



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 AM UTC

PDB ID : 6XZT / pdb_00006xzt
Title : Crystal structure of helicase Pif1 from *Thermus oshimai* mutant G110C-E410C
Authors : Dai, Y.X.; Chen, W.F.; Teng, F.Y.; Liu, N.N.; Hou, X.M.; Dou, S.X.; Rety, S.; Xi, X.G.
Deposited on : 2020-02-05
Resolution : 3.34 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

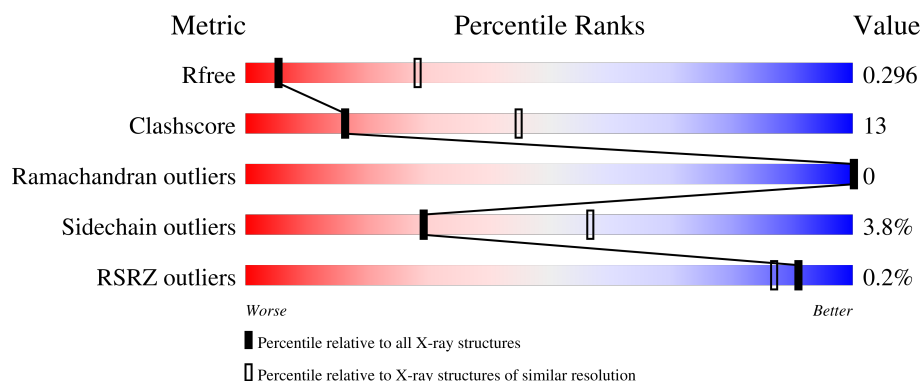
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	446	 67% 28% ...
1	B	446	 71% 24% ...

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7008 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 PIF1 helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3504	2240	641	618	5			
1	B	436	Total	C	N	O	S	0	0	0
			3504	2240	641	618	5			

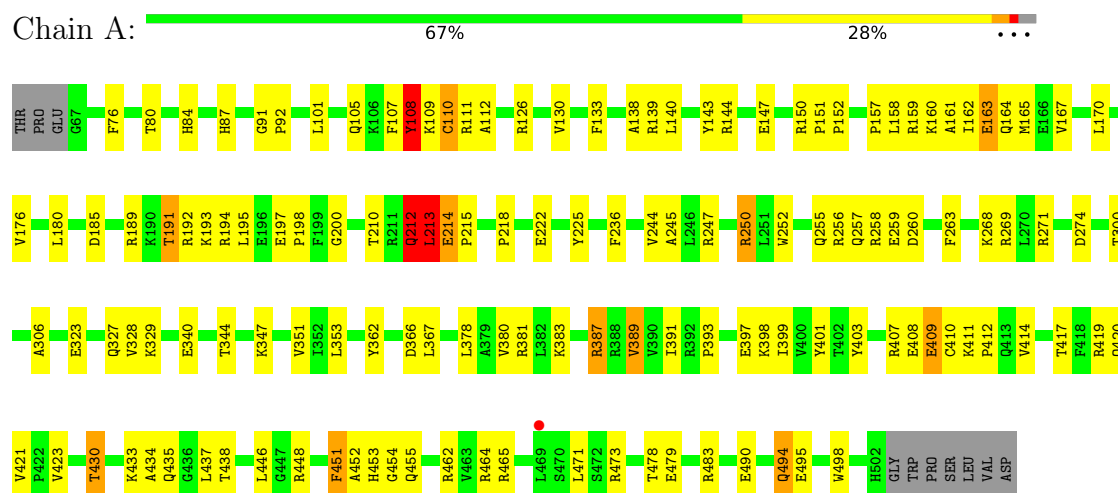
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	-	expression tag	UNP K7RJ88
A	106	LYS	GLU	conflict	UNP K7RJ88
A	110	CYS	GLY	engineered mutation	UNP K7RJ88
A	162	ILE	MET	conflict	UNP K7RJ88
A	410	CYS	ILE	engineered mutation	UNP K7RJ88
A	456	LEU	PRO	conflict	UNP K7RJ88
A	508	VAL	-	expression tag	UNP K7RJ88
A	509	ASP	-	expression tag	UNP K7RJ88
B	64	THR	-	expression tag	UNP K7RJ88
B	106	LYS	GLU	conflict	UNP K7RJ88
B	110	CYS	GLY	engineered mutation	UNP K7RJ88
B	162	ILE	MET	conflict	UNP K7RJ88
B	410	CYS	ILE	engineered mutation	UNP K7RJ88
B	456	LEU	PRO	conflict	UNP K7RJ88
B	508	VAL	-	expression tag	UNP K7RJ88
B	509	ASP	-	expression tag	UNP K7RJ88

