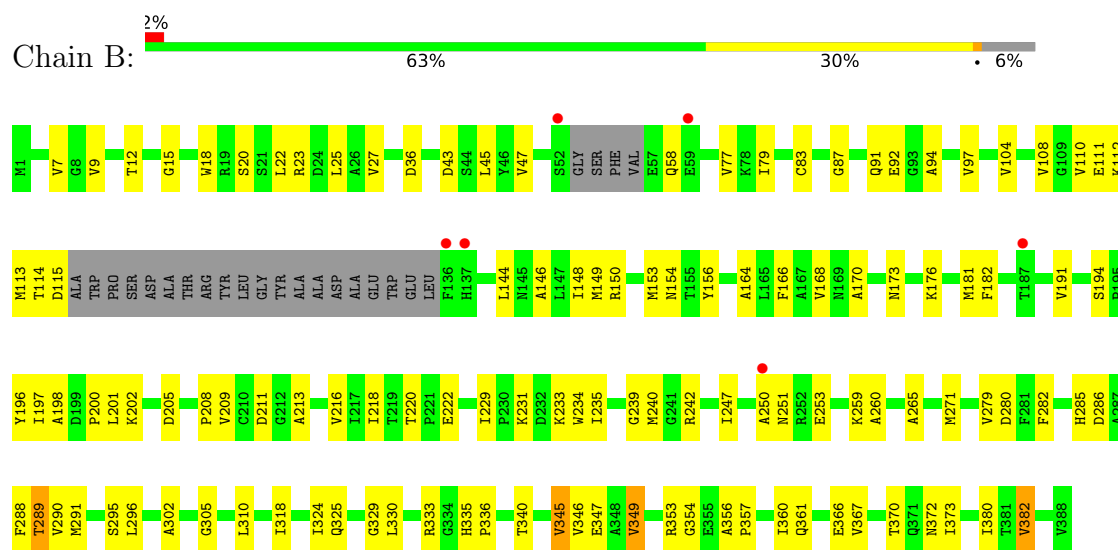
3 Residue-property plots

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: Acetyl-CoA acetyltransferase



• Molecule 1: Acetyl-CoA acetyltransferase



• Molecule 1: Acetyl-CoA acetyltransferase



R333	G334	R335	F336	V337	G338	A339	T340	V346	V349	L350	Q351	L352	R353	A356	I360	Q361	V362	A365	F366	V367	G368	L369	N372	I373	G377	S378	N379	I380	R386	R387	VAL														
I217	I235	E236	I237	A238	G239	I247	E253	L256	K259	A260	I263	K270	M271	V279	F282	H285	D286	A287	F288	T289	V290	M291	S295	L296	V301	G305	A308	A311	I312	I316	A317	I318	D319	I324	Q325	T326	K327	G328	G329	L330	K331	A332			
TYR	LEU	GLY	TYR	ALA	ASP	ALA	GLU	TRP	GLU	LEU	PHE	HIS	G138	F141	N145	A146	M149	R150	L151	Y152	M153	Y156	G157	Y158	K159	D162	L165	V168	N169	A170	H171	I186	V191	S194	P195	Y196	I197	P200	L201	K202	D205	A206	S207	C210	
MET	R2	K3	A4	V9	G10	M11	T12	P13	H17	S20	S21	L22	R23	A26	I30	M34	D40	A51	SER	GLY	SER	SER	PHE	VAL	E57	Q58	E59	N60	L61	W63	G87	A94	L93	L106	E111	K112	D115	ALA	TRP	PRO	SER	ASP	ALA	THR	ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 113.48Å 107.53Å 90.00° 123.03° 90.00°	Depositor
Resolution (Å)	48.03 – 2.70 48.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.03-2.70) 99.6 (48.03-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.209 , 0.252 0.209 , 0.250	Depositor DCC
R_{free} test set	2487 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7760	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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](#)

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	0.27	0/2675	0.52	0/3640
1	B	0.28	0/2630	0.53	0/3585
1	C	0.29	0/2569	0.54	1/3506 (0.0%)
All	All	0.28	0/7874	0.53	1/10731 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	GLY	N-CA-C	-5.57	107.32	115.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	336	PRO	Peptide

5.2 Too-close contacts [i](#)

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	2637	0	2614	64	0
1	B	2592	0	2538	78	0
1	C	2531	0	2463	72	0
All	All	7760	0	7615	214	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 14.

