



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:27 AM UTC

PDB ID : 2QUQ / pdb_00002quq
Title : Crystal Structure of the Essential Inner Kinetochore Protein Cep3p
Authors : Bellizzi III, J.J.; Harrison, S.C.
Deposited on : 2007-08-06
Resolution : 2.80 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

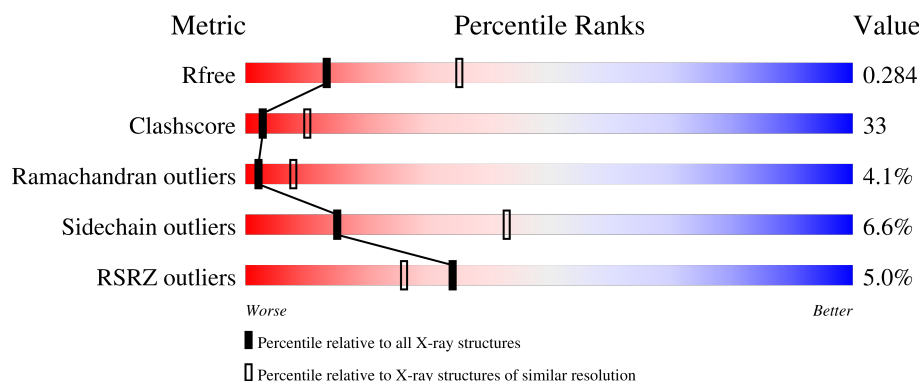
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	562	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4307 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 Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4292	2796	690	785	21			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.63Å 84.63Å 230.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.80 45.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.00-2.80) 94.3 (45.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.285 0.228 , 0.284	Depositor DCC
R_{free} test set	2003 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.48	0/4397	1.03	30/5955 (0.5%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	SER	N-CA-C	-9.01	99.35	110.61
1	A	150	LYS	N-CA-C	-8.53	102.66	113.23
1	A	205	GLN	N-CA-C	-7.76	102.14	111.69
1	A	71	TRP	N-CA-C	7.31	119.33	111.36
1	A	207	VAL	N-CA-C	-7.12	105.58	111.91
1	A	420	ILE	N-CA-C	6.76	117.38	110.82
1	A	416	LYS	N-CA-C	-6.37	104.34	111.28
1	A	155	ASP	N-CA-C	-6.37	104.61	112.38
1	A	100	MET	N-CA-C	-6.33	106.09	113.88
1	A	114	LEU	N-CA-C	-6.28	104.35	111.07
1	A	446	PHE	N-CA-C	-6.11	104.53	112.23
1	A	122	LEU	N-CA-C	6.05	120.17	113.21
1	A	165	SER	N-CA-C	-5.97	104.71	112.23
1	A	68	TYR	N-CA-C	-5.79	104.88	111.07
1	A	529	SER	N-CA-C	-5.74	105.78	112.89
1	A	381	GLN	N-CA-C	-5.73	104.67	111.03
1	A	295	ARG	N-CA-C	-5.70	104.68	111.69
1	A	62	LEU	N-CA-C	-5.42	105.03	111.69
1	A	224	ASP	N-CA-C	-5.42	104.17	111.54
1	A	261	ILE	N-CA-C	-5.41	105.22	110.42
1	A	209	CYS	N-CA-C	-5.36	106.44	112.87
1	A	305	GLY	CA-C-N	5.35	124.86	119.19
1	A	305	GLY	C-N-CA	5.35	124.86	119.19
1	A	258	THR	N-CA-C	-5.30	105.51	111.28
1	A	365	PRO	CA-C-N	-5.26	114.53	119.90
1	A	365	PRO	C-N-CA	-5.26	114.53	119.90
1	A	344	LEU	N-CA-C	-5.25	105.73	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LEU	N-CA-C	-5.18	105.71	111.36
1	A	117	PHE	N-CA-C	-5.10	105.61	111.07
1	A	352	ASP	N-CA-C	-5.09	105.81	111.36

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	4292	0	4270	281	0
2	A	15	0	0	1	0
All	All	4307	0	4270	281	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 33.

