



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 AM UTC

PDB ID : 6JJ4 / pdb_00006jj4
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)

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

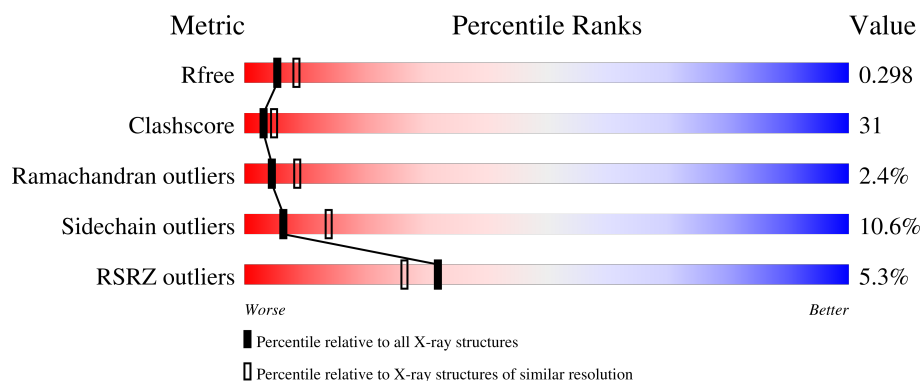
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	467	5% 51% 36% 8% ..

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	C	N	O	S	0	0	0
			3495	2203	611	666	15			

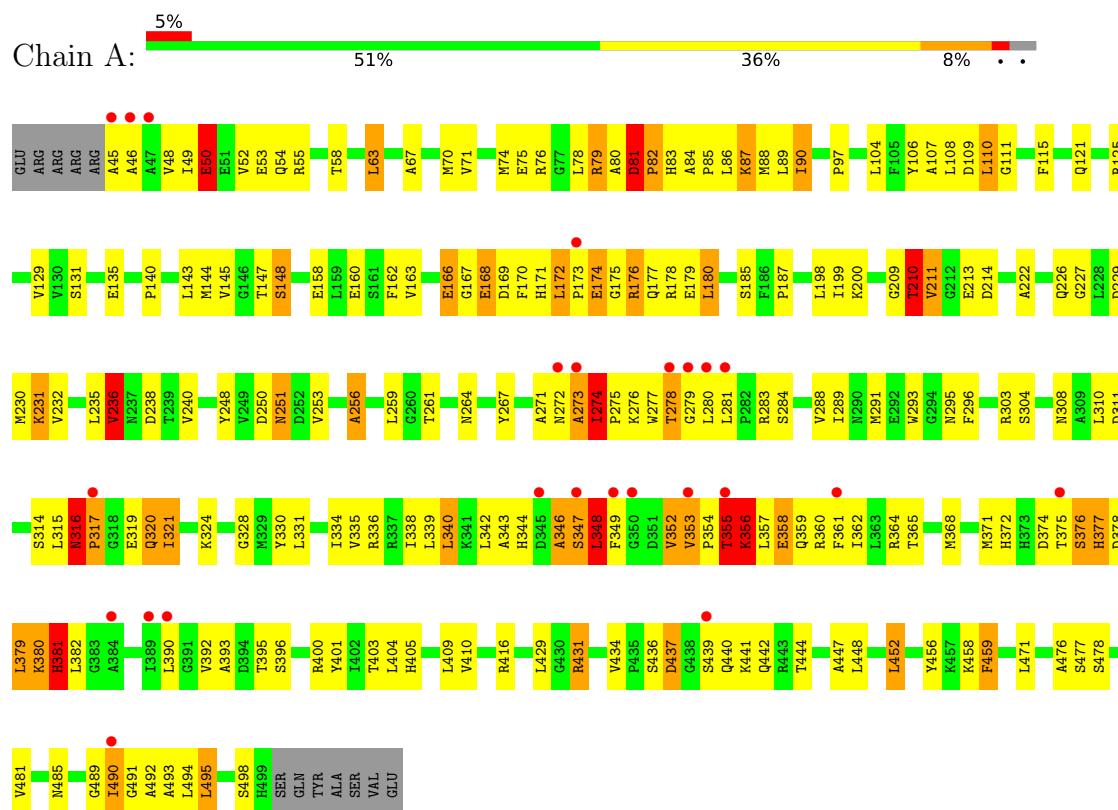
- Molecule 2 is water.

