Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 10:03 AM GMT

PDB ID	:	6S3E
Title	:	Crystal structure of helicase Pif1 from Thermus oshimai in apo form
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	:	2019-06-25
Resolution	:	3.79 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 following versions of software and data (see references ⓘ) were used in the production of this report:

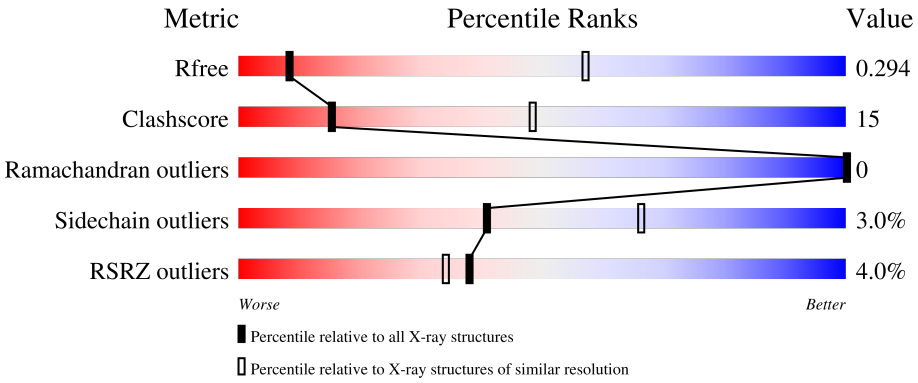
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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}	130704	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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 <=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	444	2% 66% 28%
1	B	444	6% 68% 29%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7024 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	2241	640	620	3			
1	B	438	Total	C	N	O	S	0	0	0
			3520	2251	642	624	3			

There are 6 discrepancies between the modelled and reference sequences:

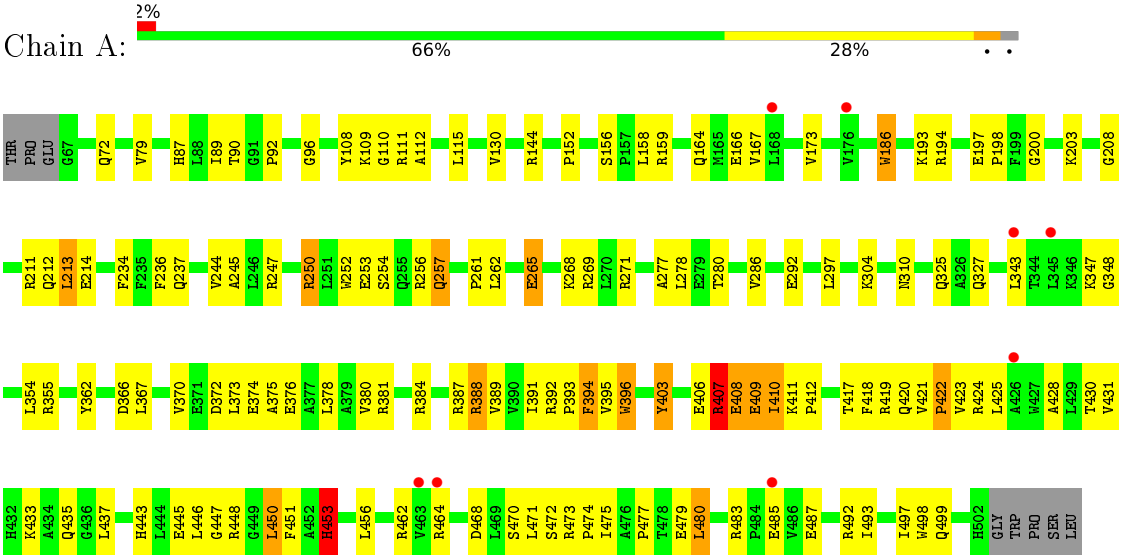
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	ALA	conflict	UNP K7RJ88
A	162	ILE	MET	conflict	UNP K7RJ88
A	456	LEU	PRO	conflict	UNP K7RJ88
B	64	THR	ALA	conflict	UNP K7RJ88
B	162	ILE	MET	conflict	UNP K7RJ88
B	456	LEU	PRO	conflict	UNP K7RJ88

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.