All (214) 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:113:MET:HE1	1:B:209:VAL:HG12	1.38	1.04
1:C:9:VAL:HG21	1:C:349:VAL:HG21	1.55	0.88
1:A:15:GLY:HA2	1:A:181:MET:HG3	1.55	0.87
1:B:356:ALA:HB3	1:B:361:GLN:HG2	1.61	0.82
1:A:164:ALA:HB1	1:A:191:VAL:HG21	1.62	0.81
1:C:356:ALA:HB3	1:C:361:GLN:HG2	1.66	0.77
1:C:279:VAL:HA	1:C:367:VAL:HG13	1.68	0.75
1:C:327:MET:HG2	1:C:360:ILE:HD12	1.67	0.75
1:B:91:GLN:HE22	1:B:242:ARG:HB2	1.50	0.74
1:B:113:MET:CE	1:B:209:VAL:HG12	2.17	0.74
1:A:237:ILE:HG21	1:A:240:MET:HE3	1.69	0.73
1:C:168:VAL:HG12	1:C:186:ILE:HG13	1.69	0.73
1:B:335:HIS:ND1	1:B:340:THR:HG21	2.04	0.72
1:A:91:GLN:HA	1:A:240:MET:HE2	1.72	0.71
1:B:279:VAL:HG13	1:B:367:VAL:HG12	1.73	0.71
1:B:291:MET:O	1:B:295:SER:OG	2.11	0.69
1:B:357:PRO:HG2	1:B:360:ILE:HD11	1.73	0.69
1:B:345:VAL:O	1:B:349:VAL:HG12	1.93	0.68
1:A:151:LEU:HB3	1:A:256:LEU:HD21	1.73	0.68
1:B:47:VAL:HG23	1:B:108:VAL:HG13	1.76	0.67
1:C:259:LYS:HG2	1:C:263:ILE:HD11	1.74	0.67
1:A:87:GLY:H	1:A:372:ASN:HD22	1.44	0.66
1:B:265:ALA:HA	1:B:382:VAL:HG21	1.78	0.66
1:A:308:ALA:O	1:A:312:ILE:HD12	1.96	0.66
1:A:12:THR:HG22	1:A:28:GLU:HG2	1.78	0.65
1:B:15:GLY:HA2	1:B:181:MET:HG3	1.77	0.65
1:A:94:ALA:HB3	1:A:240:MET:HE1	1.76	0.65
1:B:197:ILE:HD11	1:B:201:LEU:HD22	1.79	0.65
1:C:239:GLY:HA2	1:C:271:MET:HE2	1.80	0.64
1:A:23:ARG:O	1:A:27:VAL:HG22	1.98	0.64
1:A:327:MET:HA	1:A:360:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:THR:HB	1:C:351:GLN:HE21	1.63	0.63
1:C:259:LYS:O	1:C:263:ILE:HD12	1.98	0.63
1:C:171:HIS:HE1	1:C:331:LYS:HE3	1.63	0.62
1:C:171:HIS:CE1	1:C:331:LYS:HE3	2.35	0.62
1:C:87:GLY:H	1:C:372:ASN:HD22	1.46	0.62
1:B:112:LYS:HE2	1:B:115:ASP:OD1	2.00	0.61
1:C:279:VAL:HG12	1:C:367:VAL:HG22	1.82	0.61
1:B:253:GLU:OE2	1:B:259:LYS:NZ	2.34	0.61
1:C:111:GLU:HG3	1:C:338:GLY:H	1.65	0.61
1:C:335:HIS:ND1	1:C:340:THR:HG21	2.16	0.61
1:A:91:GLN:HA	1:A:240:MET:CE	2.31	0.61
1:A:242:ARG:HG3	1:A:381:THR:HG22	1.83	0.61
1:B:45:LEU:HD11	1:B:108:VAL:HG12	1.81	0.61
1:B:149:MET:HG3	1:B:290:VAL:CG2	2.31	0.60
1:B:191:VAL:O	1:B:194:SER:OG	2.20	0.60
1:B:150:ARG:HA	1:B:153:MET:HG2	1.85	0.59
1:C:197:ILE:HG13	1:C:201:LEU:HD23	1.84	0.59
1:C:201:LEU:HD11	1:C:288:PHE:CD1	2.37	0.59