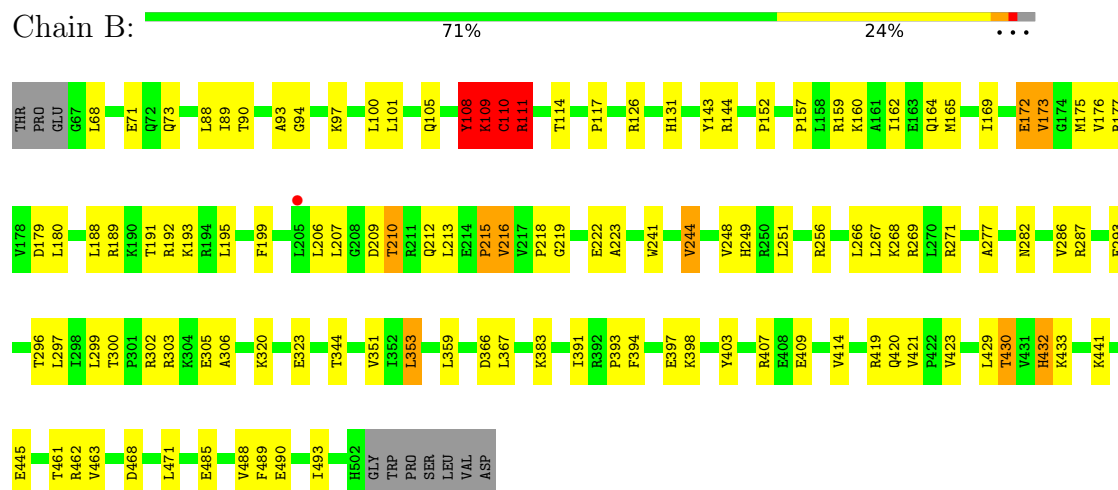
3 Residue-property plots

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: PIF1 helicase



• Molecule 1: PIF1 helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.07Å 58.68Å 118.16Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	52.55 – 3.34 52.55 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.55-3.34) 99.7 (52.55-3.34)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.252 , 0.291 0.263 , 0.296	Depositor DCC
R_{free} test set	756 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	137.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 105.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	0.26	0/3587	0.73	8/4867 (0.2%)
1	B	0.30	0/3587	0.88	17/4867 (0.3%)
All	All	0.28	0/7174	0.81	25/9734 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	1	6
All	All	1	11

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LYS	CA-C-N	15.28	150.72	121.54
1	B	109	LYS	C-N-CA	15.28	150.72	121.54
1	B	109	LYS	N-CA-CB	13.83	133.21	110.39
1	B	110	CYS	CA-C-N	13.67	144.38	123.47
1	B	110	CYS	C-N-CA	13.67	144.38	123.47
1	A	212	GLN	CA-C-N	13.60	146.06	122.12
1	A	212	GLN	C-N-CA	13.60	146.06	122.12
1	B	111	ARG	N-CA-C	12.29	128.22	113.23
1	B	108	TYR	CA-C-N	11.16	138.37	122.85
1	B	108	TYR	C-N-CA	11.16	138.37	122.85
1	A	214	GLU	N-CA-C	10.08	132.09	109.81
1	B	109	LYS	O-C-N	7.36	131.92	122.87
1	B	108	TYR	O-C-N	7.35	131.98	122.43
1	B	111	ARG	CB-CG-CD	6.53	126.31	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	GLU	N-CA-CB	-6.44	98.91	110.37
1	B	215	PRO	N-CA-C	6.11	125.06	112.47
1	A	108	TYR	CA-C-N	6.04	133.09	121.54
1	A	108	TYR	C-N-CA	6.04	133.09	121.54
1	B	110	CYS	CB-CA-C	5.97	122.30	110.42
1	B	94	GLY	CA-C-N	5.77	132.57	121.54
1	B	94	GLY	C-N-CA	5.77	132.57	121.54
1	B	109	LYS	N-CA-C	-5.54	97.44	107.75
1	A	213	LEU	CA-C-N	5.30	134.72	121.80
1	A	213	LEU	C-N-CA	5.30	134.72	121.80
1	B	111	ARG	CA-CB-CG	-5.07	103.96	114.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	109	LYS	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Peptide
1	A	109	LYS	Peptide
1	A	163	GLU	Peptide
1	A	213	LEU	Mainchain
1	A	494	GLN	Peptide
1	B	108	TYR	Peptide
1	B	109	LYS	Peptide
1	B	110	CYS	Peptide,Mainchain
1	B	432	HIS	Peptide
1	B	93	ALA	Peptide

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	3504	0	3563	102	0
1	B	3504	0	3563	84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7008	0	7126	184	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 13.