All (281) 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:190:GLU:CD	1:A:191:TYR:H	1.66	1.04
1:A:384:VAL:HG21	1:A:407:ILE:HD11	1.49	0.94
1:A:499:ILE:HD13	1:A:499:ILE:H	1.31	0.93
1:A:157:LYS:HE3	1:A:222:GLN:HE22	1.36	0.90
1:A:130:ILE:HD11	1:A:162:LEU:HD11	1.52	0.89
1:A:594:VAL:HG23	1:A:595:GLU:H	1.38	0.88
1:A:157:LYS:HE3	1:A:222:GLN:NE2	1.89	0.87
1:A:198:LEU:HD22	1:A:204:MET:HE3	1.58	0.86
1:A:203:GLY:O	1:A:207:VAL:HG23	1.78	0.84
1:A:195:ASN:C	1:A:197:ARG:H	1.82	0.83
1:A:127:PHE:CD1	1:A:131:GLY:HA2	2.14	0.82
1:A:467:VAL:HG22	1:A:489:LEU:HB3	1.62	0.80
1:A:594:VAL:HG23	1:A:595:GLU:N	1.97	0.80
1:A:126:TYR:CZ	1:A:133:ILE:HG13	2.18	0.79
1:A:55:LYS:HE3	1:A:521:TRP:HH2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HA	1:A:446:PHE:CE1	2.21	0.76
1:A:82:GLN:C	1:A:83:ARG:HD2	2.11	0.76
1:A:276:LEU:H	1:A:276:LEU:HD23	1.50	0.76
1:A:483:LYS:O	1:A:487:VAL:HG23	1.85	0.75
1:A:446:PHE:HA	1:A:451:GLU:HG2	1.68	0.74
1:A:81:LYS:HG2	1:A:83:ARG:HD3	1.69	0.74
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.53	0.74
1:A:442:ILE:CD1	1:A:463:ILE:HD11	2.17	0.74
1:A:374:ARG:HG2	1:A:374:ARG:HH11	1.53	0.73
1:A:139:ARG:HH11	1:A:139:ARG:CG	2.01	0.73
1:A:513:ARG:HG3	1:A:513:ARG:HH11	1.54	0.73
1:A:319:LEU:HD21	1:A:347:LYS:HD2	1.69	0.72
1:A:184:SER:O	1:A:187:PRO:HD2	1.90	0.72
1:A:58:LEU:HD12	1:A:61:LEU:HD23	1.73	0.71
1:A:231:ILE:H	1:A:231:ILE:HD12	1.55	0.71
1:A:543:ASN:HA	1:A:546:LYS:HG2	1.73	0.71
1:A:83:ARG:HD2	1:A:83:ARG:N	2.04	0.71
1:A:115:MET:HE1	1:A:166:VAL:HG11	1.73	0.70
1:A:592:THR:O	1:A:596:GLU:HG3	1.90	0.70
1:A:66:GLN:HE22	1:A:417:MET:HE2	1.57	0.69
1:A:536:PRO:O	1:A:540:ILE:HG13	1.93	0.69
1:A:57:TYR:CD1	1:A:58:LEU:N	2.61	0.68
1:A:158:TYR:HB3	1:A:232:ARG:NH1	2.08	0.68
1:A:385:ASP:HA	1:A:400:LYS:NZ	2.10	0.67
1:A:475:ILE:HG22	1:A:518:LYS:HB2	1.76	0.66
1:A:590:PHE:HA	1:A:593:ILE:HG12	1.77	0.66
1:A:105:TYR:OH	1:A:183:PHE:HB3	1.95	0.66
1:A:366:PRO:HG2	1:A:369:THR:OG1	1.95	0.66
1:A:499:ILE:H	1:A:499:ILE:CD1	2.01	0.66
1:A:179:LEU:HD22	1:A:205:GLN:NE2	2.11	0.66
1:A:190:GLU:CD	1:A:191:TYR:N	2.49	0.65
1:A:90:ALA:O	1:A:91:ASN:HB3	1.95	0.65
1:A:439:ILE:HG23	1:A:492:LEU:HD22	1.77	0.65
1:A:202:ASP:CG	1:A:203:GLY:H	2.04	0.65
1:A:562:LEU:C	1:A:564:SER:H	2.04	0.65
1:A:446:PHE:HA	1:A:451:GLU:CG	2.27	0.64
1:A:517:LEU:HD22	1:A:537:VAL:HG13	1.80	0.64
1:A:377:LEU:HD12	1:A:414:LEU:HD22	1.80	0.64
