



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:19 AM UTC

PDB ID : 1FOT / pdb_00001fot
Title : STRUCTURE OF THE UNLIGANDED CAMP-DEPENDENT PROTEIN
KINASE CATALYTIC SUBUNIT FROM SACCHAROMYCES CERE-
VISIAE
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Deposited on : 2000-08-28
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
Mogul : 2022.3.0, CSD as543be (2022)
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

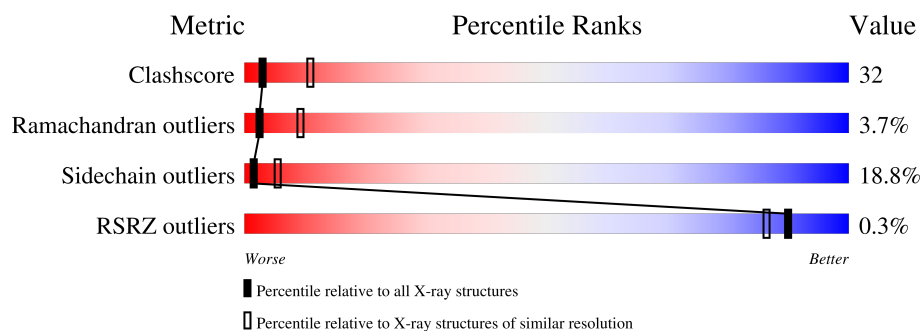
1 Overall quality at a glance

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))
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	318	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2497 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 CAMP-DEPENDENT PROTEIN KINASE TYPE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	P	S	0	0	0
			2495	1619	413	453	1	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	PRO	-	SEE REMARK 999	UNP P06244
A	241	TPO	THR	modified residue	UNP P06244

- Molecule 2 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 61.00Å 322.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.1 (20.00-2.80) 81.8 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.30 (at 2.51Å)	Xtriage
Refinement program	CNS 0.5, X-PLOR	Depositor
R, R_{free}	0.194 , 0.243 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2497	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	0.53	1/2550 (0.0%)	1.14	27/3453 (0.8%)

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	PRO	CA-C	5.96	1.55	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	O-C-N	10.38	134.42	123.00
1	A	208	TYR	O-C-N	-8.79	112.89	122.03
1	A	180	GLN	N-CA-C	7.87	127.56	110.80
1	A	208	TYR	N-CA-C	7.80	119.47	110.97
1	A	209	ARG	N-CA-CB	-7.38	105.75	114.17
1	A	235	VAL	CA-C-N	6.82	126.28	118.85
1	A	235	VAL	C-N-CA	6.82	126.28	118.85
1	A	213	PRO	N-CA-C	-6.58	105.63	113.86
1	A	361	PRO	N-CA-C	6.50	122.59	111.03
1	A	208	TYR	CA-C-N	-6.29	115.32	126.45
1	A	208	TYR	C-N-CA	-6.29	115.32	126.45
1	A	209	ARG	N-CA-C	6.25	123.09	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	N-CA-C	5.96	117.60	110.44
1	A	297	ALA	N-CA-C	5.91	118.40	109.23
1	A	388	ASP	CA-C-N	5.86	125.54	119.56
1	A	388	ASP	C-N-CA	5.86	125.54	119.56
1	A	361	PRO	CA-C-N	5.74	132.03	121.70
1	A	361	PRO	C-N-CA	5.74	132.03	121.70
1	A	245	THR	CA-C-N	5.72	126.99	119.84
1	A	245	THR	C-N-CA	5.72	126.99	119.84
1	A	175	LEU	N-CA-C	-5.44	105.43	111.36
1	A	168	GLU	N-CA-C	5.41	117.17	111.28
1	A	146	PHE	N-CA-C	5.30	119.74	113.16
1	A	125	ARG	N-CA-C	-5.25	104.98	111.33
1	A	335	VAL	N-CA-C	-5.17	105.81	110.82
1	A	101	VAL	N-CA-C	-5.08	101.16	108.42
1	A	102	HIS	N-CA-C	5.06	117.36	109.52

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLU	Peptide
1	A	179	SER	Mainchain
1	A	181	ARG	Sidechain
1	A	315	ARG	Sidechain

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	2495	0	2463	158	0
2	A	2	0	0	0	0
All	All	2497	0	2463	158	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 32.