All (184) 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:108:TYR:HB3	1:A:111:ARG:HB2	1.41	0.99
1:A:212:GLN:OE1	1:A:435:GLN:NE2	2.02	0.93
1:A:212:GLN:HE22	1:A:435:GLN:HG3	1.36	0.90
1:A:212:GLN:NE2	1:A:435:GLN:HG3	1.88	0.87
1:A:271:ARG:NH2	1:A:490:GLU:OE1	2.08	0.84
1:B:111:ARG:HH11	1:B:164:GLN:HB2	1.44	0.82
1:B:111:ARG:HG3	1:B:165:MET:HA	1.60	0.81
1:A:194:ARG:HB2	1:A:200:GLY:HA2	1.62	0.80
1:A:161:ALA:HB2	1:A:403:TYR:HB2	1.66	0.78
1:B:219:GLY:HA2	1:B:223:ALA:HB2	1.67	0.76
1:A:451:PHE:HD1	1:A:479:GLU:HG2	1.50	0.76
1:A:258:ARG:HG2	1:A:464:ARG:HD2	1.69	0.75
1:B:303:ARG:HA	1:B:430:THR:HG21	1.68	0.73
1:B:172:GLU:H	1:B:172:GLU:CD	1.96	0.73
1:B:300:THR:HG22	1:B:445:GLU:HB3	1.72	0.71
1:A:110:CYS:SG	1:A:411:LYS:N	2.61	0.71
1:B:157:PRO:HA	1:B:160:LYS:HE2	1.73	0.70
1:B:241:TRP:HD1	1:B:244:VAL:HG23	1.56	0.70
1:A:250:ARG:HG3	1:A:252:TRP:CE3	2.27	0.70
1:B:403:TYR:HA	1:B:409:GLU:HG2	1.72	0.69
1:B:173:VAL:HG11	1:B:206:LEU:HD22	1.77	0.67
1:A:112:ALA:HB2	1:A:167:VAL:HB	1.75	0.67
1:B:209:ASP:HB3	1:B:212:GLN:HG2	1.77	0.67
1:A:403:TYR:HA	1:A:410:CYS:HA	1.77	0.66
1:B:463:VAL:HG21	1:B:468:ASP:HB2	1.78	0.66
1:B:109:LYS:HB3	1:B:110:CYS:HB3	1.78	0.66
1:A:140:LEU:HD22	1:A:222:GLU:HG3	1.79	0.65
1:A:157:PRO:HA	1:A:160:LYS:HZ2	1.61	0.64
1:A:151:PRO:HB3	1:A:191:THR:HG23	1.80	0.64
1:B:297:LEU:HD11	1:B:429:LEU:HB3	1.81	0.63
1:A:170:LEU:HD21	1:A:176:VAL:HG21	1.80	0.62
1:A:80:THR:HG22	1:A:108:TYR:OH	1.98	0.62
1:A:353:LEU:HD12	1:A:366:ASP:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD21	1:A:391:ILE:HG21	1.81	0.61
1:B:393:PRO:HB2	1:B:419:ARG:HE	1.65	0.61
1:A:189:ARG:HB3	1:A:195:LEU:HA	1.82	0.61
1:A:143:TYR:OH	1:A:144:ARG:NH1	2.34	0.60
1:A:397:GLU:HB3	1:A:414:VAL:HG13	1.82	0.60
1:A:198:PRO:HG3	1:A:244:VAL:HB	1.82	0.60
1:A:260:ASP:O	1:A:263:PHE:N	2.34	0.60
1:A:157:PRO:HA	1:A:160:LYS:NZ	2.17	0.60
1:B:367:LEU:HD23	1:B:383:LYS:HD3	1.83	0.60
1:A:407:ARG:O	1:A:408:GLU:HG2	2.02	0.60
1:A:367:LEU:HD23	1:A:383:LYS:HD3	1.83	0.59
1:A:329:LYS:HB2	1:A:417:THR:HB	1.83	0.59
1:A:185:ASP:O	1:A:189:ARG:HG3	2.02	0.58
1:A:471:LEU:H	1:A:471:LEU:HD23	1.68	0.58
1:B:143:TYR:OH	1:B:144:ARG:NH1	2.36	0.58
1:A:126:ARG:HG2	1:A:399:ILE:HD12	1.84	0.58
1:B:306:ALA:CB	1:B:430:THR:HG22	2.34	0.58
1:A:152:PRO:HD2	1:A:191:THR:HG21	1.85	0.57
1:B:177:ARG:NH2	1:B:179:ASP:OD2	2.37	0.57