1:A:65:TRP:HH2	1:A:468:SER:HB3	1.63	0.64
1:A:162:LEU:O	1:A:166:VAL:HG23	1.98	0.63
1:A:544:ASP:HA	1:A:603:ILE:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:HB2	1:A:346:TRP:HH2	1.62	0.63
1:A:138:LEU:O	1:A:142:GLN:HG3	1.99	0.63
1:A:144:TRP:HA	1:A:147:ARG:HB2	1.81	0.62
1:A:499:ILE:HD13	1:A:499:ILE:N	2.09	0.62
1:A:179:LEU:HD22	1:A:205:GLN:HE21	1.62	0.62
1:A:535:HIS:CG	1:A:536:PRO:HD2	2.35	0.62
1:A:391:PHE:HD1	1:A:391:PHE:H	1.45	0.62
1:A:548:ILE:CD1	1:A:607:LEU:HD21	2.30	0.62
1:A:594:VAL:CG2	1:A:595:GLU:H	2.11	0.61
1:A:419:LEU:HB2	1:A:427:SER:HB3	1.82	0.61
1:A:313:HIS:HB2	1:A:346:TRP:CH2	2.35	0.61
1:A:513:ARG:HG3	1:A:513:ARG:NH1	2.15	0.61
1:A:195:ASN:C	1:A:197:ARG:N	2.54	0.61
1:A:487:VAL:O	1:A:491:GLU:HG3	2.00	0.61
1:A:562:LEU:O	1:A:564:SER:N	2.34	0.61
1:A:546:LYS:HG3	1:A:547:ILE:HG13	1.83	0.60
1:A:533:PHE:N	1:A:533:PHE:CD1	2.69	0.60
1:A:535:HIS:HD2	1:A:537:VAL:H	1.49	0.60
1:A:543:ASN:HB3	1:A:547:ILE:HD11	1.82	0.60
1:A:202:ASP:CG	1:A:203:GLY:N	2.60	0.59
1:A:200:TRP:HA	1:A:200:TRP:CE3	2.38	0.59
1:A:460:MET:HB2	1:A:500:PHE:CE1	2.37	0.59
1:A:234:VAL:O	1:A:238:LEU:HG	2.02	0.59
1:A:178:LYS:O	1:A:182:ILE:HG13	2.02	0.59
1:A:107:GLN:HB2	1:A:110:GLN:HG3	1.84	0.58
1:A:133:ILE:O	1:A:136:LEU:N	2.31	0.58
1:A:498:THR:C	1:A:500:PHE:H	2.11	0.58
1:A:185:VAL:HB	1:A:189:HIS:NE2	2.18	0.58
1:A:129:SER:HB2	2:A:619:HOH:O	2.04	0.58
1:A:546:LYS:HG3	1:A:547:ILE:N	2.19	0.58
1:A:603:ILE:HD12	1:A:604:SER:H	1.69	0.58
1:A:502:SER:O	1:A:506:LYS:HG2	2.05	0.57
1:A:509:TYR:CD1	1:A:509:TYR:C	2.82	0.57
1:A:112:PHE:O	1:A:116:ASN:ND2	2.38	0.57
1:A:160:ASP:HB3	1:A:219:GLN:OE1	2.05	0.57
1:A:412:TRP:CZ2	1:A:466:VAL:HA	2.39	0.57
1:A:132:ASP:OD2	1:A:134:SER:HB2	2.05	0.57
1:A:217:LEU:CD1	1:A:252:LEU:HD21	2.35	0.57
1:A:594:VAL:CG2	1:A:595:GLU:N	2.68	0.57
1:A:498:THR:C	1:A:500:PHE:N	2.62	0.56
1:A:200:TRP:HA	1:A:200:TRP:HE3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:O	1:A:56:GLU:N	2.36	0.56
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.87	0.56
1:A:391:PHE:CD1	1:A:391:PHE:N	2.73	0.56
1:A:545:ILE:O	1:A:549:GLU:HB2	2.05	0.56
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.64	0.56
1:A:171:ILE:HG21	1:A:208:MET:HB3	1.86	0.56
1:A:543:ASN:C	1:A:547:ILE:HD12	2.30	0.56
1:A:82:GLN:N	1:A:83:ARG:HH11	2.04	0.56
1:A:467:VAL:CG2	1:A:489:LEU:HB3	2.34	0.56
1:A:157:LYS:CE	1:A:222:GLN:HE22	2.15	0.55