All (158) 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:208:TYR:O	1:A:209:ARG:HB2	1.58	0.97
1:A:312:LEU:HD22	1:A:316:LEU:HD22	1.48	0.94
1:A:309:VAL:HG13	1:A:340:TRP:CE2	2.06	0.90
1:A:166:TYR:HE2	1:A:168:GLU:OE2	1.53	0.90
1:A:157:ALA:CB	1:A:385:GLN:HA	2.03	0.88
1:A:242:LEU:O	1:A:242:LEU:HG	1.70	0.83
1:A:207:ILE:HG13	1:A:209:ARG:HG3	1.59	0.83
1:A:157:ALA:HB3	1:A:385:GLN:HA	1.63	0.80
1:A:207:ILE:HD11	1:A:209:ARG:HD3	1.63	0.79
1:A:166:TYR:CE2	1:A:168:GLU:OE2	2.36	0.79
1:A:321:LEU:HD12	1:A:321:LEU:H	1.48	0.77
1:A:212:LYS:HD3	1:A:245:THR:OG1	1.85	0.77
1:A:306:ASN:O	1:A:309:VAL:HG23	1.87	0.75
1:A:100:ARG:HH11	1:A:100:ARG:HB3	1.51	0.74
1:A:120:LYS:O	1:A:124:VAL:HG23	1.87	0.73
1:A:162:MET:HB3	1:A:164:MET:HE2	1.72	0.72
1:A:168:GLU:HG3	1:A:220:LYS:NZ	2.04	0.72
1:A:300:ARG:HD2	1:A:300:ARG:C	2.13	0.72
1:A:144:HIS:HD2	1:A:146:PHE:H	1.38	0.72
1:A:332:THR:HG22	1:A:336:LYS:HG3	1.71	0.71
1:A:100:ARG:HH11	1:A:100:ARG:CB	2.03	0.71
1:A:111:ARG:HD3	1:A:113:TYR:OH	1.90	0.71
1:A:157:ALA:HB2	1:A:385:GLN:HA	1.70	0.71
1:A:345:VAL:HG12	1:A:348:LYS:H	1.57	0.69
1:A:207:ILE:CG1	1:A:209:ARG:HG3	2.22	0.69
1:A:220:LYS:O	1:A:359:GLU:HG3	1.92	0.68
1:A:154:PHE:HE2	1:A:163:ILE:HD11	1.57	0.68
1:A:312:LEU:CD2	1:A:316:LEU:HD22	2.23	0.68
1:A:300:ARG:HH12	1:A:302:PRO:HG3	1.59	0.68
1:A:179:SER:O	1:A:181:ARG:N	2.29	0.66
1:A:207:ILE:HG13	1:A:209:ARG:CG	2.26	0.66
1:A:93:LEU:HD11	1:A:103:LEU:HB2	1.79	0.65
1:A:101:VAL:HA	1:A:115:MET:O	1.96	0.65
1:A:168:GLU:HG3	1:A:220:LYS:HZ2	1.61	0.65
1:A:395:ARG:HG3	1:A:396:ASP:N	2.12	0.65
1:A:343:GLU:H	1:A:343:GLU:CD	2.04	0.64
1:A:286:ASN:HD22	1:A:289:LYS:CG	2.11	0.63
1:A:300:ARG:HD2	1:A:301:PHE:N	2.14	0.63
1:A:144:HIS:CD2	1:A:146:PHE:H	2.18	0.62
1:A:352:ARG:HH11	1:A:352:ARG:HB2	1.63	0.61
1:A:100:ARG:CD	1:A:100:ARG:H	2.13	0.61
1:A:184:ASN:HB3	1:A:185:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:HB2	1:A:275:MET:O	2.01	0.61
1:A:188:LYS:HE2	1:A:340:TRP:O	2.01	0.61
1:A:215:ASN:O	1:A:227:THR:HG22	2.00	0.60
1:A:220:LYS:HA	1:A:360:PRO:HG2	1.83	0.60
1:A:309:VAL:HG13	1:A:340:TRP:NE1	2.16	0.59
1:A:289:LYS:O	1:A:292:GLU:HB2	2.02	0.59
1:A:286:ASN:HD22	1:A:289:LYS:HG3	1.67	0.59
1:A:109:ASN:OD1	1:A:111:ARG:HB2	2.03	0.58
1:A:342:LYS:HD2	1:A:342:LYS:O	2.04	0.58
1:A:163:ILE:C	1:A:164:MET:HG2	2.26	0.58
1:A:207:ILE:HD11	1:A:209:ARG:CD	2.34	0.58
1:A:286:ASN:ND2	1:A:289:LYS:H	2.02	0.57
1:A:242:LEU:O	1:A:242:LEU:CG	2.46	0.57