1:B:89:ILE:HB	1:B:207:LEU:HD12	1.86	0.57
1:A:84:HIS:NE2	1:A:245:ALA:O	2.38	0.57
1:A:269:ARG:NH1	1:A:274:ASP:OD2	2.37	0.56
1:A:110:CYS:HB3	1:A:409:GLU:HG3	1.88	0.56
1:B:105:GLN:HE22	1:B:126:ARG:HG3	1.71	0.56
1:A:362:TYR:HD2	1:A:389:VAL:HG11	1.70	0.56
1:A:189:ARG:HH11	1:A:198:PRO:HA	1.71	0.56
1:A:257:GLN:C	1:A:259:GLU:H	2.13	0.56
1:B:191:THR:HG23	1:B:192:ARG:HD3	1.88	0.55
1:A:260:ASP:HB2	1:A:465:ARG:HG2	1.89	0.55
1:A:451:PHE:HB3	1:A:478:THR:HG23	1.89	0.55
1:A:189:ARG:HD2	1:A:197:GLU:O	2.07	0.55
1:A:212:GLN:HE22	1:A:435:GLN:CG	2.14	0.55
1:A:393:PRO:HA	1:A:421:VAL:HA	1.89	0.54
1:B:111:ARG:NH1	1:B:164:GLN:HB2	2.17	0.54
1:A:446:LEU:HG	1:A:448:ARG:H	1.73	0.54
1:A:323:GLU:HG2	1:A:344:THR:HG22	1.89	0.54
1:B:111:ARG:NE	1:B:409:GLU:O	2.41	0.54
1:B:296:THR:HG23	1:B:441:LYS:HG2	1.90	0.53
1:A:133:PHE:O	1:A:158:LEU:HD11	2.08	0.53
1:A:381:ARG:HA	1:A:387:ARG:HB2	1.91	0.53
1:B:160:LYS:HE3	1:B:403:TYR:CG	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:HG2	1:B:344:THR:HG22	1.91	0.52
1:A:300:THR:OG1	1:A:306:ALA:HB2	2.09	0.52
1:A:110:CYS:SG	1:A:410:CYS:N	2.82	0.52
1:B:162:ILE:O	1:B:165:MET:HG2	2.10	0.52
1:B:394:PHE:O	1:B:419:ARG:HA	2.10	0.52
1:B:420:GLN:HG2	1:B:421:VAL:H	1.74	0.52
1:A:256:ARG:H	1:A:256:ARG:CD	2.23	0.52
1:B:215:PRO:O	1:B:216:VAL:HG13	2.09	0.51
1:A:271:ARG:HH22	1:A:490:GLU:CD	2.17	0.51
1:B:403:TYR:HA	1:B:409:GLU:CG	2.38	0.51
1:B:109:LYS:HB3	1:B:110:CYS:CB	2.40	0.51
1:B:114:THR:HG22	1:B:169:ILE:HB	1.93	0.51
1:B:286:VAL:HA	1:B:471:LEU:HB2	1.91	0.51
1:A:108:TYR:CE1	1:A:167:VAL:HG21	2.45	0.51
1:B:266:LEU:HD12	1:B:277:ALA:HB1	1.92	0.51
1:A:163:GLU:O	1:A:164:GLN:HG3	2.11	0.50
1:B:269:ARG:NH1	1:B:277:ALA:HB2	2.27	0.49
1:B:162:ILE:HG21	1:B:191:THR:HG21	1.94	0.49
1:A:420:GLN:HG2	1:A:421:VAL:H	1.78	0.49
1:A:256:ARG:H	1:A:256:ARG:HD3	1.76	0.49
1:B:248:VAL:HG11	1:B:493:ILE:HD12	1.95	0.49
1:A:452:ALA:HB3	1:A:455:GLN:HG3	1.95	0.49
1:B:282:ASN:O	1:B:286:VAL:HG22	2.13	0.49
1:A:192:ARG:O	1:A:193:LYS:HG2	2.13	0.49
1:A:210:THR:O	1:A:213:LEU:HG	2.12	0.49
1:B:300:THR:OG1	1:B:306:ALA:HB2	2.13	0.49
1:A:158:LEU:O	1:A:162:ILE:HG23	2.13	0.48
1:B:407:ARG:O	1:B:407:ARG:HG3	2.13	0.48
1:A:453:HIS:HB3	1:A:483:ARG:HD3	1.95	0.48
1:B:172:GLU:CD	1:B:172:GLU:N	2.68	0.48
1:B:287:ARG:NH1	1:B:293:GLU:OE2	2.46	0.48
1:A:193:LYS:O	1:B:359:LEU:HD21	2.14	0.48
1:B:101:LEU:O	1:B:105:GLN:HG2	2.15	0.47