1:A:452:PHE:CZ	1:A:453:PHE:HE1	2.24	0.55
1:A:111:SER:HA	1:A:114:LEU:HD12	1.88	0.55
1:A:389:GLU:O	1:A:389:GLU:HG3	2.05	0.55
1:A:215:CYS:O	1:A:219:GLN:HG3	2.06	0.55
1:A:274:PRO:CB	1:A:283:SER:HB3	2.35	0.55
1:A:456:HIS:CE1	1:A:458:MET:HB2	2.42	0.54
1:A:70:TYR:O	1:A:74:ASN:HB3	2.07	0.54
1:A:99:CYS:O	1:A:103:MET:HG3	2.07	0.54
1:A:466:VAL:O	1:A:470:ILE:HG12	2.07	0.54
1:A:209:CYS:O	1:A:209:CYS:SG	2.64	0.54
1:A:384:VAL:CG2	1:A:407:ILE:HD11	2.32	0.54
1:A:313:HIS:HD2	1:A:353:ARG:HH11	1.54	0.54
1:A:261:ILE:HD12	1:A:312:LEU:HB2	1.89	0.54
1:A:131:GLY:O	1:A:132:ASP:C	2.50	0.54
1:A:548:ILE:HD13	1:A:607:LEU:HD21	1.90	0.54
1:A:384:VAL:HG21	1:A:407:ILE:CD1	2.32	0.54
1:A:57:TYR:HH	1:A:521:TRP:HZ2	1.56	0.53
1:A:208:MET:C	1:A:210:GLN:N	2.66	0.53
1:A:515:SER:O	1:A:518:LYS:HB3	2.08	0.53
1:A:564:SER:C	1:A:565:LEU:O	2.46	0.53
1:A:69:GLU:O	1:A:73:THR:OG1	2.18	0.53
1:A:472:PHE:O	1:A:475:ILE:HG12	2.09	0.53
1:A:231:ILE:H	1:A:231:ILE:CD1	2.17	0.53
1:A:474:GLN:HG2	1:A:482:VAL:HG12	1.90	0.53
1:A:126:TYR:CE1	1:A:133:ILE:HG13	2.42	0.53
1:A:374:ARG:HG2	1:A:374:ARG:NH1	2.21	0.53
1:A:474:GLN:HG3	1:A:486:LEU:HD22	1.91	0.53
1:A:536:PRO:HD3	1:A:590:PHE:CD1	2.43	0.53
1:A:274:PRO:HB3	1:A:283:SER:HB3	1.91	0.52
1:A:164:TRP:CD1	1:A:219:GLN:HE22	2.28	0.52
1:A:385:ASP:HA	1:A:400:LYS:HZ1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:HG12	1:A:525:GLN:N	2.25	0.52
1:A:80:THR:O	1:A:81:LYS:HB2	2.10	0.52
1:A:133:ILE:O	1:A:134:SER:C	2.50	0.52
1:A:96:THR:O	1:A:100:MET:HB2	2.10	0.52
1:A:157:LYS:CE	1:A:222:GLN:NE2	2.69	0.52
1:A:455:ARG:HG2	1:A:499:ILE:CG1	2.40	0.51
1:A:198:LEU:HD23	1:A:202:ASP:OD2	2.09	0.51
1:A:351:LEU:HD22	1:A:373:ILE:HG23	1.92	0.51
1:A:341:THR:HG23	1:A:342:GLU:N	2.25	0.51
1:A:140:VAL:O	1:A:143:TYR:HB3	2.10	0.51
1:A:204:MET:HA	1:A:207:VAL:HG23	1.92	0.51
1:A:117:PHE:CZ	1:A:175:PRO:HD3	2.46	0.51
1:A:593:ILE:HA	1:A:596:GLU:OE2	2.10	0.51
1:A:381:GLN:O	1:A:385:ASP:OD1	2.29	0.50
1:A:437:VAL:O	1:A:440:SER:HB3	2.11	0.50
1:A:358:TYR:HA	1:A:361:LYS:HB2	1.93	0.50
1:A:535:HIS:CD2	1:A:537:VAL:H	2.27	0.50
1:A:61:LEU:HD21	1:A:476:PHE:CE2	2.47	0.50
1:A:160:ASP:O	1:A:163:ILE:HG12	2.11	0.50
1:A:206:LEU:O	1:A:206:LEU:HG	2.12	0.50
1:A:543:ASN:HD22	1:A:598:GLN:NE2	2.08	0.50
1:A:114:LEU:HD23	1:A:174:MET:CE	2.41	0.50
1:A:123:GLY:HA2	1:A:126:TYR:CE2	2.47	0.50
1:A:195:ASN:HB2	1:A:197:ARG:HB3	1.94	0.50
1:A:208:MET:C	1:A:210:GLN:H	2.18	0.50
