Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 03:31 PM JST

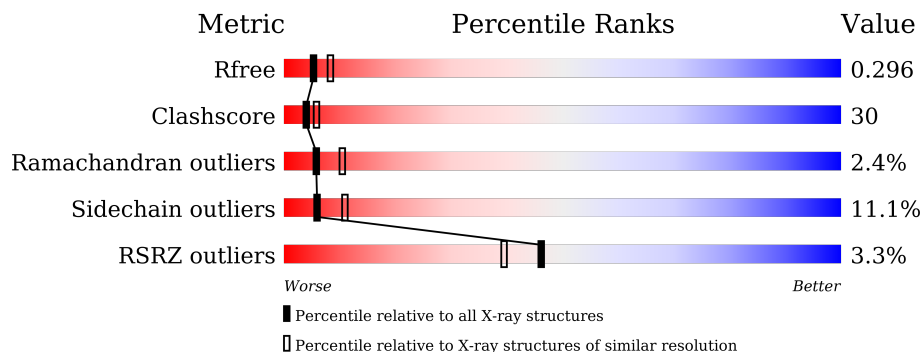|		
PDB ID	:	6JJ4
Title	:	Crystal structure of OsHXK6-apo form
Authors	:	He, C.; Wei, P.; Chen, J.; Wang, H.; Wan, Y.; Zhou, J.; Zhu, Y.; Huang, W.; Yin, L.
Deposited on	:	2019-02-25
Resolution	:	2.60 Å(reported)

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 2.60 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	Percentile Ranks	Value
Rfree		0.296
Clashscore		30
Ramachandran outliers		2.4%
Sidechain outliers		11.1%
RSRZ outliers		3.3%

Worse ← → Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	467	3% / 54% / 36% / 6% · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3539 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 Hexokinase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total 3495	C 2203	N 611	O 666	S 15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total 44	O 44	0	0

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: Hexokinase-6
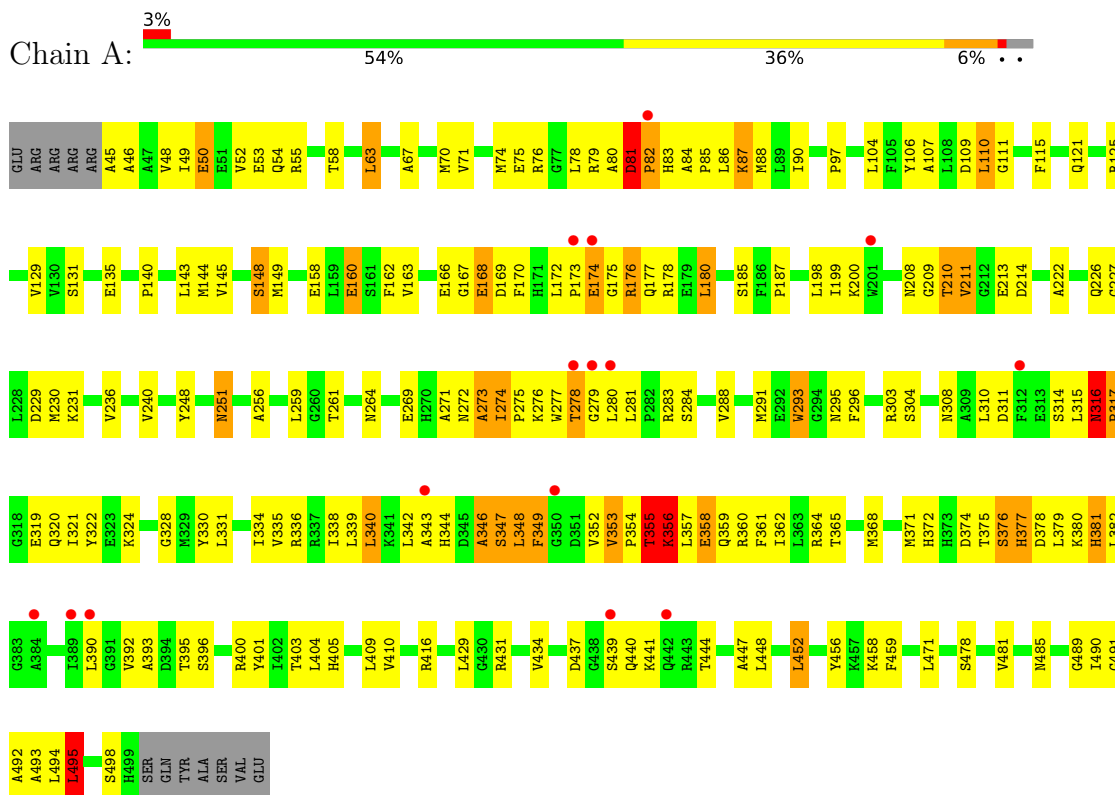
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	65.89Å 65.89Å 170.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.28 – 2.60 47.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.28-2.60) 96.3 (47.43-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.58 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.250 , 0.319 0.247 , 0.296	Depositor DCC
R_{free} test set	1350 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3539	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.92	2/3557 (0.1%)	0.94	16/4811 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	TYR	CE1-CZ	-6.23	1.30	1.38
1	A	269	GLU	CD-OE2	-5.95	1.19	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ILE	N-CA-C	-11.30	80.49	111.00
1	A	176	ARG	N-CA-C	-9.53	85.28	111.00
1	A	109	ASP	CB-CG-OD2	8.55	126.00	118.30
1	A	485	ASN	N-CA-C	8.13	132.95	111.00
1	A	316	ASN	N-CA-C	-7.26	91.41	111.00
1	A	278	THR	N-CA-C	-6.47	93.54	111.00
1	A	273	ALA	N-CA-C	6.32	128.06	111.00
1	A	169	ASP	N-CA-C	-6.03	94.73	111.00
1	A	316	ASN	C-N-CD	5.65	140.26	128.40
1	A	471	LEU	N-CA-C	-5.46	96.25	111.00