1:A:104:ILE:HD13	1:A:115:MET:HG3	1.87	0.56
1:A:135:GLU:HG3	1:A:230:GLY:HA2	1.87	0.56
1:A:240:TYR:O	1:A:241:TPO:C	2.53	0.56
1:A:88:GLN:HG2	1:A:88:GLN:O	2.05	0.56
1:A:300:ARG:NH1	1:A:302:PRO:HG3	2.21	0.56
1:A:105:ARG:CG	1:A:105:ARG:HH11	2.19	0.56
1:A:306:ASN:OD1	1:A:308:ASP:HB2	2.07	0.55
1:A:342:LYS:HD2	1:A:342:LYS:C	2.32	0.55
1:A:287:THR:O	1:A:290:THR:HB	2.08	0.54
1:A:300:ARG:C	1:A:300:ARG:CD	2.80	0.54
1:A:162:MET:HE2	1:A:164:MET:HE2	1.89	0.54
1:A:241:TPO:O	1:A:259:TYR:OH	2.21	0.54
1:A:100:ARG:H	1:A:100:ARG:HD2	1.72	0.54
1:A:168:GLU:CG	1:A:220:LYS:NZ	2.70	0.54
1:A:118:LEU:HD12	1:A:118:LEU:N	2.23	0.54
1:A:162:MET:HE2	1:A:164:MET:CE	2.38	0.54
1:A:234:TYR:CZ	1:A:236:PRO:HG3	2.43	0.54
1:A:162:MET:CB	1:A:164:MET:HE2	2.38	0.53
1:A:213:PRO:HD3	1:A:248:TYR:CZ	2.43	0.53
1:A:284:ASP:HB2	1:A:293:LYS:HE2	1.90	0.53
1:A:144:HIS:CD2	1:A:145:PRO:HD2	2.45	0.52
1:A:380:ILE:O	1:A:380:ILE:HG23	2.08	0.52
1:A:153:THR:O	1:A:154:PHE:HB3	2.10	0.52
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.23	0.52
1:A:273:TYR:CG	1:A:281:PRO:HG3	2.44	0.52
1:A:105:ARG:NH1	1:A:110:GLY:O	2.43	0.51
1:A:168:GLU:CG	1:A:220:LYS:HZ2	2.23	0.51
1:A:249:ILE:HG22	1:A:294:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HH11	1:A:352:ARG:CG	2.23	0.51
1:A:390:TYR:O	1:A:391:ALA:C	2.53	0.51
1:A:246:PRO:O	1:A:294:ILE:HD11	2.10	0.50
1:A:395:ARG:HG3	1:A:396:ASP:H	1.75	0.50
1:A:93:LEU:CD1	1:A:103:LEU:HB2	2.41	0.50
1:A:207:ILE:O	1:A:232:ALA:HA	2.11	0.50
1:A:352:ARG:HH11	1:A:352:ARG:CB	2.25	0.49
1:A:208:TYR:O	1:A:209:ARG:CB	2.31	0.49
1:A:175:LEU:HD13	1:A:182:PHE:CZ	2.48	0.49
1:A:83:SER:O	1:A:86:ASP:HB2	2.13	0.48
1:A:253:VAL:HG13	1:A:259:TYR:CE2	2.48	0.48
1:A:167:ILE:HG21	1:A:217:LEU:HB3	1.96	0.48
1:A:293:LYS:O	1:A:294:ILE:C	2.57	0.48
1:A:88:GLN:O	1:A:88:GLN:CG	2.62	0.48
1:A:221:ASN:HD22	1:A:221:ASN:C	2.22	0.48
1:A:219:ASP:OD1	1:A:221:ASN:ND2	2.47	0.48
1:A:117:VAL:C	1:A:118:LEU:HD12	2.39	0.47
1:A:283:TYR:CG	1:A:284:ASP:N	2.82	0.47
1:A:317:ILE:HG22	1:A:317:ILE:O	2.14	0.47
1:A:160:ILE:HD12	1:A:397:PHE:CE1	2.49	0.47
1:A:282:PHE:HB3	1:A:293:LYS:HB2	1.95	0.47
1:A:297:ALA:H	1:A:319:ARG:NH2	2.13	0.47
1:A:207:ILE:CG1	1:A:209:ARG:CG	2.90	0.47
1:A:309:VAL:HG13	1:A:340:TRP:CZ2	2.48	0.47
1:A:362:ILE:C	1:A:362:ILE:HD13	2.40	0.47
1:A:207:ILE:HD11	1:A:209:ARG:CG	2.46	0.46
1:A:234:TYR:CE2	1:A:236:PRO:HG3	2.49	0.46
1:A:138:MET:O	1:A:142:VAL:HG22	2.16	0.46