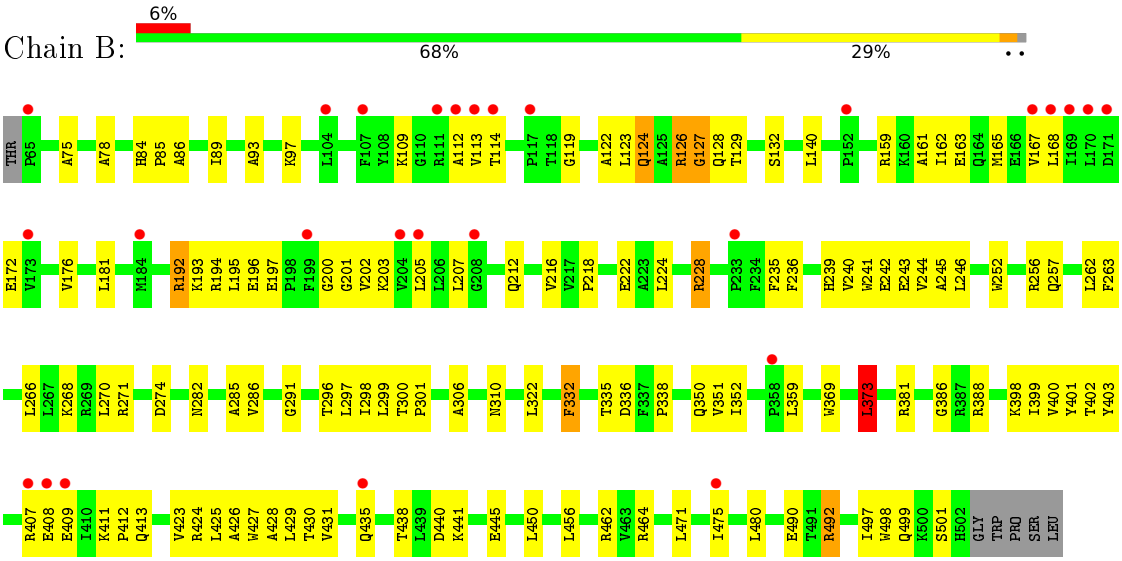
- Molecule 1: PIF1 helicase

Chain A:



- Molecule 1: PIF1 helicase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.27Å 59.41Å 117.15Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	36.71 – 3.79 74.23 – 3.79	Depositor EDS
% Data completeness (in resolution range)	96.8 (36.71-3.79) 96.9 (74.23-3.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.14rc1_3177: ???)	Depositor
R, R_{free}	0.237 , 0.295 0.237 , 0.294	Depositor DCC
R_{free} test set	530 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	132.9	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 105.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/3587	0.59	2/4868 (0.0%)
1	B	0.30	0/3604	0.60	2/4891 (0.0%)
All	All	0.30	0/7191	0.59	4/9759 (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	A	0	10
1	B	0	4
All	All	0	14

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	480	LEU	CA-CB-CG	9.54	137.24	115.30
1	B	127	GLY	N-CA-C	6.19	128.58	113.10
1	A	480	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	B	373	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	LEU	Peptide
1	A	254	SER	Peptide
1	A	388	ARG	Peptide
1	A	396	TRP	Peptide
1	A	407	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	409	GLU	Peptide
1	A	410	ILE	Peptide
1	A	422	PRO	Peptide
1	A	450	LEU	Peptide
1	A	453	HIS	Peptide
1	B	124	GLN	Peptide
1	B	407	ARG	Peptide
1	B	408	GLU	Peptide
1	B	431	VAL	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	3504	0	3562	120	0
1	B	3520	0	3576	92	0
All	All	7024	0	7138	211	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 (211) 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:451:PHE:HB2	1:A:479:GLU:HB3	1.35	1.07
1:A:250:ARG:NH1	1:A:253:GLU:OE1	1.93	0.99
1:A:450:LEU:HD12	1:A:451:PHE:H	1.29	0.96
1:B:411:LYS:HG2	1:B:412:PRO:HD2	1.48	0.95
1:B:85:PRO:HB3	1:B:203:LYS:HA	1.49	0.94
1:A:378:LEU:HG	1:A:391:ILE:HG12	1.51	0.93
1:A:411:LYS:HD3	1:A:412:PRO:HD3	1.60	0.84
1:B:127:GLY:HA2	1:B:401:TYR:OH	1.80	0.81
1:A:92:PRO:HD3	1:A:252:TRP:HD1	1.44	0.81
1:B:271:ARG:HH21	1:B:490:GLU:HG3	1.52	0.75