1:A:138:ALA:O	1:A:139:ARG:HG3	2.15	0.47
1:B:89:ILE:HA	1:B:249:HIS:O	2.15	0.47
1:B:299:LEU:HD23	1:B:429:LEU:O	2.14	0.47
1:B:108:TYR:O	1:B:109:LYS:HE2	2.15	0.47
1:A:218:PRO:HG2	1:A:222:GLU:HB3	1.97	0.46
1:A:268:LYS:HA	1:A:271:ARG:HD3	1.96	0.46
1:A:152:PRO:HG3	1:A:158:LEU:HD23	1.97	0.46
1:B:117:PRO:HD2	1:B:172:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:O	1:B:222:GLU:HB2	2.15	0.46
1:A:143:TYR:CE1	1:A:144:ARG:HG3	2.51	0.46
1:B:189:ARG:HB3	1:B:195:LEU:HA	1.96	0.46
1:A:362:TYR:CD2	1:A:389:VAL:HG11	2.50	0.46
1:A:454:GLY:HA2	1:A:479:GLU:O	2.16	0.46
1:A:401:TYR:CD2	1:A:412:PRO:HB3	2.51	0.46
1:B:302:ARG:HB3	1:B:305:GLU:OE1	2.16	0.45
1:A:159:ARG:HA	1:A:162:ILE:HG12	1.98	0.45
1:A:87:HIS:CE1	1:A:247:ARG:HD3	2.52	0.45
1:B:164:GLN:NE2	1:B:409:GLU:OE2	2.48	0.45
1:A:87:HIS:HE1	1:A:247:ARG:HD3	1.81	0.45
1:B:157:PRO:HA	1:B:160:LYS:CE	2.45	0.45
1:B:256:ARG:NH1	1:B:461:THR:O	2.50	0.45
1:B:489:PHE:O	1:B:493:ILE:HG12	2.17	0.45
1:A:236:PHE:HB2	1:A:498:TRP:CH2	2.53	0.44
1:A:193:LYS:HB2	1:B:359:LEU:HD22	1.97	0.44
1:A:162:ILE:O	1:A:165:MET:HG2	2.17	0.44
1:B:131:HIS:NE2	1:B:180:LEU:HD13	2.32	0.44
1:B:193:LYS:HE2	1:B:193:LYS:HB3	1.84	0.44
1:B:173:VAL:O	1:B:176:VAL:HG22	2.17	0.44
1:A:347:LYS:H	1:A:347:LYS:HG2	1.56	0.44
1:A:430:THR:HG23	1:A:433:LYS:HB2	1.99	0.44
1:B:88:LEU:HB3	1:B:248:VAL:HG22	1.99	0.44
1:A:351:VAL:HB	1:A:423:VAL:HG22	1.99	0.44
1:A:407:ARG:HG3	1:A:409:GLU:CB	2.48	0.44
1:A:152:PRO:HG3	1:A:158:LEU:CD2	2.49	0.43
1:B:210:THR:HB	1:B:490:GLU:OE1	2.18	0.43
1:B:485:GLU:O	1:B:488:VAL:HG12	2.19	0.43
1:B:191:THR:HG23	1:B:192:ARG:CD	2.47	0.43
1:B:268:LYS:HA	1:B:271:ARG:HD3	2.01	0.43
1:A:112:ALA:HA	1:A:167:VAL:O	2.19	0.43
1:B:100:LEU:HD22	1:B:207:LEU:HD11	2.01	0.43
1:A:435:GLN:HA	1:A:462:ARG:CZ	2.50	0.42
1:B:306:ALA:HB2	1:B:430:THR:HG22	2.01	0.42
1:B:97:LYS:HE2	1:B:207:LEU:HG	2.01	0.42
1:A:451:PHE:CD1	1:A:479:GLU:HG2	2.41	0.42
1:B:393:PRO:HA	1:B:421:VAL:HA	2.02	0.42
1:A:101:LEU:O	1:A:105:GLN:HG2	2.19	0.42
1:B:152:PRO:HB2	1:B:159:ARG:HB2	2.02	0.42
1:B:188:LEU:HB3	1:B:199:PHE:O	2.20	0.42
1:B:351:VAL:HB	1:B:423:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:HB3	1:B:414:VAL:HG13	2.01	0.42
1:A:147:GLU:O	1:A:150:ARG:NH2	2.52	0.42
1:A:160:LYS:HZ3	1:A:403:TYR:HB3	1.84	0.42
1:B:219:GLY:HA2	1:B:223:ALA:CB	2.44	0.42
1:A:255:GLN:O	1:A:259:GLU:HG2	2.20	0.42