1:C:9:VAL:HG13	1:C:346:VAL:HG13	1.83	0.59
1:A:333:ARG:HD3	1:A:347:GLU:OE2	2.02	0.59
1:C:165:LEU:HA	1:C:168:VAL:HG22	1.85	0.59
1:C:362:VAL:HG23	1:C:365:ALA:HB2	1.85	0.59
1:C:253:GLU:OE2	1:C:259:LYS:NZ	2.21	0.59
1:B:149:MET:HG3	1:B:290:VAL:HG22	1.83	0.58
1:A:149:MET:O	1:A:153:MET:HG3	2.03	0.58
1:C:260:ALA:HB3	1:C:380:ILE:HD12	1.86	0.58
1:B:198:ALA:O	1:B:201:LEU:N	2.37	0.58
1:A:103:ASP:O	1:A:219:THR:HG22	2.04	0.57
1:B:302:ALA:HB2	1:B:310:LEU:HD11	1.86	0.57
1:C:30:ILE:HD13	1:C:106:LEU:HD21	1.86	0.57
1:A:279:VAL:HA	1:A:367:VAL:HB	1.87	0.57
1:B:280:ASP:OD2	1:B:366:GLU:N	2.31	0.56
1:B:20:SER:O	1:B:112:LYS:NZ	2.34	0.56
1:C:191:VAL:O	1:C:194:SER:OG	2.22	0.56
1:B:354:GLY:HA2	1:B:361:GLN:NE2	2.21	0.56
1:A:285:HIS:CD2	1:A:373:ILE:H	2.24	0.56
1:C:318:ILE:HD11	1:C:360:ILE:HG22	1.86	0.56
1:A:247:ILE:HD12	1:A:248:ASN:N	2.21	0.56
1:B:12:THR:HG22	1:B:213:ALA:H	1.71	0.56
1:B:239:GLY:HA2	1:B:271:MET:HE2	1.88	0.56
1:B:285:HIS:HB3	1:B:373:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG21	1:C:349:VAL:CG2	2.32	0.56
1:A:113:MET:HE2	1:A:209:VAL:HB	1.89	0.55
1:B:250:ALA:O	1:B:251:ASN:ND2	2.39	0.55
1:C:235:ILE:HD11	1:C:353:ARG:HG2	1.89	0.55
1:C:196:TYR:CE1	1:C:202:LYS:HG2	2.42	0.55
1:B:79:ILE:HD12	1:B:92:GLU:HG3	1.87	0.55
1:B:36:ASP:OD2	1:B:353:ARG:NH2	2.40	0.54
1:C:34:MET:HG2	1:C:217:ILE:HD11	1.88	0.54
1:C:291:MET:O	1:C:295:SER:OG	2.23	0.54
1:C:351:GLN:OE1	1:C:361:GLN:HA	2.08	0.54
1:C:23:ARG:HG3	1:C:68:TRP:CD2	2.44	0.53
1:B:146:ALA:HB1	1:B:200:PRO:HG2	1.91	0.53
1:B:279:VAL:HB	1:B:282:PHE:CZ	2.43	0.53
1:C:158:TYR:CE1	1:C:308:ALA:HB3	2.42	0.53
1:B:354:GLY:HA2	1:B:361:GLN:HE21	1.73	0.53
1:C:326:THR:HB	1:C:351:GLN:NE2	2.23	0.53
1:A:287:ALA:HB3	1:A:291:MET:HE3	1.90	0.53
1:C:151:LEU:HG	1:C:256:LEU:HD11	1.90	0.52
1:B:329:GLY:O	1:B:333:ARG:HB3	2.09	0.52
1:C:282:PHE:HD2	1:C:369:LEU:HD22	1.75	0.52
1:A:17:HIS:HB3	1:A:20:SER:HB2	1.90	0.52
1:A:164:ALA:CB	1:A:191:VAL:HG21	2.38	0.52
1:C:286:ASP:OD1	1:C:330:LEU:HB2	2.09	0.52
1:A:162:ASP:HB3	1:A:312:ILE:HD11	1.92	0.51
1:A:197:ILE:HD11	1:A:203:LEU:HD12	1.92	0.51
1:A:91:GLN:HG2	1:A:240:MET:HE2	1.93	0.51
1:C:170:ALA:HB2	1:C:325:GLN:NE2	2.25	0.51