1	A	495	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	274	ILE	C-N-CD	5.39	139.72	128.40
1	A	175	GLY	N-CA-C	-5.30	99.85	113.10
1	A	346	ALA	N-CA-C	5.24	125.16	111.00
1	A	214	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	82	PRO	CA-N-CD	-5.09	104.37	111.50

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	3495	0	3490	211	0
2	A	44	0	0	9	0
All	All	3539	0	3490	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 30.

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:278:THR:CG2	1:A:283:ARG:HH11	1.60	1.12
1:A:346:ALA:HB3	1:A:347:SER:HA	1.36	1.03
1:A:311:ASP:OD1	1:A:317:PRO:O	1.80	0.99
1:A:278:THR:HG22	1:A:283:ARG:HH11	1.26	0.96
1:A:58:THR:HB	1:A:63:LEU:HD11	1.48	0.95
1:A:374:ASP:OD2	1:A:376:SER:OG	1.85	0.95
1:A:340:LEU:O	1:A:343:ALA:N	2.00	0.92
1:A:76:ARG:HG2	1:A:79:ARG:HH12	1.36	0.91
1:A:278:THR:HG22	1:A:283:ARG:NH1	1.86	0.90
1:A:278:THR:HG23	1:A:283:ARG:HH11	1.36	0.90
1:A:278:THR:HB	1:A:279:GLY:HA2	1.52	0.89
1:A:277:TRP:O	1:A:283:ARG:NH1	2.07	0.86
1:A:311:ASP:CG	1:A:317:PRO:O	2.14	0.86
1:A:180:LEU:C	1:A:180:LEU:HD12	1.96	0.85
1:A:278:THR:CG2	1:A:283:ARG:NH1	2.39	0.85
1:A:491:GLY:N	2:A:603:HOH:O	2.10	0.85
1:A:328:GLY:O	1:A:365:THR:OG1	1.93	0.85
1:A:346:ALA:CB	1:A:347:SER:HA	2.04	0.84
1:A:173:PRO:CB	1:A:174:GLU:HG2	2.07	0.84
1:A:303:ARG:NH2	1:A:308:ASN:OD1	2.10	0.84
1:A:319:GLU:O	1:A:324:LYS:NZ	2.10	0.83
1:A:314:SER:OG	1:A:316:ASN:O	1.96	0.82
1:A:172:LEU:HD22	1:A:176:ARG:CZ	2.11	0.81
1:A:173:PRO:HB2	1:A:174:GLU:CG	2.11	0.80
1:A:271:ALA:O	1:A:273:ALA:HA	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:O	1:A:357:LEU:HD23	1.80	0.80
1:A:172:LEU:H	1:A:172:LEU:HD12	1.47	0.79
1:A:173:PRO:CB	1:A:174:GLU:CG	2.62	0.78
1:A:180:LEU:HD12	1:A:180:LEU:O	1.85	0.76
1:A:490:ILE:HG22	1:A:493:ALA:H	1.50	0.76
1:A:76:ARG:HG2	1:A:79:ARG:NH1	1.99	0.76
1:A:78:LEU:O	1:A:275:PRO:HD2	1.85	0.75
1:A:371:MET:HB3	1:A:382:LEU:HD13	1.67	0.74
1:A:167:GLY:HA3	1:A:168:GLU:HB3	1.69	0.74
1:A:490:ILE:HA	1:A:492:ALA:H	1.52	0.74
1:A:81:ASP:N	1:A:81:ASP:OD1	2.21	0.73
1:A:173:PRO:HB2	1:A:174:GLU:HG3	1.70	0.73
1:A:67:ALA:O	1:A:71:VAL:HG23	1.89	0.72
1:A:311:ASP:OD2	1:A:317:PRO:O	2.07	0.72
1:A:226:GLN:H	1:A:227:GLY:HA2	1.56	0.71
1:A:352:VAL:O	1:A:354:PRO:HD3	1.90	0.71