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

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: Hexokinase-6



4 Data and refinement statistics

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 40.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.28-2.60) 96.2 (40.28-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.58 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.250 , 0.319 0.248 , 0.298	Depositor DCC
R_{free} test set	1350 reflections (9.74%)	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)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	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.*

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	1.21	20/3557 (0.6%)	1.19	37/4811 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ALA	C-O	-7.17	1.15	1.23
1	A	109	ASP	C-O	-6.65	1.16	1.23
1	A	250	ASP	C-O	-6.46	1.16	1.24
1	A	471	LEU	C-O	-6.35	1.15	1.23
1	A	490	ILE	C-O	-6.33	1.16	1.24
1	A	179	GLU	C-O	-6.28	1.16	1.24
1	A	147	THR	CA-C	-6.01	1.44	1.53
1	A	108	LEU	C-O	-5.80	1.17	1.24
1	A	231	LYS	C-O	-5.53	1.17	1.24
1	A	89	LEU	C-O	-5.38	1.17	1.23
1	A	471	LEU	CA-C	-5.36	1.45	1.53
1	A	431	ARG	C-O	-5.34	1.16	1.24
1	A	477	SER	C-O	-5.33	1.17	1.24
1	A	235	LEU	C-O	-5.25	1.18	1.24
1	A	238	ASP	C-O	-5.25	1.17	1.24
1	A	253	VAL	C-O	-5.21	1.18	1.24
1	A	214	ASP	C-O	-5.18	1.18	1.24
1	A	232	VAL	C-O	-5.07	1.18	1.24
1	A	476	ALA	C-O	-5.02	1.18	1.24
1	A	459	PHE	C-O	-5.01	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	N-CA-C	16.57	132.95	111.75
1	A	176	ARG	N-CA-C	-16.03	85.28	109.81
1	A	274	ILE	N-CA-C	-13.14	80.49	108.88
1	A	278	THR	N-CA-C	-13.00	93.54	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	LEU	N-CA-C	-11.07	96.25	110.53
1	A	437	ASP	N-CA-C	9.33	122.55	108.46
1	A	169	ASP	N-CA-C	-9.23	94.73	109.59
1	A	79	ARG	N-CA-C	8.72	124.28	112.68
1	A	348	LEU	N-CA-C	8.41	121.66	111.40
1	A	316	ASN	N-CA-C	-8.33	91.41	109.81
1	A	442	GLN	N-CA-C	-7.74	98.01	109.15
1	A	381	HIS	N-CA-C	-7.11	102.94	111.69
1	A	346	ALA	N-CA-C	6.74	125.16	110.80
1	A	352	VAL	N-CA-C	6.67	118.08	108.48
1	A	89	LEU	N-CA-C	6.59	120.03	110.28
1	A	81	ASP	C-N-CD	6.56	135.02	120.60
1	A	380	LYS	N-CA-C	6.56	119.42	111.82
1	A	320	GLN	N-CA-C	6.50	120.38	111.54
1	A	236	VAL	N-CA-C	6.32	118.85	108.99
1	A	273	ALA	N-CA-C	6.09	128.06	111.00
1	A	172	LEU	CA-C-N	-6.04	113.55	119.90
1	A	172	LEU	C-N-CA	-6.04	113.55	119.90
1	A	321	ILE	N-CA-C	5.81	116.00	110.42
1	A	166	GLU	N-CA-C	5.74	123.03	110.80
1	A	316	ASN	CA-C-N	-5.72	112.69	119.84
1	A	316	ASN	C-N-CA	-5.72	112.69	119.84
1	A	436	SER	O-C-N	5.69	127.93	122.07
1	A	175	GLY	N-CA-C	-5.63	99.85	113.18
1	A	210	THR	N-CA-C	-5.51	99.06	110.80
1	A	490	ILE	N-CA-C	5.50	120.78	109.34
1	A	278	THR	N-CA-CB	5.49	115.11	109.51
1	A	471	LEU	CA-C-O	-5.35	115.79	121.94
1	A	439	SER	N-CA-C	-5.29	106.78	113.23
1	A	278	THR	CA-C-O	-5.12	116.50	120.19
1	A	82	PRO	CA-N-CD	-5.09	104.37	111.50
1	A	274	ILE	CA-C-N	-5.08	114.43	119.56
1	A	274	ILE	C-N-CA	-5.08	114.43	119.56

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	218	0
2	A	44	0	0	9	0
All	All	3539	0	3490	218	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 31.