1:A:211:ARG:HH22	1:A:256:ARG:NH1	1.86	0.73
1:A:381:ARG:HG2	1:A:387:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:O	1:B:401:TYR:OH	2.04	0.72
1:B:126:ARG:HB2	1:B:399:ILE:HD12	1.70	0.72
1:A:355:ARG:NH2	1:A:392:ARG:O	2.21	0.72
1:B:212:GLN:OE1	1:B:435:GLN:NE2	2.13	0.72
1:A:250:ARG:HE	1:A:252:TRP:HE3	1.36	0.72
1:A:262:LEU:O	1:A:265:GLU:HG3	1.93	0.69
1:B:306:ALA:HB2	1:B:430:THR:HG23	1.75	0.68
1:A:212:GLN:HE21	1:A:435:GLN:HB3	1.58	0.68
1:B:86:ALA:HB1	1:B:246:LEU:HA	1.74	0.68
1:B:499:GLN:HG3	1:B:501:SER:H	1.59	0.66
1:B:301:PRO:HG3	1:B:450:LEU:HD11	1.77	0.66
1:A:451:PHE:CB	1:A:479:GLU:HB3	2.20	0.66
1:A:492:ARG:NH1	1:A:499:GLN:O	2.29	0.66
1:B:239:HIS:ND1	1:B:242:GLU:OE2	2.26	0.65
1:A:422:PRO:O	1:A:423:VAL:HG13	1.98	0.64
1:A:109:LYS:HG3	1:A:411:LYS:NZ	2.13	0.64
1:A:111:ARG:HB2	1:A:166:GLU:HB2	1.80	0.64
1:A:343:LEU:HD21	1:A:423:VAL:HG23	1.79	0.64
1:B:128:GLN:NE2	1:B:400:VAL:HG23	2.13	0.64
1:B:300:THR:HG22	1:B:445:GLU:HB3	1.80	0.64
1:A:403:TYR:HE1	1:A:408:GLU:HA	1.62	0.63
1:B:297:LEU:HD11	1:B:429:LEU:HD23	1.79	0.63
1:A:213:LEU:HD22	1:A:234:PHE:CD2	2.34	0.63
1:B:381:ARG:NH2	1:B:386:GLY:O	2.29	0.63
1:A:374:GLU:HG2	1:A:375:ALA:H	1.63	0.62
1:A:450:LEU:HD12	1:A:451:PHE:N	2.08	0.62
1:A:388:ARG:HB3	1:A:389:VAL:HG13	1.81	0.62
1:A:450:LEU:CD1	1:A:451:PHE:H	2.08	0.60
1:A:451:PHE:HB2	1:A:479:GLU:CB	2.23	0.60
1:A:213:LEU:HD23	1:A:214:GLU:HA	1.84	0.60
1:B:245:ALA:HB1	1:B:497:ILE:HB	1.83	0.60
1:A:173:VAL:HG12	1:A:208:GLY:HA3	1.83	0.59
1:A:144:ARG:HB2	1:A:186:TRP:CE2	2.38	0.59
1:A:327:GLN:HG3	1:A:419:ARG:HB3	1.85	0.59
1:B:86:ALA:CB	1:B:246:LEU:HA	2.32	0.58
1:A:297:LEU:HD11	1:A:367:LEU:HD21	1.85	0.58
1:A:443:HIS:HA	1:A:470:SER:O	2.02	0.58
1:B:123:LEU:HD21	1:B:336:ASP:O	2.04	0.58
1:B:140:LEU:HD22	1:B:222:GLU:HG3	1.84	0.58
1:B:195:LEU:HD12	1:B:196:GLU:HG3	1.86	0.58
1:B:192:ARG:NH1	1:B:200:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:HIS:CG	1:A:483:ARG:HE	2.21	0.58
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.84	0.58
1:A:109:LYS:HG3	1:A:411:LYS:HZ2	1.68	0.57
1:B:114:THR:O	1:B:401:TYR:CZ	2.56	0.57
1:A:395:VAL:HB	1:A:419:ARG:HB2	1.87	0.57