1:A:340:LEU:CD2	1:A:344:HIS:HD2	2.03	0.71
1:A:236:VAL:HG11	1:A:494:LEU:HD23	1.74	0.70
1:A:177:GLN:HG3	1:A:229:ASP:OD1	1.91	0.69
1:A:381:HIS:H	1:A:381:HIS:CD2	2.08	0.69
1:A:275:PRO:O	1:A:278:THR:O	2.11	0.69
1:A:379:LEU:N	1:A:379:LEU:HD23	2.08	0.69
1:A:342:LEU:HA	1:A:346:ALA:CB	2.23	0.68
1:A:172:LEU:HB2	1:A:176:ARG:HD3	1.75	0.68
1:A:490:ILE:C	2:A:603:HOH:O	2.31	0.67
1:A:110:LEU:HD23	1:A:115:PHE:HB3	1.76	0.67
1:A:264:ASN:HA	1:A:293:TRP:CD1	2.29	0.67
1:A:173:PRO:C	1:A:174:GLU:HG3	2.15	0.67
1:A:173:PRO:HB2	1:A:174:GLU:HG2	1.76	0.67
1:A:339:LEU:HD21	1:A:403:THR:HG23	1.77	0.66
1:A:490:ILE:O	2:A:603:HOH:O	2.13	0.66
1:A:209:GLY:O	1:A:211:VAL:HG12	1.95	0.66
1:A:55:ARG:HE	1:A:304:SER:HA	1.61	0.65
1:A:335:VAL:O	1:A:339:LEU:HD13	1.96	0.65
1:A:340:LEU:HD22	1:A:344:HIS:HD2	1.59	0.65
1:A:173:PRO:HB3	1:A:174:GLU:HG2	1.79	0.64
1:A:178:ARG:HB2	1:A:230:MET:HE3	1.80	0.64
1:A:283:ARG:O	1:A:284:SER:HB3	1.98	0.63
1:A:498:SER:OG	2:A:602:HOH:O	2.01	0.62
1:A:167:GLY:CA	1:A:168:GLU:HB3	2.30	0.62
1:A:278:THR:CB	1:A:279:GLY:HA2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HB2	1:A:248:TYR:HB2	1.81	0.62
1:A:226:GLN:N	1:A:227:GLY:HA2	2.15	0.62
1:A:180:LEU:C	1:A:180:LEU:CD1	2.67	0.62
1:A:81:ASP:HB2	1:A:82:PRO:C	2.21	0.61
1:A:213:GLU:OE2	1:A:213:GLU:HA	1.99	0.61
1:A:58:THR:O	1:A:416:ARG:NH1	2.33	0.61
1:A:320:GLN:O	1:A:324:LYS:HG3	2.00	0.61
1:A:81:ASP:OD1	1:A:82:PRO:HA	2.02	0.60
1:A:121:GLN:HB3	1:A:131:SER:HB2	1.82	0.60
1:A:78:LEU:HA	1:A:276:LYS:HE2	1.84	0.60
1:A:76:ARG:NH1	1:A:85:PRO:HD3	2.16	0.60
1:A:353:VAL:O	1:A:353:VAL:HG23	2.00	0.60
1:A:104:LEU:O	2:A:605:HOH:O	2.16	0.59
1:A:278:THR:CG2	1:A:283:ARG:HE	2.16	0.59
1:A:490:ILE:CG2	1:A:493:ALA:H	2.15	0.59
1:A:76:ARG:HH11	1:A:85:PRO:HD3	1.67	0.58
1:A:396:SER:O	1:A:400:ARG:N	2.33	0.58
1:A:489:GLY:C	1:A:490:ILE:HG13	2.22	0.58
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.68	0.58
1:A:178:ARG:HB3	1:A:230:MET:HE2	1.86	0.58
1:A:199:ILE:HG22	1:A:200:LYS:HG2	1.85	0.58
1:A:342:LEU:HA	1:A:346:ALA:HB2	1.84	0.58
1:A:79:ARG:N	1:A:80:ALA:HB2	2.18	0.58
1:A:378:ASP:OD1	1:A:380:LYS:HG2	2.04	0.58
1:A:355:THR:C	1:A:357:LEU:H	2.07	0.58
1:A:335:VAL:HG11	1:A:368:MET:HE3	1.86	0.57
1:A:344:HIS:NE2	1:A:358:GLU:OE2	2.38	0.57