1:B:91:GLN:HE21	1:B:242:ARG:HH11	1.58	0.51
1:A:230:PRO:HG2	1:A:233:LYS:HG3	1.93	0.51
1:C:58:GLN:O	1:C:61:LEU:HB2	2.11	0.50
1:C:59:GLU:O	1:C:60:ASN:HB2	2.11	0.50
1:B:23:ARG:O	1:B:27:VAL:HG23	2.12	0.50
1:B:260:ALA:HB3	1:B:380:ILE:HD12	1.93	0.50
1:C:349:VAL:O	1:C:353:ARG:HG3	2.11	0.50
1:B:166:PHE:HB2	1:B:289:THR:HG22	1.95	0.49
1:A:80:GLU:HA	1:A:85:SER:HB3	1.94	0.49
1:B:144:LEU:O	1:B:148:ILE:HG12	2.12	0.49
1:B:9:VAL:HB	1:B:346:VAL:HG13	1.93	0.49
1:B:111:GLU:HG3	1:B:113:MET:HG3	1.95	0.49
1:B:9:VAL:HG11	1:B:349:VAL:HG11	1.95	0.49
1:C:373:ILE:HG23	1:C:380:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:HD12	1:B:318:ILE:H	1.77	0.49
1:B:370:THR:O	1:B:382:VAL:HA	2.13	0.49
1:C:17:HIS:HB3	1:C:20:SER:OG	2.13	0.48
1:C:11:MET:SD	1:C:346:VAL:HG11	2.53	0.48
1:C:156:TYR:CD2	1:C:305:GLY:HA2	2.48	0.48
1:C:308:ALA:O	1:C:312:ILE:HG13	2.13	0.48
1:C:159:LYS:N	1:C:162:ASP:OD1	2.43	0.48
1:A:87:GLY:H	1:A:372:ASN:ND2	2.08	0.48
1:B:156:TYR:CD1	1:B:305:GLY:HA2	2.49	0.48
1:B:182:PHE:HE2	1:B:208:PRO:HG3	1.79	0.48
1:C:22:LEU:HD12	1:C:112:LYS:HB2	1.96	0.48
1:A:191:VAL:HG12	1:A:204:PHE:HB3	1.95	0.48
1:B:233:LYS:HA	1:B:353:ARG:HD3	1.97	0.47
1:B:110:VAL:HG23	1:B:213:ALA:HB2	1.96	0.47
1:C:111:GLU:CG	1:C:338:GLY:H	2.26	0.47
1:C:279:VAL:HG23	1:C:282:PHE:CZ	2.49	0.47
1:A:282:PHE:HB2	1:A:324:ILE:HG22	1.97	0.47
1:C:9:VAL:CG1	1:C:346:VAL:HG13	2.44	0.47
1:C:286:ASP:OD2	1:C:325:GLN:HG2	2.14	0.47
1:B:43:ASP:HB2	1:B:104:VAL:O	2.15	0.47
1:B:336:PRO:HD2	1:B:340:THR:HG22	1.98	0.46
1:A:94:ALA:CB	1:A:240:MET:HE1	2.45	0.46
1:B:231:LYS:HA	1:B:234:TRP:CG	2.51	0.46
1:C:296:LEU:HD21	1:C:324:ILE:HG21	1.97	0.46
1:A:173:ASN:CG	1:A:318:ILE:HD11	2.40	0.46
1:C:205:ASP:OD2	1:C:289:THR:OG1	2.26	0.46
1:A:32:ASN:N	1:A:32:ASN:HD22	2.14	0.46
1:C:149:MET:O	1:C:153:MET:HG3	2.16	0.45
1:B:170:ALA:HB2	1:B:325:GLN:NE2	2.30	0.45
1:B:173:ASN:OD1	1:B:318:ILE:HD11	2.16	0.45
1:B:9:VAL:HG11	1:B:349:VAL:CG1	2.46	0.45
1:C:316:ILE:HB	1:C:324:ILE:HG12	1.97	0.45
1:A:110:VAL:HG23	1:A:213:ALA:HB2	1.98	0.45
1:A:23:ARG:HG3	1:A:68:TRP:CD2	2.52	0.45
1:B:222:GLU:CD	1:B:222:GLU:H	2.25	0.45
1:B:91:GLN:HG2	1:B:240:MET:HG2	1.99	0.45
1:A:92:GLU:O	1:A:95:LYS:HG2	2.17	0.45