1:A:126:TYR:HB3	1:A:169:MET:HE1	1.94	0.50
1:A:231:ILE:HD12	1:A:231:ILE:N	2.23	0.50
1:A:275:LEU:O	1:A:278:ASP:HB2	2.12	0.50
1:A:603:ILE:HD12	1:A:604:SER:N	2.27	0.49
1:A:497:PRO:HB2	1:A:499:ILE:HD11	1.94	0.49
1:A:540:ILE:HD13	1:A:597:PHE:CD2	2.46	0.49
1:A:104:ASN:C	1:A:104:ASN:HD22	2.19	0.49
1:A:424:THR:HG22	1:A:425:ALA:H	1.77	0.49
1:A:455:ARG:HG2	1:A:499:ILE:HD11	1.94	0.49
1:A:55:LYS:HE3	1:A:521:TRP:CH2	2.37	0.49
1:A:319:LEU:HD13	1:A:350:SER:OG	2.13	0.49
1:A:428:LEU:O	1:A:432:ILE:HG13	2.12	0.49
1:A:442:ILE:HD12	1:A:463:ILE:HD11	1.92	0.49
1:A:403:ALA:O	1:A:407:ILE:HG13	2.12	0.49
1:A:513:ARG:NH1	1:A:601:TYR:O	2.40	0.49
1:A:185:VAL:HG21	1:A:199:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD13	1:A:233:LEU:CD1	2.43	0.49
1:A:146:ARG:HD2	1:A:152:HIS:NE2	2.28	0.48
1:A:297:CYS:HB3	1:A:346:TRP:CZ3	2.49	0.48
1:A:562:LEU:C	1:A:564:SER:N	2.71	0.48
1:A:186:TYR:HB3	1:A:187:PRO:HD3	1.95	0.48
1:A:425:ALA:O	1:A:426:ASP:HB2	2.14	0.48
1:A:127:PHE:O	1:A:128:GLY:C	2.57	0.48
1:A:513:ARG:HD3	1:A:514:LEU:HD12	1.95	0.47
1:A:433:HIS:O	1:A:437:VAL:HG23	2.14	0.47
1:A:452:PHE:HA	1:A:455:ARG:HD3	1.95	0.47
1:A:423:ASP:CG	1:A:423:ASP:O	2.56	0.47
1:A:406:GLN:HG2	1:A:458:MET:SD	2.54	0.47
1:A:544:ASP:HB3	1:A:603:ILE:HG21	1.95	0.47
1:A:127:PHE:CE1	1:A:131:GLY:HA2	2.49	0.47
1:A:365:PRO:O	1:A:366:PRO:C	2.55	0.47
1:A:190:GLU:O	1:A:191:TYR:C	2.58	0.47
1:A:526:LEU:HD11	1:A:533:PHE:HB3	1.95	0.47
1:A:597:PHE:CE1	1:A:601:TYR:HD2	2.33	0.47
1:A:347:LYS:O	1:A:350:SER:HB3	2.14	0.46
1:A:67:ASN:N	1:A:67:ASN:HD22	2.13	0.46
1:A:198:LEU:HD12	1:A:198:LEU:N	2.31	0.46
1:A:61:LEU:HD21	1:A:476:PHE:CD2	2.51	0.46
1:A:377:LEU:CD1	1:A:414:LEU:HD22	2.46	0.46
1:A:535:HIS:CD2	1:A:536:PRO:HD2	2.51	0.46
1:A:603:ILE:O	1:A:605:ASP:N	2.49	0.46
1:A:186:TYR:CD1	1:A:196:LYS:NZ	2.83	0.46
1:A:117:PHE:O	1:A:121:ASN:HB2	2.16	0.46
1:A:196:LYS:HD2	1:A:196:LYS:O	2.15	0.46
1:A:299:CYS:O	1:A:303:GLN:HG3	2.16	0.46
1:A:455:ARG:HG3	1:A:497:PRO:HG3	1.98	0.46
1:A:82:GLN:C	1:A:83:ARG:HH11	2.24	0.45
1:A:402:ILE:HG23	1:A:458:MET:HE1	1.98	0.45
1:A:390:ASP:C	1:A:392:ARG:H	2.24	0.45
1:A:186:TYR:CB	1:A:187:PRO:CD	2.94	0.45
1:A:197:ARG:O	1:A:197:ARG:HG2	2.17	0.45
1:A:274:PRO:HB2	1:A:283:SER:HB3	1.98	0.45
1:A:154:VAL:HG13	1:A:223:CYS:HB3	1.99	0.45
1:A:394:ASN:OD1	1:A:397:ARG:NH2	2.50	0.44
1:A:496:LEU:O	1:A:497:PRO:C	2.60	0.44
1:A:101:PHE:O	1:A:104:ASN:HB3	2.17	0.44