1:A:140:PRO:HD2	1:A:143:LEU:HD12	1.86	0.57
1:A:348:LEU:HD13	1:A:349:PHE:CZ	2.40	0.57
1:A:88:MET:SD	1:A:291:MET:HG2	2.46	0.56
1:A:381:HIS:CD2	1:A:381:HIS:N	2.73	0.56
1:A:49:ILE:O	1:A:52:VAL:N	2.37	0.56
1:A:211:VAL:HG22	1:A:211:VAL:O	2.05	0.56
1:A:148:SER:OG	1:A:210:THR:OG1	2.22	0.55
1:A:58:THR:HB	1:A:63:LEU:CD1	2.30	0.54
1:A:340:LEU:HD21	1:A:358:GLU:HG2	1.89	0.54
1:A:173:PRO:CB	1:A:174:GLU:HG3	2.33	0.54
1:A:86:LEU:HD22	1:A:293:TRP:HA	1.90	0.54
1:A:365:THR:HA	1:A:368:MET:HG2	1.89	0.54
1:A:76:ARG:NH1	1:A:84:ALA:HA	2.23	0.53
1:A:81:ASP:CG	1:A:82:PRO:HA	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:CB	1:A:82:PRO:HA	2.37	0.53
1:A:81:ASP:CB	1:A:82:PRO:CA	2.85	0.53
1:A:172:LEU:HD22	1:A:176:ARG:NH2	2.23	0.53
1:A:198:LEU:HD23	1:A:211:VAL:N	2.24	0.53
1:A:104:LEU:HD21	1:A:106:TYR:CE2	2.44	0.53
1:A:50:GLU:O	1:A:54:GLN:HG3	2.09	0.52
1:A:278:THR:HG21	1:A:283:ARG:HE	1.74	0.52
1:A:359:GLN:HG2	1:A:360:ARG:N	2.23	0.52
1:A:335:VAL:HG12	1:A:410:VAL:HG21	1.92	0.52
1:A:379:LEU:HD13	1:A:382:LEU:HD23	1.91	0.52
1:A:86:LEU:CD2	1:A:293:TRP:HA	2.41	0.51
1:A:172:LEU:HD13	1:A:176:ARG:HE	1.75	0.51
1:A:395:THR:O	1:A:400:ARG:NH2	2.42	0.51
1:A:49:ILE:HG22	1:A:53:GLU:HG3	1.92	0.51
1:A:222:ALA:O	1:A:226:GLN:HG2	2.11	0.50
1:A:342:LEU:HA	1:A:346:ALA:HB3	1.92	0.50
1:A:170:PHE:CD1	1:A:170:PHE:C	2.85	0.50
1:A:198:LEU:HD23	1:A:211:VAL:HB	1.92	0.50
1:A:340:LEU:HA	1:A:343:ALA:HB3	1.93	0.50
1:A:135:GLU:HG2	1:A:162:PHE:CE2	2.47	0.50
1:A:360:ARG:O	1:A:362:ILE:N	2.45	0.49
1:A:173:PRO:CA	1:A:174:GLU:CG	2.91	0.49
1:A:259:LEU:O	1:A:452:LEU:HB2	2.11	0.49
1:A:342:LEU:O	1:A:348:LEU:N	2.45	0.49
1:A:90:ILE:HD11	1:A:274:ILE:HG21	1.95	0.49
1:A:259:LEU:HD13	1:A:459:PHE:HE2	1.77	0.49
1:A:490:ILE:HG23	1:A:492:ALA:HB3	1.94	0.49
1:A:448:LEU:HD13	1:A:481:VAL:HG13	1.94	0.49
1:A:272:ASN:OD1	1:A:272:ASN:N	2.38	0.49
1:A:148:SER:HB2	1:A:209:GLY:HA3	1.95	0.48
1:A:48:VAL:HG12	1:A:48:VAL:O	2.14	0.48
1:A:87:LYS:O	1:A:88:MET:C	2.50	0.48
1:A:86:LEU:HB3	1:A:88:MET:HG2	1.96	0.48
1:A:240:VAL:HG13	1:A:288:VAL:HG11	1.96	0.48
1:A:478:SER:HB3	2:A:633:HOH:O	2.14	0.48
1:A:357:LEU:HD12	1:A:390:LEU:HD13	1.96	0.47
1:A:278:THR:HG22	1:A:283:ARG:CZ	2.44	0.47
1:A:167:GLY:HA3	1:A:168:GLU:CB	2.41	0.47