1:A:263:ILE:HG13	1:A:264:ASP:N	2.30	0.46
1:A:104:ILE:HG21	1:A:115:MET:HE2	1.98	0.45
1:A:157:ALA:HB2	1:A:385:GLN:CA	2.44	0.45
1:A:307:GLU:O	1:A:310:LYS:HB2	2.16	0.45
1:A:383:GLY:O	1:A:384:VAL:C	2.59	0.45
1:A:357:PRO:O	1:A:358:TYR:HB2	2.16	0.45
1:A:338:HIS:CE1	1:A:339:PRO:HD2	2.52	0.45
1:A:379:ASP:CG	1:A:380:ILE:N	2.74	0.45
1:A:105:ARG:CG	1:A:105:ARG:NH1	2.80	0.45
1:A:301:PHE:HE2	1:A:313:LEU:HB2	1.82	0.45
1:A:207:ILE:HD12	1:A:263:ILE:HD11	1.99	0.44
1:A:120:LYS:O	1:A:121:GLU:C	2.60	0.44
1:A:151:TRP:H	1:A:151:TRP:CD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASP:OD2	1:A:391:ALA:N	2.50	0.44
1:A:213:PRO:HD2	1:A:214:GLU:OE1	2.18	0.43
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.53	0.43
1:A:307:GLU:O	1:A:308:ASP:C	2.61	0.43
1:A:352:ARG:CG	1:A:352:ARG:NH1	2.81	0.43
1:A:338:HIS:CG	1:A:339:PRO:HD2	2.54	0.43
1:A:100:ARG:CG	1:A:100:ARG:NH1	2.79	0.43
1:A:221:ASN:O	1:A:356:THR:HG21	2.19	0.43
1:A:193:GLU:OE2	1:A:349:LEU:HD11	2.18	0.42
1:A:287:THR:O	1:A:290:THR:N	2.48	0.42
1:A:291:TYR:O	1:A:295:LEU:HB2	2.19	0.42
1:A:122:ILE:O	1:A:123:VAL:C	2.62	0.42
1:A:379:ASP:CG	1:A:380:ILE:H	2.27	0.42
1:A:212:LYS:HE2	1:A:214:GLU:HB2	2.02	0.42
1:A:362:ILE:O	1:A:362:ILE:HG12	2.20	0.42
1:A:259:TYR:CE1	1:A:263:ILE:HD13	2.55	0.42
1:A:100:ARG:HG3	1:A:102:HIS:HE2	1.85	0.41
1:A:298:GLU:O	1:A:298:GLU:HG3	2.20	0.41
1:A:158:GLN:HB2	1:A:159:GLN:NE2	2.35	0.41
1:A:200:TYR:O	1:A:201:LEU:C	2.62	0.41
1:A:349:LEU:CD1	1:A:354:ILE:HG21	2.50	0.41
1:A:177:ARG:HA	1:A:177:ARG:HD3	1.88	0.41
1:A:302:PRO:HA	1:A:303:PRO:HD3	1.95	0.41
1:A:145:PRO:HB3	1:A:352:ARG:CZ	2.51	0.41
1:A:209:ARG:HG2	1:A:263:ILE:HD11	2.02	0.41
1:A:168:GLU:HG3	1:A:220:LYS:CE	2.51	0.41
1:A:219:ASP:O	1:A:220:LYS:C	2.64	0.41
1:A:98:PHE:HE1	1:A:126:LEU:HD12	1.85	0.41
1:A:353:ASN:HD22	1:A:353:ASN:HA	1.68	0.41
1:A:144:HIS:O	1:A:145:PRO:C	2.63	0.40
1:A:217:LEU:CD1	1:A:227:THR:HB	2.51	0.40
1:A:288:MET:H	1:A:288:MET:HG3	1.63	0.40
1:A:116:LYS:HD2	1:A:118:LEU:HD11	2.03	0.40
1:A:147:ILE:CD1	1:A:201:LEU:HD21	2.52	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	295/318 (93%)	245 (83%)	39 (13%)	11 (4%)	2 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	154	PHE
1	A	285	SER
1	A	220	LYS
1	A	246	PRO
1	A	184	ASN
1	A	228	ASP
1	A	358	TYR
1	A	384	VAL
1	A	317	ILE
1	A	123	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	272/288 (94%)	221 (81%)	51 (19%)	1 5