1:B:286:ASP:OD2	1:B:330:LEU:N	2.47	0.45
1:C:329:GLY:O	1:C:333:ARG:HB3	2.17	0.45
1:C:165:LEU:HD23	1:C:311:ALA:O	2.17	0.45
1:C:26:ALA:O	1:C:30:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ALA:HB1	1:C:200:PRO:HD2	1.98	0.44
1:C:238:ALA:HB2	1:C:386:ARG:HD2	1.99	0.44
1:A:324:ILE:HD12	1:A:325:GLN:HG3	1.99	0.44
1:C:141:PHE:O	1:C:145:ASN:ND2	2.49	0.44
1:A:223:LYS:HE3	1:A:227:LEU:HD21	2.00	0.44
1:A:318:ILE:HD12	1:A:318:ILE:H	1.83	0.44
1:B:333:ARG:NE	1:B:347:GLU:OE2	2.50	0.44
1:B:201:LEU:HD11	1:B:288:PHE:CD1	2.53	0.44
1:A:329:GLY:O	1:A:333:ARG:HB3	2.17	0.44
1:A:335:HIS:CE1	1:A:337:VAL:HG12	2.53	0.44
1:C:23:ARG:HG3	1:C:68:TRP:CG	2.52	0.43
1:C:270:LYS:HD3	1:C:270:LYS:HA	1.60	0.43
1:A:84:ALA:HA	1:A:372:ASN:ND2	2.33	0.43
1:B:22:LEU:HA	1:B:25:LEU:HD12	1.99	0.43
1:B:149:MET:HE1	1:B:205:ASP:CG	2.43	0.43
1:B:234:TRP:O	1:B:235:ILE:HD13	2.19	0.43
1:C:4:ALA:HB2	1:C:98:LEU:CD1	2.48	0.43
1:C:285:HIS:O	1:C:330:LEU:HD13	2.17	0.43
1:A:150:ARG:HD3	1:A:150:ARG:HA	1.81	0.43
1:A:340:THR:O	1:A:344:GLN:HG3	2.19	0.43
1:A:343:TYR:HA	1:A:346:VAL:HG22	2.00	0.43
1:A:330:LEU:HD12	1:A:333:ARG:NH2	2.33	0.43
1:B:164:ALA:O	1:B:168:VAL:HG13	2.19	0.43
1:C:207:SER:HB3	1:C:330:LEU:O	2.18	0.43
1:C:247:ILE:CD1	1:C:378:SER:HB3	2.49	0.43
1:B:149:MET:O	1:B:153:MET:HG2	2.19	0.43
1:A:113:MET:CE	1:A:209:VAL:HB	2.48	0.43
1:B:196:TYR:CE1	1:B:202:LYS:HG2	2.54	0.43
1:B:235:ILE:CG1	1:B:349:VAL:HG23	2.49	0.42
1:A:318:ILE:HD12	1:A:318:ILE:N	2.34	0.42
1:C:13:PRO:O	1:C:17:HIS:NE2	2.42	0.42
1:A:111:GLU:O	1:A:211:ASP:HA	2.20	0.42
1:B:113:MET:HE1	1:B:209:VAL:C	2.44	0.42
1:C:40:ASP:OD1	1:C:40:ASP:N	2.53	0.42
1:B:296:LEU:HD21	1:B:324:ILE:HG21	2.00	0.42
1:B:182:PHE:CE2	1:B:208:PRO:HG3	2.54	0.42
1:A:296:LEU:HD23	1:A:310:LEU:HD12	2.01	0.42
1:A:356:ALA:HB3	1:A:361:GLN:OE1	2.19	0.42
1:A:9:VAL:HG12	1:A:216:VAL:HG22	2.01	0.41
1:A:114:THR:O	1:A:114:THR:OG1	2.38	0.41
1:A:237:ILE:HD13	1:A:385:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TRP:CZ3	1:B:114:THR:HB	2.55	0.41
1:C:165:LEU:HA	1:C:168:VAL:CG2	2.49	0.41
1:B:94:ALA:O	1:B:97:VAL:HG22	2.21	0.41
1:A:92:GLU:OE1	1:A:242:ARG:NH1	2.44	0.41
1:A:34:MET:HE2	1:A:34:MET:HB3	1.86	0.41
1:A:6:ILE:HD11	1:A:237:ILE:HD11	2.02	0.41