1:A:278:THR:HG21	1:A:283:ARG:HB2	1.97	0.47
1:A:295:ASN:HA	1:A:320:GLN:HA	1.96	0.47
1:A:490:ILE:HA	1:A:492:ALA:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HA	1:A:163:VAL:HB	1.96	0.47
1:A:158:GLU:OE1	2:A:606:HOH:O	2.20	0.47
1:A:173:PRO:HA	1:A:174:GLU:HA	1.68	0.47
1:A:178:ARG:HB3	1:A:230:MET:CE	2.45	0.47
1:A:178:ARG:CB	1:A:230:MET:HE3	2.43	0.47
1:A:356:LYS:HB2	1:A:356:LYS:HE2	1.74	0.46
1:A:371:MET:HB2	1:A:371:MET:HE2	1.80	0.46
1:A:375:THR:O	1:A:375:THR:OG1	2.31	0.46
1:A:178:ARG:CB	1:A:230:MET:CE	2.94	0.46
1:A:83:HIS:O	1:A:83:HIS:CG	2.69	0.46
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.27	0.46
1:A:278:THR:HG23	1:A:283:ARG:NH1	2.17	0.46
1:A:340:LEU:C	1:A:343:ALA:H	2.08	0.46
1:A:107:ALA:HB2	1:A:492:ALA:HB2	1.98	0.45
1:A:84:ALA:HB1	2:A:608:HOH:O	2.16	0.45
1:A:495:LEU:HD13	1:A:495:LEU:HA	1.83	0.45
1:A:377:HIS:CE1	1:A:378:ASP:OD2	2.69	0.45
1:A:81:ASP:CB	1:A:82:PRO:C	2.85	0.44
1:A:261:THR:OG1	2:A:604:HOH:O	2.12	0.44
1:A:251:ASN:N	1:A:251:ASN:OD1	2.50	0.44
1:A:86:LEU:HD21	1:A:296:PHE:HB2	1.98	0.44
1:A:334:ILE:O	1:A:338:ILE:HG13	2.18	0.44
1:A:381:HIS:H	1:A:381:HIS:HD2	1.60	0.44
1:A:379:LEU:N	1:A:379:LEU:CD2	2.78	0.43
1:A:172:LEU:HD13	1:A:176:ARG:NE	2.33	0.43
1:A:71:VAL:O	1:A:75:GLU:HG3	2.17	0.43
1:A:340:LEU:HD22	1:A:344:HIS:CD2	2.47	0.43
1:A:259:LEU:HD13	1:A:459:PHE:CE2	2.53	0.43
1:A:70:MET:O	1:A:74:MET:HG3	2.19	0.43
1:A:187:PRO:HB2	1:A:199:ILE:HB	2.01	0.43
1:A:198:LEU:HD23	1:A:211:VAL:CA	2.49	0.43
1:A:173:PRO:CA	1:A:174:GLU:HG3	2.49	0.42
1:A:81:ASP:HB2	1:A:83:HIS:N	2.34	0.42
1:A:429:LEU:HB2	1:A:431:ARG:HG2	2.02	0.42
1:A:331:LEU:O	1:A:335:VAL:HG13	2.19	0.42
1:A:104:LEU:CD2	1:A:106:TYR:CE2	3.02	0.42
1:A:336:ARG:HD2	1:A:362:ILE:HG22	2.02	0.42
1:A:340:LEU:CD2	1:A:344:HIS:CD2	2.93	0.42
1:A:271:ALA:C	1:A:273:ALA:HA	2.38	0.42
1:A:256:ALA:HA	1:A:447:ALA:O	2.20	0.41
1:A:278:THR:CG2	1:A:283:ARG:NE	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:HD13	1:A:321:ILE:HA	1.74	0.41
1:A:340:LEU:HD21	1:A:344:HIS:HD2	1.83	0.41
1:A:88:MET:HA	1:A:291:MET:HA	2.03	0.41
1:A:401:TYR:CD1	1:A:404:LEU:HD23	2.56	0.41
1:A:148:SER:HG	1:A:210:THR:HG1	1.65	0.41
1:A:275:PRO:HA	1:A:278:THR:O	2.21	0.41
1:A:354:PRO:HB2	1:A:357:LEU:HD13	2.03	0.41