1:B:75:ALA:O	1:B:78:ALA:N	2.37	0.57
1:B:89:ILE:HB	1:B:207:LEU:HG	1.86	0.56
1:A:453:HIS:CD2	1:A:483:ARG:HG2	2.39	0.56
1:B:402:THR:HG22	1:B:403:TYR:N	2.19	0.56
1:A:115:LEU:HD23	1:A:130:VAL:HA	1.88	0.56
1:A:237:GLN:NE2	1:A:485:GLU:OE1	2.38	0.56
1:B:159:ARG:NH1	1:B:163:GLU:OE2	2.38	0.56
1:B:224:LEU:HD22	1:B:228:ARG:HH21	1.71	0.56
1:A:72:GLN:NE2	1:A:96:GLY:O	2.39	0.55
1:A:410:ILE:HB	1:A:411:LYS:HE2	1.88	0.55
1:B:335:THR:HG22	1:B:336:ASP:H	1.71	0.55
1:A:250:ARG:CZ	1:A:252:TRP:HB2	2.37	0.55
1:A:374:GLU:HG2	1:A:375:ALA:N	2.21	0.55
1:A:393:PRO:HA	1:A:421:VAL:HA	1.89	0.55
1:A:445:GLU:O	1:A:446:LEU:HD23	2.07	0.54
1:A:245:ALA:HB1	1:A:497:ILE:HG23	1.88	0.54
1:B:167:VAL:HA	1:B:203:LYS:O	2.06	0.54
1:B:402:THR:HG22	1:B:403:TYR:H	1.73	0.54
1:B:426:ALA:HA	1:B:429:LEU:HD21	1.89	0.54
1:B:291:GLY:HA2	1:B:298:ILE:HD11	1.89	0.53
1:A:110:GLY:O	1:A:410:ILE:HG12	2.08	0.53
1:B:128:GLN:HB3	1:B:401:TYR:CD2	2.43	0.53
1:A:194:ARG:HB2	1:A:200:GLY:HA2	1.91	0.53
1:A:456:LEU:HG	1:A:480:LEU:HD23	1.90	0.53
1:B:129:THR:O	1:B:132:SER:N	2.36	0.53
1:A:167:VAL:HG22	1:A:203:LYS:HB3	1.91	0.52
1:A:456:LEU:CG	1:A:480:LEU:HD23	2.40	0.52
1:B:270:LEU:HD23	1:B:480:LEU:HD21	1.91	0.52
1:A:271:ARG:HG3	1:A:487:GLU:OE2	2.10	0.52
1:B:93:ALA:HA	1:B:97:LYS:HB3	1.92	0.52
1:B:128:GLN:OE1	1:B:401:TYR:N	2.38	0.52
1:A:79:VAL:HG21	1:A:89:ILE:HD11	1.90	0.51
1:B:426:ALA:HA	1:B:429:LEU:CD2	2.41	0.51
1:A:355:ARG:NE	1:A:422:PRO:HG3	2.25	0.51
1:B:425:LEU:H	1:B:425:LEU:HD12	1.76	0.51
1:B:122:ALA:O	1:B:126:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HD12	1:A:473:ARG:HB3	1.93	0.51
1:A:411:LYS:HD3	1:A:412:PRO:CD	2.38	0.51
1:A:277:ALA:O	1:A:280:THR:HG22	2.11	0.51
1:A:430:THR:HG23	1:A:433:LYS:H	1.76	0.51
1:A:325:GLN:O	1:A:420:GLN:NE2	2.44	0.50
1:A:395:VAL:HA	1:A:418:PHE:O	2.10	0.50
1:A:109:LYS:HE2	1:A:411:LYS:HZ2	1.76	0.50
1:B:240:VAL:O	1:B:243:GLU:HG2	2.11	0.50
1:A:493:ILE:HG22	1:A:498:TRP:HB2	1.93	0.50
1:B:310:ASN:OD1	1:B:427:TRP:HB2	2.12	0.50
1:A:395:VAL:CG2	1:A:417:THR:HB	2.42	0.50
1:A:278:LEU:HD23	1:A:480:LEU:HD11	1.93	0.50
1:A:213:LEU:HD22	1:A:234:PHE:CE2	2.47	0.50