All (218) 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:311:ASP:CG	1:A:317:PRO:O	2.14	0.90
1:A:278:THR:HG22	1:A:283:ARG:NH1	1.86	0.90
1:A:180:LEU:C	1:A:180:LEU:HD12	1.96	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: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
1:A:357:LEU:O	1:A:357:LEU:HD23	1.80	0.80
1:A:178:ARG:HB3	1:A:230:MET:HE2	1.64	0.79
1:A:172:LEU:HD12	1:A:172:LEU:H	1.47	0.79
1:A:173:PRO:CB	1:A:174:GLU:CG	2.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:490:ILE:C	2:A:603:HOH:O	2.31	0.71
1:A:173:PRO:C	1:A:174:GLU:HG3	2.15	0.71
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:CD2	1:A:381:HIS:H	2.08	0.69
1:A:275:PRO:O	1:A:278:THR:O	2.11	0.69
1:A:379:LEU:HD23	1:A:379:LEU:N	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:180:LEU:C	1:A:180:LEU:CD1	2.67	0.68
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: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:81:ASP:HB2	1:A:82:PRO:C	2.21	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:267:TYR:CD2	1:A:291:MET:HE2	2.31	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:368:MET:HA	1:A:371:MET:HE2	1.78	0.64
1:A:283:ARG:O	1:A:284:SER:HB3	1.98	0.63
1:A:267:TYR:HD2	1:A:291:MET:HE2	1.64	0.63
1:A:489:GLY:C	1:A:490:ILE:HG13	2.22	0.63
1:A:355:THR:C	1:A:357:LEU:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:213:GLU:HA	1:A:213:GLU:OE2	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:HG23	1:A:353:VAL:O	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:178:ARG:HG3	1:A:178:ARG:HH11	1.68	0.58
1:A:81:ASP:CG	1:A:82:PRO:HA	2.29	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: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:178:ARG:CB	1:A:230:MET:HE2	2.33	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:170:PHE:CD1	1:A:170:PHE:C	2.85	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:CB	1:A:82:PRO:HA	2.37	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: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:87:LYS:O	1:A:88:MET:C	2.50	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:340:LEU:C	1:A:343:ALA:H	2.08	0.50
1:A:342:LEU:HA	1:A:346:ALA:HB3	1.92	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:81:ASP:CB	1:A:82:PRO:C	2.85	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:86:LEU:HB3	1:A:88:MET:HG2	1.96	0.48
1:A:81:ASP:CG	1:A:82:PRO:C	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HA	1:A:492:ALA:N	2.26	0.47
1:A:160:GLU:HA	1:A:163:VAL:HB	1.96	0.47
1:A:88:MET:HE3	1:A:289:ILE:HG21	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:271:ALA:C	1:A:273:ALA:HA	2.38	0.46
1:A:356:LYS:HB2	1:A:356:LYS:HE2	1.74	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:CG	1:A:83:HIS:O	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:355:THR:C	1:A:357:LEU:N	2.74	0.46
1:A:377:HIS:ND1	1:A:377:HIS:C	2.72	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:261:THR:OG1	2:A:604:HOH:O	2.12	0.44
1:A:340:LEU:C	1:A:342:LEU:N	2.74	0.44
1:A:251:ASN:OD1	1:A:251:ASN:N	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:171:HIS:O	1:A:172:LEU:C	2.61	0.43
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:173:PRO:C	1:A:174:GLU:CG	2.90	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:88:MET:HE3	1:A:88:MET:HB3	1.87	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:368:MET:HE2	1:A:456:TYR:OH	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:HA	1:A:447:ALA:O	2.20	0.41
1:A:173:PRO:CA	1:A:174:GLU:HG3	2.49	0.41
1:A:278:THR:CG2	1:A:283:ARG:NE	2.82	0.41
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:81:ASP:HB2	1:A:83:HIS:N	2.34	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: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: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:52:VAL:C	1:A:54:GLN:H	2.28	0.40
1:A:310:LEU:HD21	1:A:330:TYR:CD1	2.56	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:381:HIS:O	1:A:382:LEU:C	2.61	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 ⓘ

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	453/467 (97%)	402 (89%)	40 (9%)	11 (2%)	4 9

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 [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	368/379 (97%)	329 (89%)	39 (11%)	6 14

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	63	LEU
1	A	81	ASP
1	A	87	LYS
1	A	90	ILE
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	168	GLU
1	A	174	GLU
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	210	THR
1	A	231	LYS
1	A	236	VAL
1	A	251	ASN
1	A	274	ILE
1	A	315	LEU
1	A	316	ASN
1	A	340	LEU
1	A	347	SER
1	A	348	LEU
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	379	LEU
1	A	381	HIS
1	A	434	VAL
1	A	437	ASP
1	A	440	GLN
1	A	441	LYS
1	A	444	THR
1	A	452	LEU
1	A	495	LEU

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	177	GLN
1	A	208	ASN
1	A	237	ASN
1	A	286	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 [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	455/467 (97%)	0.46	24 (5%) 32 26	18, 32, 61, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	5.9
1	A	350	GLY	4.1
1	A	173	PRO	4.0
1	A	353	VAL	3.5
1	A	278	THR	3.3
1	A	280	LEU	3.3
1	A	390	LEU	3.0
1	A	384	ALA	3.0
1	A	46	ALA	2.7
1	A	347	SER	2.5
1	A	281	LEU	2.5
1	A	439	SER	2.5
1	A	47	ALA	2.5
1	A	361	PHE	2.4
1	A	349	PHE	2.4
1	A	45	ALA	2.4
1	A	375	THR	2.3
1	A	317	PRO	2.3
1	A	389	ILE	2.3
1	A	273	ALA	2.2
1	A	345	ASP	2.2
1	A	355	THR	2.1
1	A	272	ASN	2.1
1	A	490	ILE	2.1

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.