1:A:377:HIS:ND1	1:A:377:HIS:C	2.72	0.41
1:A:81:ASP:HB2	1:A:82:PRO:CA	2.49	0.41
1:A:283:ARG:HE	1:A:283:ARG:HB2	1.59	0.41
1:A:355:THR:O	1:A:357:LEU:N	2.54	0.41
1:A:45:ALA:HA	1:A:46:ALA:HB2	2.02	0.41
1:A:111:GLY:HA2	1:A:185:SER:HB2	2.02	0.41
1:A:405:HIS:CD2	1:A:409:LEU:HD11	2.55	0.41
1:A:310:LEU:HD21	1:A:330:TYR:CD1	2.56	0.40
1:A:340:LEU:C	1:A:342:LEU:N	2.74	0.40
1:A:405:HIS:NE2	1:A:409:LEU:HD11	2.37	0.40
1:A:278:THR:CG2	1:A:283:ARG:CZ	2.99	0.40
1:A:280:LEU:HA	1:A:281:LEU:HA	1.93	0.40
1:A:372:HIS:CD2	1:A:458:LYS:HD3	2.56	0.40
1:A:53:GLU:OE1	1:A:405:HIS:NE2	2.55	0.40
1:A:378:ASP:OD1	1:A:380:LYS:CG	2.70	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	453/467 (97%)	402 (89%)	40 (9%)	11 (2%)	6	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	THR
1	A	356	LYS
1	A	361	PHE
1	A	393	ALA
1	A	81	ASP
1	A	50	GLU
1	A	166	GLU
1	A	317	PRO
1	A	353	VAL
1	A	392	VAL
1	A	211	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	368/379 (97%)	327 (89%)	41 (11%)	6	11

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	81	ASP
1	A	87	LYS
1	A	110	LEU
1	A	125	ARG
1	A	129	VAL
1	A	144	MET
1	A	145	VAL
1	A	148	SER
1	A	149	MET
1	A	160	GLU
1	A	168	GLU
1	A	174	GLU
1	A	180	LEU
1	A	208	ASN
1	A	210	THR

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Mol	Chain	Res	Type
1	A	231	LYS
1	A	251	ASN
1	A	293	TRP
1	A	315	LEU
1	A	316	ASN
1	A	340	LEU
1	A	347	SER
1	A	348	LEU
1	A	349	PHE
1	A	355	THR
1	A	356	LYS
1	A	358	GLU
1	A	364	ARG
1	A	376	SER
1	A	377	HIS
1	A	381	HIS
1	A	434	VAL
1	A	437	ASP
1	A	439	SER
1	A	440	GLN
1	A	441	LYS
1	A	444	THR
1	A	452	LEU
1	A	456	TYR
1	A	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	208	ASN
1	A	316	ASN
1	A	344	HIS
1	A	359	GLN
1	A	381	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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(Å²)	Q<0.9
1	A	455/467 (97%)	0.03	15 (3%)	46	39	18, 32, 61, 79	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	6.3
1	A	350	GLY	5.7
1	A	173	PRO	4.5
1	A	384	ALA	3.4
1	A	390	LEU	3.0
1	A	278	THR	2.8
1	A	439	SER	2.7
1	A	82	PRO	2.7
1	A	389	ILE	2.5
1	A	343	ALA	2.4
1	A	312	PHE	2.3
1	A	280	LEU	2.3
1	A	174	GLU	2.2
1	A	442	GLN	2.1
1	A	201	TRP	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.