1:B:113:VAL:HG12	1:B:165:MET:SD	2.52	0.50
1:B:306:ALA:CB	1:B:430:THR:HG23	2.40	0.50
1:B:492:ARG:HG2	1:B:498:TRP:HD1	1.77	0.50
1:A:268:LYS:O	1:A:271:ARG:HG2	2.12	0.49
1:B:332:PHE:CZ	1:B:398:LYS:HB2	2.47	0.49
1:B:128:GLN:HB3	1:B:401:TYR:CE2	2.46	0.49
1:B:109:LYS:HG3	1:B:409:GLU:OE2	2.13	0.49
1:B:262:LEU:HD12	1:B:263:PHE:N	2.27	0.49
1:B:298:ILE:O	1:B:428:ALA:HA	2.12	0.49
1:B:351:VAL:HB	1:B:423:VAL:HG13	1.94	0.49
1:A:257:GLN:NE2	1:A:464:ARG:O	2.46	0.48
1:A:90:THR:HA	1:A:208:GLY:O	2.14	0.48
1:A:366:ASP:OD2	1:A:384:ARG:HB2	2.13	0.48
1:A:108:TYR:HD1	1:A:111:ARG:HG3	1.78	0.48
1:B:256:ARG:HH12	1:B:438:THR:HB	1.78	0.48
1:A:355:ARG:HD3	1:A:396:TRP:CZ3	2.49	0.48
1:B:285:ALA:O	1:B:471:LEU:N	2.46	0.48
1:A:164:GLN:HG2	1:A:409:GLU:HA	1.95	0.47
1:A:193:LYS:HB3	1:B:359:LEU:HA	1.96	0.47
1:A:194:ARG:NH2	1:A:197:GLU:OE1	2.47	0.47
1:A:250:ARG:NE	1:A:252:TRP:HE3	2.08	0.47
1:A:403:TYR:CE1	1:A:408:GLU:HA	2.45	0.47
1:B:411:LYS:CG	1:B:412:PRO:HD2	2.33	0.47
1:A:447:GLY:O	1:A:448:ARG:HG2	2.15	0.47
1:A:111:ARG:C	1:A:410:ILE:HD11	2.35	0.47
1:A:424:ARG:HB2	1:A:433:LYS:HZ1	1.79	0.47
1:B:270:LEU:HA	1:B:274:ASP:OD1	2.15	0.47
1:A:406:GLU:OE1	1:A:407:ARG:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ALA:HA	1:B:403:TYR:HE1	1.80	0.47
1:A:261:PRO:HG2	1:A:262:LEU:HD22	1.96	0.47
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.69	0.47
1:A:198:PRO:HG3	1:A:244:VAL:HG22	1.96	0.46
1:A:268:LYS:HA	1:A:271:ARG:HD3	1.98	0.46
1:A:348:GLY:N	1:A:370:VAL:O	2.37	0.46
1:B:193:LYS:HD2	1:B:193:LYS:H	1.80	0.46
1:B:97:LYS:NZ	1:B:207:LEU:HB3	2.31	0.46
1:A:376:GLU:OE1	1:A:419:ARG:NH2	2.48	0.46
1:B:194:ARG:NH2	1:B:197:GLU:OE1	2.49	0.46
1:B:216:VAL:O	1:B:218:PRO:HD3	2.16	0.45
1:B:235:PHE:CE1	1:B:236:PHE:HD1	2.34	0.45
1:A:167:VAL:HA	1:A:203:LYS:O	2.17	0.45
1:A:378:LEU:H	1:A:391:ILE:HG13	1.81	0.45
1:A:362:TYR:HD2	1:A:389:VAL:HG11	1.82	0.45
1:A:380:VAL:HG23	1:A:389:VAL:HG23	1.99	0.44
1:A:473:ARG:O	1:A:473:ARG:HG3	2.16	0.44
1:B:322:LEU:HB2	1:B:373:LEU:HD22	1.97	0.44
1:A:354:LEU:HD11	1:A:433:LYS:HZ1	1.81	0.44
1:B:351:VAL:HA	1:B:426:ALA:H	1.83	0.44
1:A:152:PRO:HG3	1:A:158:LEU:HD22	2.00	0.44