1:A:61:LEU:HD21	1:A:476:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:C	1:A:186:TYR:H	2.26	0.44
1:A:603:ILE:C	1:A:605:ASP:N	2.73	0.44
1:A:184:SER:C	1:A:186:TYR:N	2.75	0.44
1:A:238:LEU:O	1:A:241:ALA:HB3	2.17	0.44
1:A:346:TRP:O	1:A:347:LYS:C	2.59	0.44
1:A:364:LYS:HE2	1:A:422:TYR:CZ	2.52	0.44
1:A:507:LEU:O	1:A:507:LEU:HD22	2.17	0.44
1:A:590:PHE:HA	1:A:593:ILE:CG1	2.46	0.44
1:A:603:ILE:C	1:A:605:ASP:H	2.26	0.44
1:A:138:LEU:O	1:A:141:GLU:HB3	2.18	0.44
1:A:526:LEU:HD13	1:A:535:HIS:HB2	1.99	0.44
1:A:104:ASN:C	1:A:104:ASN:ND2	2.75	0.43
1:A:158:TYR:CB	1:A:232:ARG:NH1	2.77	0.43
1:A:186:TYR:HB3	1:A:187:PRO:CD	2.48	0.43
1:A:155:ASP:OD1	1:A:232:ARG:NH2	2.51	0.43
1:A:195:ASN:O	1:A:197:ARG:N	2.51	0.43
1:A:164:TRP:CG	1:A:219:GLN:HE22	2.36	0.43
1:A:412:TRP:CZ3	1:A:416:LYS:HD3	2.53	0.43
1:A:435:SER:O	1:A:439:ILE:HG13	2.18	0.43
1:A:452:PHE:CZ	1:A:453:PHE:CE1	3.06	0.43
1:A:257:LEU:HD21	1:A:300:ASP:HA	2.00	0.43
1:A:220:LEU:HD13	1:A:233:LEU:HD12	2.01	0.43
1:A:407:ILE:HG13	1:A:407:ILE:H	1.45	0.43
1:A:543:ASN:O	1:A:547:ILE:HD12	2.19	0.43
1:A:82:GLN:N	1:A:83:ARG:NH1	2.66	0.43
1:A:126:TYR:CD1	1:A:126:TYR:C	2.96	0.43
1:A:127:PHE:O	1:A:129:SER:N	2.52	0.43
1:A:217:LEU:HD13	1:A:252:LEU:HD21	2.00	0.43
1:A:462:THR:O	1:A:466:VAL:HG23	2.19	0.43
1:A:367:LEU:HD11	1:A:418:TYR:HE1	1.84	0.42
1:A:202:ASP:C	1:A:204:MET:H	2.28	0.42
1:A:245:PHE:N	1:A:246:PRO:HD2	2.34	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.71	0.42
1:A:171:ILE:HD12	1:A:208:MET:HE2	2.00	0.42
1:A:224:ASP:O	1:A:226:MET:N	2.53	0.42
1:A:341:THR:CG2	1:A:342:GLU:N	2.83	0.42
1:A:144:TRP:O	1:A:147:ARG:HB3	2.20	0.41
1:A:154:VAL:C	1:A:156:GLY:N	2.75	0.41
1:A:344:LEU:CD1	1:A:380:PHE:HD1	2.33	0.41
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.83	0.41
1:A:535:HIS:HB3	1:A:538:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:HE2	1:A:422:TYR:OH	2.21	0.41
1:A:384:VAL:HG11	1:A:407:ILE:HD11	2.02	0.41
1:A:96:THR:HG22	1:A:218:PHE:HE1	1.86	0.41
1:A:180:ALA:HA	1:A:200:TRP:CD1	2.56	0.41
1:A:424:THR:HG22	1:A:425:ALA:N	2.35	0.41
1:A:98:GLU:C	1:A:100:MET:H	2.29	0.41
1:A:204:MET:HA	1:A:207:VAL:CG2	2.51	0.41
1:A:543:ASN:ND2	1:A:598:GLN:NE2	2.68	0.41
1:A:139:ARG:HD3	1:A:142:GLN:OE1	2.21	0.41
1:A:295:ARG:HD2	1:A:295:ARG:HA	1.97	0.41
1:A:452:PHE:HA	1:A:455:ARG:CD	2.51	0.41
1:A:58:LEU:O	1:A:61:LEU:HB3	2.21	0.40
1:A:239:ILE:HD13	1:A:239:ILE:HA	1.91	0.40