1:A:30:ILE:O	1:A:34:MET:HG3	2.20	0.41
1:B:7:VAL:HB	1:B:229:ILE:HG21	2.03	0.41
1:A:180:ALA:O	1:A:183:LYS:HE2	2.20	0.41
1:A:191:VAL:O	1:A:194:SER:OG	2.37	0.41
1:B:47:VAL:HA	1:B:108:VAL:O	2.21	0.41
1:B:87:GLY:H	1:B:372:ASN:HD22	1.66	0.41
1:A:188:VAL:O	1:A:191:VAL:HG22	2.21	0.40
1:B:150:ARG:O	1:B:154:ASN:HB2	2.22	0.40
1:B:220:THR:OG1	1:B:222:GLU:OE2	2.38	0.40
1:A:46:TYR:HD2	1:A:79:ILE:HD11	1.86	0.40
1:C:94:ALA:HB2	1:C:237:ILE:HD13	2.02	0.40
1:A:354:GLY:HA2	1:A:361:GLN:HE22	1.86	0.40
1:B:197:ILE:HD11	1:B:201:LEU:CD2	2.50	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	362/388 (93%)	350 (97%)	12 (3%)	0	100	100
1	B	358/388 (92%)	348 (97%)	10 (3%)	0	100	100
1	C	353/388 (91%)	340 (96%)	13 (4%)	0	100	100
All	All	1073/1164 (92%)	1038 (97%)	35 (3%)	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	257/290 (89%)	248 (96%)	9 (4%)	32	61
1	B	249/290 (86%)	237 (95%)	12 (5%)	23	50
1	C	239/290 (82%)	235 (98%)	4 (2%)	53	79
All	All	745/870 (86%)	720 (97%)	25 (3%)	32	62

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	CYS
1	A	97	VAL
1	A	187	THR
1	A	201	LEU
1	A	220	THR
1	A	244	ILE
1	A	277	GLU
1	A	331	LYS
1	A	333	ARG
1	B	58	GLN
1	B	77	VAL
1	B	83	CYS
1	B	176	LYS
1	B	211	ASP
1	B	216	VAL
1	B	218	ILE
1	B	247	ILE
1	B	289	THR
1	B	345	VAL
1	B	349	VAL
1	B	382	VAL
1	C	210	CYS
1	C	301	VAL
1	C	319	ASP
1	C	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	169	ASN
1	A	285	HIS
1	A	325	GLN
1	A	372	ASN
1	A	379	ASN
1	B	58	GLN
1	B	91	GLN
1	B	251	ASN
1	C	58	GLN
1	C	169	ASN
1	C	325	GLN
1	C	372	ASN
1	C	379	ASN

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	368/388 (94%)	0.07	4 (1%) 78 76	57, 86, 119, 160	0
1	B	364/388 (93%)	0.15	6 (1%) 70 68	65, 87, 111, 145	0
1	C	359/388 (92%)	0.14	5 (1%) 73 72	72, 93, 118, 136	0
All	All	1091/1164 (93%)	0.12	15 (1%) 73 72	57, 89, 117, 160	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ALA	2.7
1	A	198	ALA	2.5
1	C	115	ASP	2.5
1	A	80	GLU	2.4
1	A	56	VAL	2.4
1	B	136	PHE	2.3
1	B	59	GLU	2.3
1	C	279	VAL	2.3
1	B	52	SER	2.2
1	B	137	HIS	2.2
1	C	57	GLU	2.2
1	A	247	ILE	2.2
1	C	51	ALA	2.1
1	B	187	THR	2.1
1	C	319	ASP	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.