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.86	0.44
1:A:286:VAL:CG2	1:A:474:PRO:HB3	2.48	0.44
1:B:296:THR:OG1	1:B:441:LYS:HD2	2.17	0.44
1:B:119:GLY:HA3	1:B:336:ASP:CG	2.37	0.44
1:B:299:LEU:O	1:B:445:GLU:N	2.50	0.44
1:A:156:SER:OG	1:A:159:ARG:HB2	2.17	0.44
1:A:92:PRO:HD3	1:A:252:TRP:CD1	2.37	0.44
1:A:468:ASP:OD1	1:A:468:ASP:N	2.50	0.44
1:B:338:PRO:O	1:B:424:ARG:NH2	2.51	0.44
1:A:388:ARG:HD3	1:A:388:ARG:HA	1.78	0.43
1:A:236:PHE:O	1:A:498:TRP:HH2	2.00	0.43
1:A:310:ASN:OD1	1:A:428:ALA:N	2.47	0.43
1:B:176:VAL:HG11	1:B:181:LEU:HG	1.99	0.43
1:B:300:THR:O	1:B:430:THR:HG22	2.17	0.43
1:A:462:ARG:HD3	1:A:462:ARG:HA	1.70	0.43
1:B:123:LEU:HD12	1:B:124:GLN:H	1.84	0.43
1:A:355:ARG:CZ	1:A:394:PHE:HB2	2.48	0.43
1:A:87:HIS:HA	1:A:247:ARG:O	2.18	0.43
1:B:301:PRO:HB3	1:B:450:LEU:HD21	2.00	0.43
1:B:413:GLN:HG3	1:B:413:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HA	1:A:407:ARG:NE	2.34	0.43
1:A:112:ALA:HA	1:A:167:VAL:O	2.18	0.43
1:B:84:HIS:HE2	1:B:244:VAL:HG13	1.83	0.43
1:A:347:LYS:HE2	1:A:372:ASP:HA	2.00	0.43
1:B:268:LYS:HA	1:B:268:LYS:HD2	1.91	0.42
1:B:350:GLN:HG3	1:B:369:TRP:NE1	2.34	0.42
1:A:394:PHE:O	1:A:419:ARG:HA	2.19	0.42
1:A:304:LYS:HB2	1:A:304:LYS:HE3	1.80	0.42
1:B:112:ALA:HB2	1:B:167:VAL:HB	2.01	0.42
1:B:168:LEU:HB2	1:B:202:VAL:HG11	2.02	0.42
1:B:97:LYS:HZ1	1:B:207:LEU:HB3	1.84	0.42
1:B:440:ASP:HA	1:B:464:ARG:NH2	2.35	0.42
1:B:194:ARG:HE	1:B:201:GLY:HA3	1.85	0.42
1:B:456:LEU:HD23	1:B:475:ILE:HD13	2.01	0.42
1:A:234:PHE:CZ	1:A:483:ARG:HD2	2.55	0.42
1:A:431:VAL:O	1:A:435:GLN:HG3	2.20	0.42
1:B:381:ARG:NH1	1:B:388:ARG:HB2	2.35	0.42
1:A:269:ARG:CZ	1:A:277:ALA:HB2	2.50	0.42
1:A:278:LEU:HD21	1:A:475:ILE:O	2.20	0.42
1:B:236:PHE:HA	1:B:241:TRP:CZ3	2.55	0.41
1:B:241:TRP:CE3	1:B:246:LEU:HD11	2.55	0.41
1:A:411:LYS:HA	1:A:411:LYS:HE2	2.02	0.41
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.93	0.41
1:A:92:PRO:HG2	1:A:256:ARG:HD2	2.02	0.41
1:A:112:ALA:N	1:A:410:ILE:HD11	2.36	0.41
1:A:152:PRO:HB2	1:A:156:SER:OG	2.20	0.41
1:A:472:SER:OG	1:A:473:ARG:N	2.53	0.41
1:B:266:LEU:HD23	1:B:270:LEU:HD13	2.02	0.41