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	88	GLN
1	A	100	ARG
1	A	101	VAL
1	A	103	LEU
1	A	105	ARG
1	A	115	MET
1	A	116	LYS
1	A	119	LYS
1	A	124	VAL
1	A	125	ARG
1	A	128	GLN
1	A	130	GLU
1	A	140	SER
1	A	159	GLN
1	A	164	MET
1	A	171	GLU
1	A	172	LEU
1	A	175	LEU
1	A	178	LYS
1	A	204	LYS
1	A	207	ILE
1	A	211	LEU
1	A	221	ASN
1	A	224	ILE
1	A	242	LEU
1	A	246	PRO
1	A	249	ILE
1	A	253	VAL
1	A	255	SER
1	A	257	LYS
1	A	261	LYS
1	A	280	THR
1	A	286	ASN
1	A	288	MET
1	A	295	LEU
1	A	306	ASN
1	A	309	VAL
1	A	312	LEU
1	A	314	SER
1	A	316	LEU
1	A	320	ASP
1	A	333	GLU

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Mol	Chain	Res	Type
1	A	342	LYS
1	A	343	GLU
1	A	348	LYS
1	A	352	ARG
1	A	362	ILE
1	A	380	ILE
1	A	387	GLU
1	A	392	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	131	HIS
1	A	144	HIS
1	A	221	ASN
1	A	223	HIS
1	A	286	ASN
1	A	337	ASN
1	A	353	ASN
1	A	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	241	1	8,10,11	1.98	1 (12%)	10,14,16	2.67	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	241	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	TPO	P-OG1	-5.11	1.50	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	TPO	P-OG1-CB	-7.99	101.63	123.33
1	A	241	TPO	O-C-CA	-2.02	119.57	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	241	TPO	2	0

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 ⓘ

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	299/318 (94%)	-0.39	1 (0%) 90 86	21, 47, 79, 101	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	361	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	241	11/12	0.93	0.09	37,54,61,61	0

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.