1:A:257:LEU:O	1:A:261:ILE:HG12	2.21	0.40
1:A:417:MET:HG3	1:A:421:TYR:CE2	2.57	0.40
1:A:535:HIS:O	1:A:538:PHE:HB2	2.21	0.40
1:A:374:ARG:NH1	1:A:374:ARG:CG	2.84	0.40
1:A:184:SER:O	1:A:186:TYR:N	2.55	0.40
1:A:191:TYR:C	1:A:191:TYR:CD1	3.00	0.40
1:A:185:VAL:HB	1:A:189:HIS:CD2	2.57	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	511/562 (91%)	441 (86%)	49 (10%)	21 (4%)	2 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP

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Mol	Chain	Res	Type
1	A	388	GLU
1	A	55	LYS
1	A	131	GLY
1	A	225	PHE
1	A	501	GLY
1	A	563	GLY
1	A	81	LYS
1	A	91	ASN
1	A	128	GLY
1	A	276	LEU
1	A	565	LEU
1	A	196	LYS
1	A	391	PHE
1	A	424	THR
1	A	502	SER
1	A	604	SER
1	A	58	LEU
1	A	186	TYR
1	A	185	VAL
1	A	203	GLY

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	483/525 (92%)	451 (93%)	32 (7%)	15	43

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	86	THR
1	A	130	ILE
1	A	139	ARG
1	A	152	HIS
1	A	186	TYR

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Mol	Chain	Res	Type
1	A	190	GLU
1	A	196	LYS
1	A	200	TRP
1	A	209	CYS
1	A	223	CYS
1	A	231	ILE
1	A	276	LEU
1	A	308	LYS
1	A	343	VAL
1	A	391	PHE
1	A	407	ILE
1	A	417	MET
1	A	474	GLN
1	A	484	GLN
1	A	498	THR
1	A	499	ILE
1	A	504	LEU
1	A	507	LEU
1	A	509	TYR
1	A	513	ARG
1	A	520	LEU
1	A	525	GLN
1	A	533	PHE
1	A	541	LEU
1	A	562	LEU
1	A	603	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	67	ASN
1	A	104	ASN
1	A	121	ASN
1	A	205	GLN
1	A	211	ASN
1	A	222	GLN
1	A	262	HIS
1	A	321	GLN
1	A	445	ASN
1	A	454	ASN
1	A	461	GLN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	543	ASN
1	A	598	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 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	517/562 (91%)	0.43	26 (5%) 34 26	53, 91, 163, 201	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	CYS	9.0
1	A	299	CYS	4.5
1	A	563	GLY	3.4
1	A	275	LEU	3.3
1	A	608	SER	3.2
1	A	526	LEU	3.2
1	A	564	SER	3.1
1	A	527	LEU	3.1
1	A	565	LEU	3.1
1	A	387	LEU	3.0
1	A	92	LEU	2.9
1	A	566	VAL	2.9
1	A	590	PHE	2.8
1	A	204	MET	2.6
1	A	587	PRO	2.6
1	A	210	GLN	2.5
1	A	556	PHE	2.4
1	A	525	GLN	2.4
1	A	221	LYS	2.4
1	A	476	PHE	2.2
1	A	206	LEU	2.2
1	A	520	LEU	2.1
1	A	517	LEU	2.1
1	A	90	ALA	2.1
1	A	86	THR	2.0
1	A	491	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 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.