1:A:108:TYR:CE1	1:A:167:VAL:HG21	2.56	0.41
1:A:424:ARG:HD2	1:A:424:ARG:HA	1.95	0.40
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.86	0.40
1:B:282:ASN:HA	1:B:286:VAL:HG13	2.03	0.40
1:B:203:LYS:NZ	1:B:205:LEU:HD21	2.36	0.40
1:B:228:ARG:HD3	1:B:228:ARG:HA	1.77	0.40
1:B:352:ILE:HB	1:B:426:ALA:HB2	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	434/444 (98%)	430 (99%)	4 (1%)	0	100	100
1	B	436/444 (98%)	427 (98%)	9 (2%)	0	100	100
All	All	870/888 (98%)	857 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	364/371 (98%)	352 (97%)	12 (3%)	38	64
1	B	366/371 (99%)	356 (97%)	10 (3%)	44	69
All	All	730/742 (98%)	708 (97%)	22 (3%)	41	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	TRP
1	A	250	ARG
1	A	257	GLN
1	A	265	GLU
1	A	292	GLU
1	A	373	LEU
1	A	394	PHE
1	A	403	TYR

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Mol	Chain	Res	Type
1	A	407	ARG
1	A	408	GLU
1	A	453	HIS
1	A	471	LEU
1	B	126	ARG
1	B	172	GLU
1	B	192	ARG
1	B	228	ARG
1	B	252	TRP
1	B	257	GLN
1	B	332	PHE
1	B	373	LEU
1	B	462	ARG
1	B	492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	212	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	436/444 (98%)	0.12	8 (1%)	68	65	91, 155, 231, 396	0
1	B	438/444 (98%)	0.33	27 (6%)	20	17	100, 177, 275, 369	0
All	All	874/888 (98%)	0.23	35 (4%)	38	34	91, 165, 249, 396	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	GLU	8.3
1	B	171	ASP	5.6
1	B	104	LEU	4.8
1	B	358	PRO	4.7
1	B	408	GLU	4.7
1	B	112	ALA	4.1
1	B	169	ILE	4.0
1	A	463	VAL	3.8
1	B	170	LEU	3.7
1	B	205	LEU	3.6
1	B	208	GLY	3.4
1	B	168	LEU	3.2
1	B	111	ARG	3.1
1	B	114	THR	3.1
1	B	65	PRO	2.8
1	B	204	VAL	2.7
1	B	152	PRO	2.7
1	B	199	PHE	2.6
1	B	113	VAL	2.5
1	A	345	LEU	2.4
1	B	184	MET	2.3
1	B	167	VAL	2.3
1	B	107	PHE	2.3
1	B	407	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLN	2.2
1	B	173	VAL	2.2
1	A	426	ALA	2.2
1	A	176	VAL	2.1
1	B	475	ILE	2.1
1	A	343	LEU	2.1
1	A	464	ARG	2.1
1	B	233	PRO	2.1
1	A	168	LEU	2.1
1	B	117	PRO	2.0
1	A	485	GLU	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 monosaccharides 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.