1:A:381:ARG:HA	1:A:387:ARG:CB	2.50	0.41
1:A:140:LEU:HD21	1:A:225:TYR:CD2	2.54	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD2	1.79	0.41
1:B:175:MET:O	1:B:215:PRO:HB3	2.21	0.41
1:B:353:LEU:HD23	1:B:366:ASP:HB3	2.03	0.41
1:B:432:HIS:O	1:B:432:HIS:CG	2.71	0.41
1:A:76:PHE:HZ	1:A:107:PHE:CD1	2.39	0.41
1:A:378:LEU:HD12	1:A:380:VAL:HG13	2.02	0.41
1:B:71:GLU:OE2	1:B:251:LEU:HG	2.20	0.41
1:B:90:THR:O	1:B:251:LEU:HB3	2.21	0.41
1:A:130:VAL:HG11	1:A:180:LEU:HD21	2.01	0.41
1:A:250:ARG:HD2	1:A:494:GLN:OE1	2.20	0.41
1:A:327:GLN:OE1	1:A:419:ARG:NH2	2.54	0.41
1:A:434:ALA:HA	1:A:437:LEU:HD13	2.03	0.41
1:B:177:ARG:NE	1:B:179:ASP:OD1	2.54	0.41
1:A:471:LEU:HD12	1:A:473:ARG:O	2.21	0.40
1:B:68:LEU:HB3	1:B:73:GLN:HG3	2.02	0.40
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.84	0.40
1:A:91:GLY:HA2	1:A:92:PRO:HD3	1.95	0.40
1:A:451:PHE:HD1	1:A:479:GLU:CG	2.27	0.40
1:A:143:TYR:CD1	1:A:144:ARG:HG3	2.55	0.40
1:A:162:ILE:HG13	1:A:163:GLU:N	2.36	0.40
1:B:462:ARG:HA	1:B:462:ARG:HD3	1.97	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	434/446 (97%)	426 (98%)	8 (2%)	0	100	100
1	B	434/446 (97%)	422 (97%)	12 (3%)	0	100	100
All	All	868/892 (97%)	848 (98%)	20 (2%)	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	365/374 (98%)	351 (96%)	14 (4%)	29	57
1	B	365/374 (98%)	351 (96%)	14 (4%)	29	57
All	All	730/748 (98%)	702 (96%)	28 (4%)	29	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	CYS
1	A	191	THR
1	A	212	GLN
1	A	250	ARG
1	A	328	VAL
1	A	340	GLU
1	A	387	ARG
1	A	389	VAL
1	A	398	LYS
1	A	409	GLU
1	A	430	THR
1	A	438	THR
1	A	451	PHE
1	A	495	GLU
1	B	109	LYS
1	B	111	ARG
1	B	172	GLU
1	B	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	THR
1	B	213	LEU
1	B	216	VAL
1	B	244	VAL
1	B	320	LYS
1	B	353	LEU
1	B	391	ILE
1	B	398	LYS
1	B	430	THR
1	B	433	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	255	GLN
1	A	257	GLN
1	A	385	ASN
1	A	432	HIS
1	A	435	GLN
1	B	237	GLN
1	B	420	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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	436/446 (97%)	-0.57	1 (0%) 91 87	97, 148, 191, 234	0
1	B	436/446 (97%)	-0.51	1 (0%) 91 87	105, 155, 216, 339	0
All	All	872/892 (97%)	-0.54	2 (0%) 91 87	97, 151, 202, 339	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	2.7
1	A	469	LEU	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.